wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2023 – 10:53 PM EDT

PDB ID	:	4V99
Title	:	The Crystallographic Structure of Panicum Mosaic Virus
Authors	:	Makino, D.L.; Larson, S.B.; McPherson, A.
Deposited on	:	2012-07-04
Resolution	:	2.90 Å(reported)

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

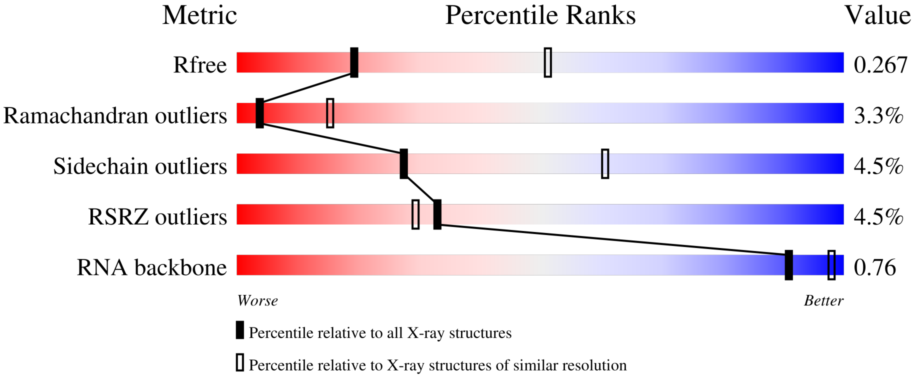
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

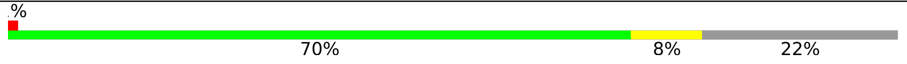
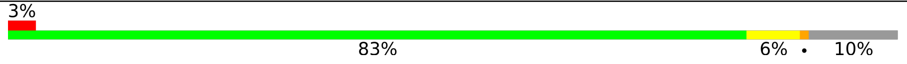
The reported resolution of this entry is 2.90 Å.

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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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

Mol	Chain	Length	Quality of chain
1	A1	242	 2% 83% 6% • 10%
1	A4	242	 71% 5% 24%
1	A5	242	 % 70% 8% 22%
1	A6	242	 3% 83% 6% • 10%
1	AA	242	 71% 5% 24%

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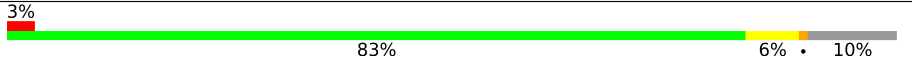
Mol	Chain	Length	Quality of chain
1	AB	242	
1	AC	242	
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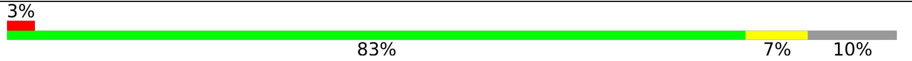
1	AG	242	
1	AH	242	
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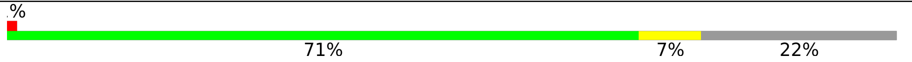
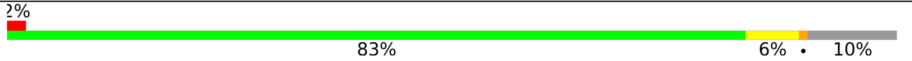
1	AL	242	
1	AM	242	
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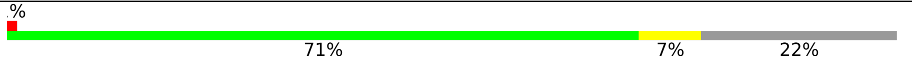
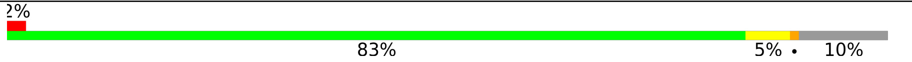
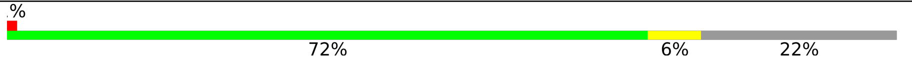
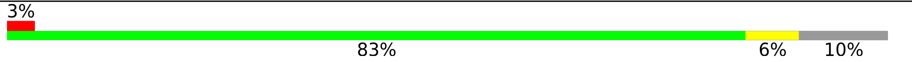
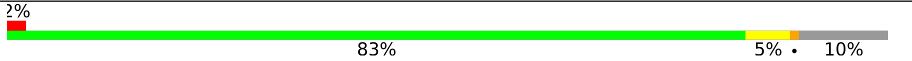
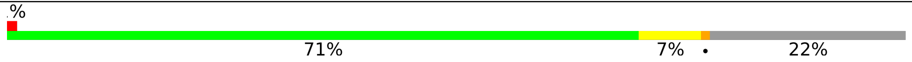
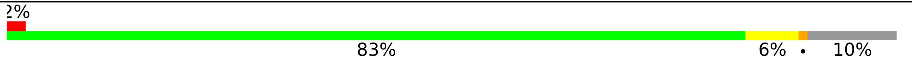
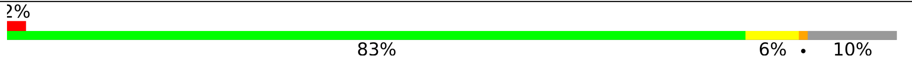
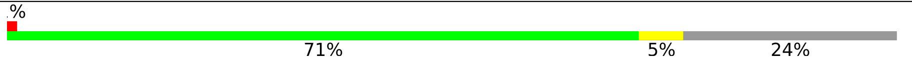
1	AQ	242	
1	AR	242	
1	AU	242	
1	AV	242	
1	AW	242	
1	AZ	242	
1	Aa	242	
1	Ab	242	
1	Ae	242	
1	Af	242	
1	Ag	242	
1	Aj	242	
1	Ak	242	
1	Al	242	
1	Ao	242	
1	Ap	242	

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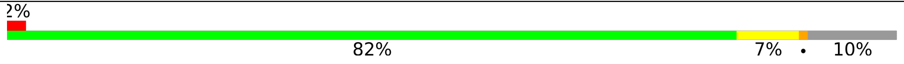
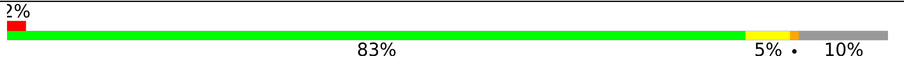
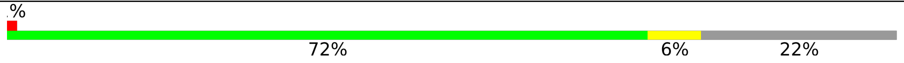
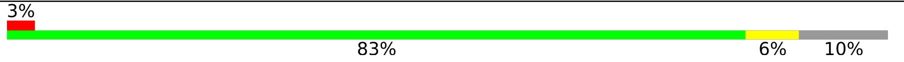
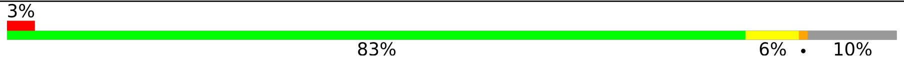
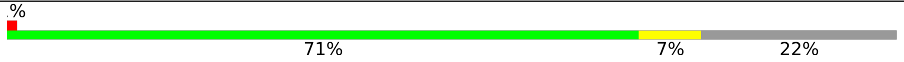
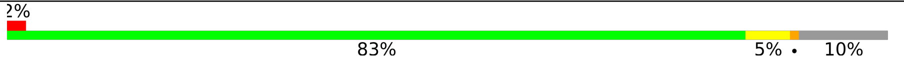
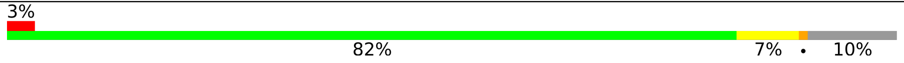
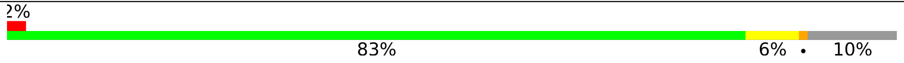
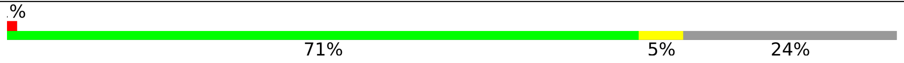
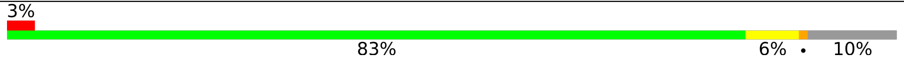
Mol	Chain	Length	Quality of chain
1	Aq	242	
1	At	242	
1	Au	242	
1	Av	242	
1	Ay	242	
1	Az	242	
1	B1	242	
1	B4	242	
1	B5	242	
1	B6	242	
1	BA	242	
1	BB	242	
1	BC	242	
1	BF	242	
1	BG	242	
1	BH	242	
1	BK	242	
1	BL	242	
1	BM	242	
1	BP	242	
1	BQ	242	
1	BR	242	
1	BU	242	
1	BV	242	
1	BW	242	

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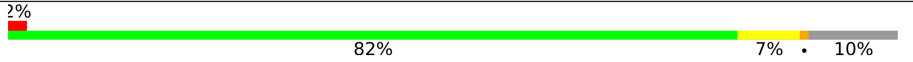
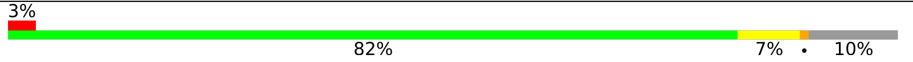
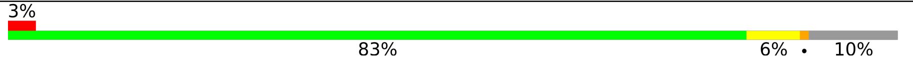
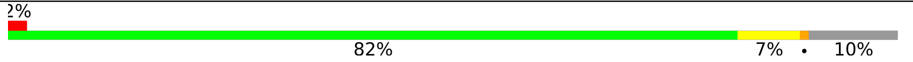
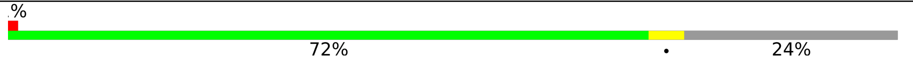
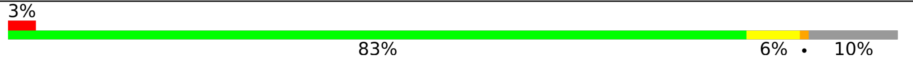
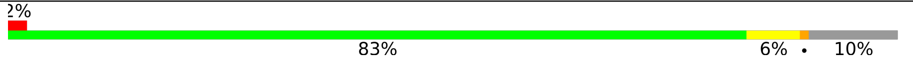
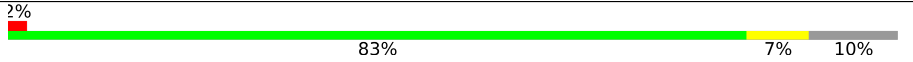
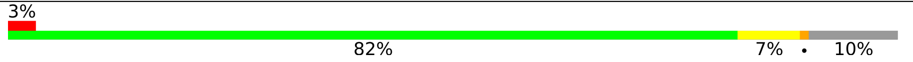
Mol	Chain	Length	Quality of chain
1	BZ	242	 71% 5% 24%
1	Ba	242	 72% 6% 22%
1	Bb	242	 2% 82% 7% • 10%
1	Be	242	 71% 5% 24%
1	Bf	242	 71% 7% 22%
1	Bg	242	 3% 82% 7% • 10%
1	Bj	242	 71% 5% 24%
1	Bk	242	 72% 6% 22%
1	Bl	242	 3% 83% 6% • 10%
1	Bo	242	 71% 5% 24%
1	Bp	242	 70% 8% 22%
1	Bq	242	 2% 82% 7% • 10%
1	Bt	242	 % 72% • 24%
1	Bu	242	 72% 6% 22%
1	Bv	242	 3% 83% 6% • 10%
1	By	242	 69% 7% 24%
1	Bz	242	 71% 7% 22%
1	C1	242	 2% 83% 6% • 10%
1	C4	242	 71% 5% • 24%
1	C5	242	 71% 7% 22%
1	C6	242	 2% 83% 7% 10%
1	CA	242	 71% 5% 24%
1	CB	242	 71% 7% 22%
1	CC	242	 3% 82% 7% • 10%
1	CF	242	 71% 5% 24%

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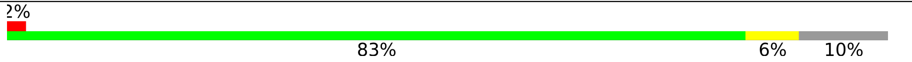
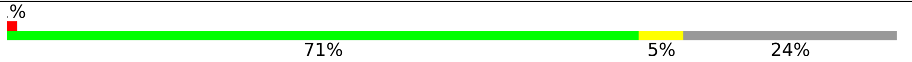
Mol	Chain	Length	Quality of chain
1	CG	242	
1	CH	242	
1	CK	242	
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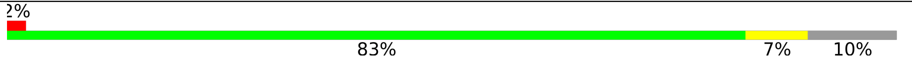
1	CM	242	
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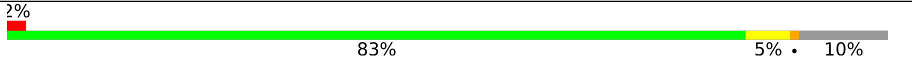
1	CQ	242	
1	CR	242	
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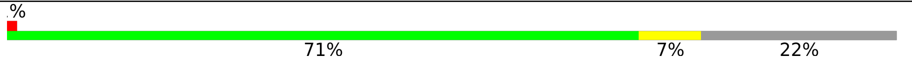
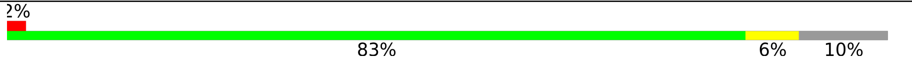
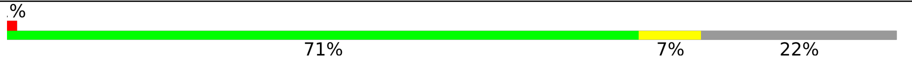
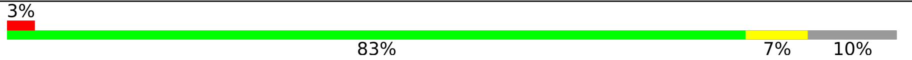
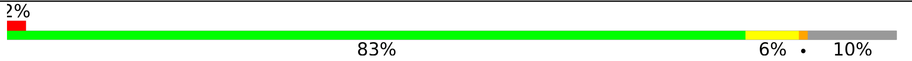
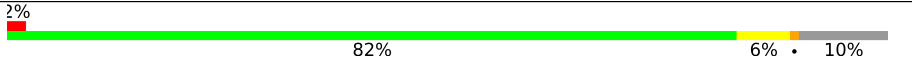
1	CV	242	
1	CW	242	
1	CZ	242	
1	Ca	242	
1	Cb	242	
1	Ce	242	
1	Cf	242	
1	Cg	242	
1	Cj	242	
1	Ck	242	
1	Cl	242	
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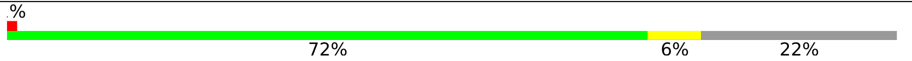
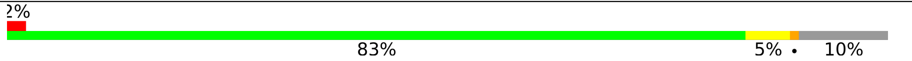
1	Cp	242	
1	Cq	242	
1	Ct	242	
1	Cu	242	

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Mol	Chain	Length	Quality of chain
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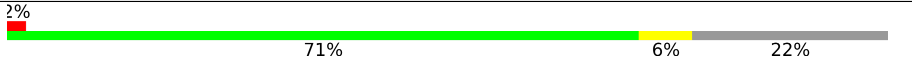
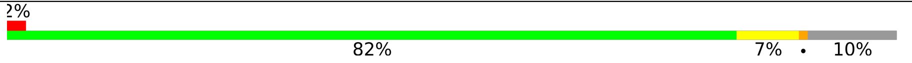
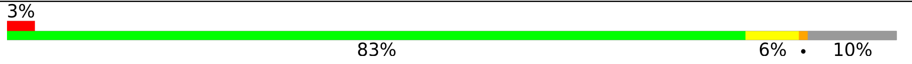
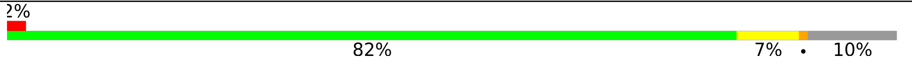
1	Cy	242	
1	Cz	242	
1	D1	242	
1	D4	242	
1	D5	242	
1	D6	242	
1	DA	242	
1	DB	242	
1	DC	242	
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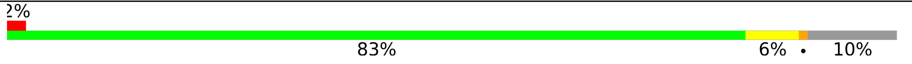
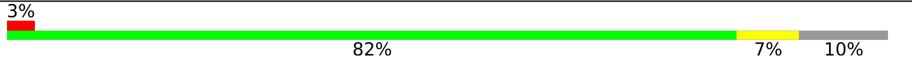
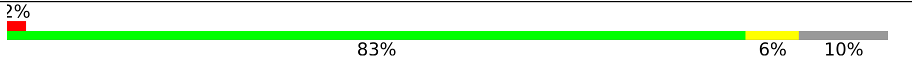
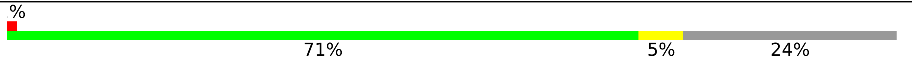
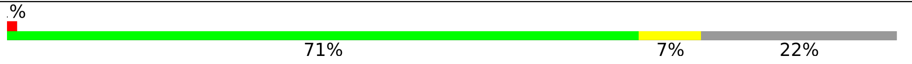
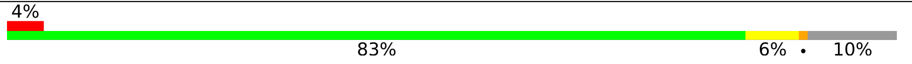
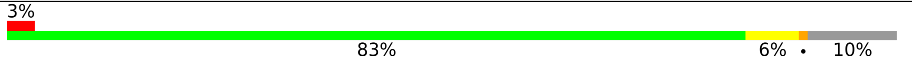
1	DG	242	
1	DH	242	
1	DK	242	
1	DL	242	
1	DM	242	
1	DP	242	
1	DQ	242	
1	DR	242	
1	DU	242	
1	DV	242	
1	DW	242	
1	DZ	242	
1	Da	242	
1	Db	242	

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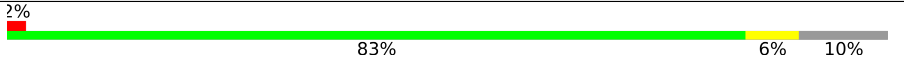
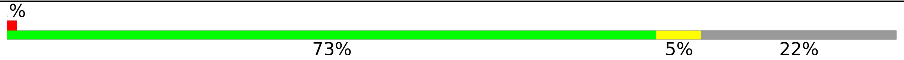
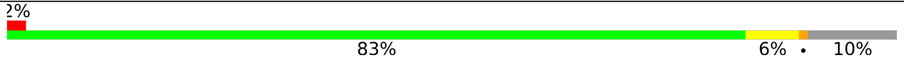
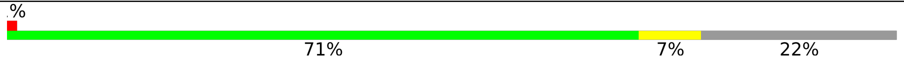
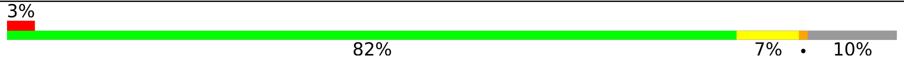
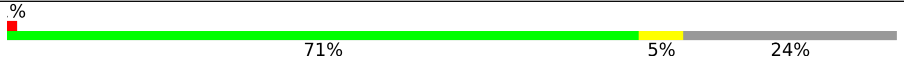
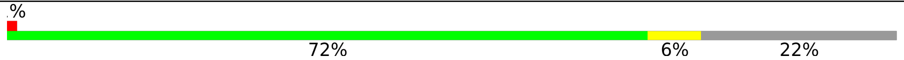
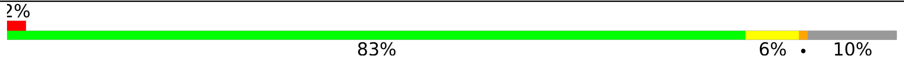
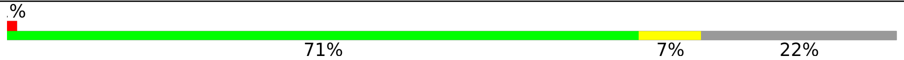
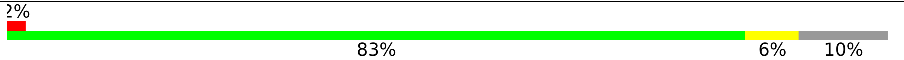
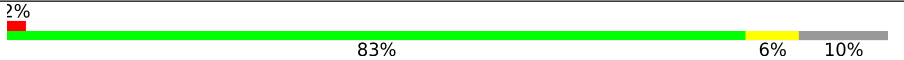
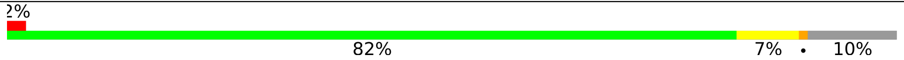
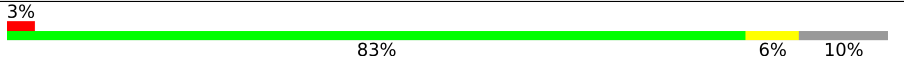
Mol	Chain	Length	Quality of chain
1	De	242	
1	Df	242	
1	Dg	242	
1	Dj	242	
1	Dk	242	
1	Dl	242	
1	Do	242	
1	Dp	242	
1	Dq	242	
1	Dt	242	
1	Du	242	
1	Dv	242	
1	Dy	242	
1	Dz	242	
1	E1	242	
1	E4	242	
1	E5	242	
1	E6	242	
1	EA	242	
1	EB	242	
1	EC	242	
1	EF	242	
1	EG	242	
1	EH	242	
1	EK	242	

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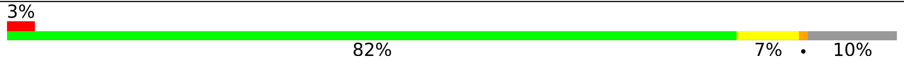
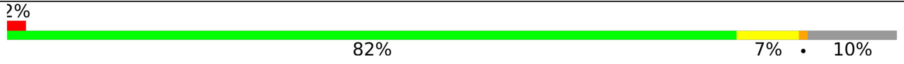
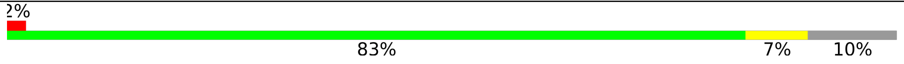
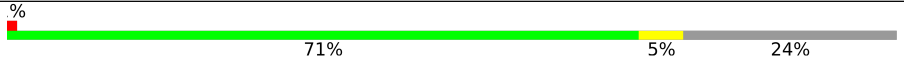
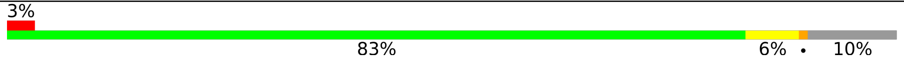
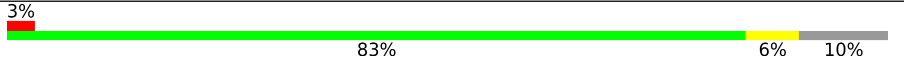
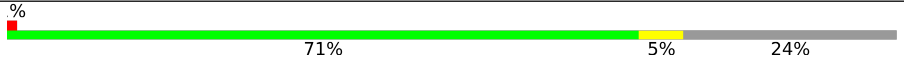
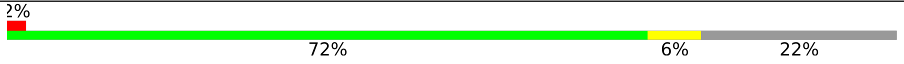
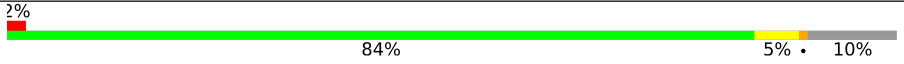
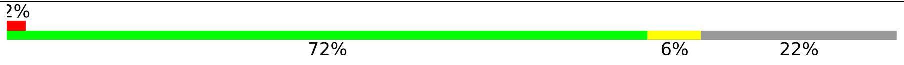
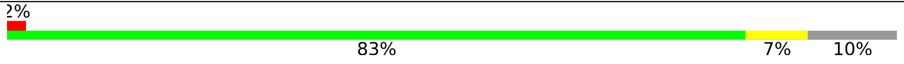
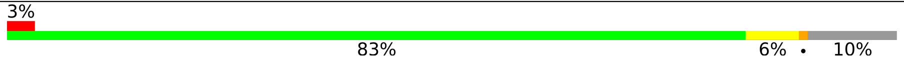
Mol	Chain	Length	Quality of chain
1	EL	242	
1	EM	242	
1	EP	242	
1	EQ	242	
1	ER	242	
1	EU	242	
1	EV	242	
1	EW	242	
1	EZ	242	
1	Ea	242	
1	Eb	242	
1	Ee	242	
1	Ef	242	
1	Eg	242	
1	Ej	242	
1	Ek	242	
1	El	242	
1	Eo	242	
1	Ep	242	
1	Eq	242	
1	Et	242	
1	Eu	242	
1	Ev	242	
1	Ey	242	
1	Ez	242	

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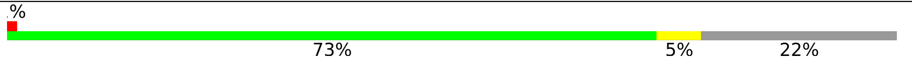
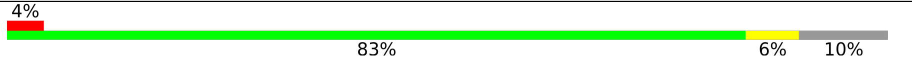
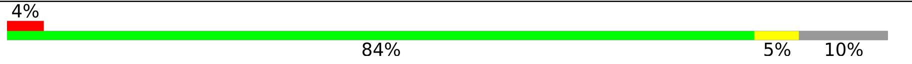
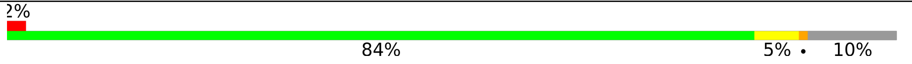
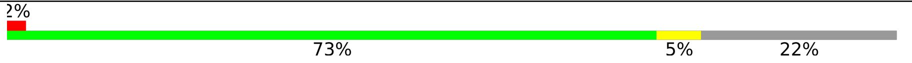
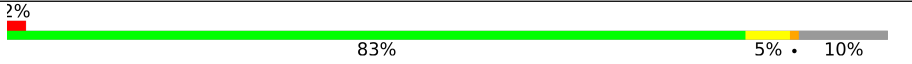
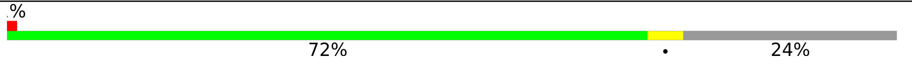
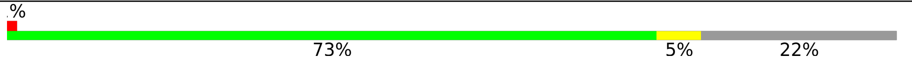
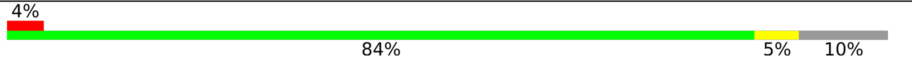
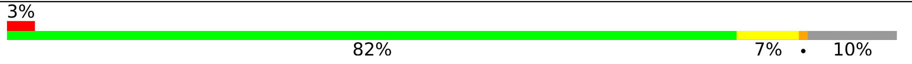
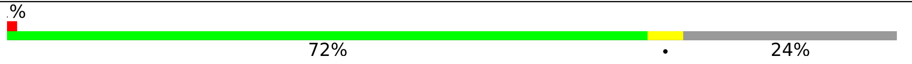
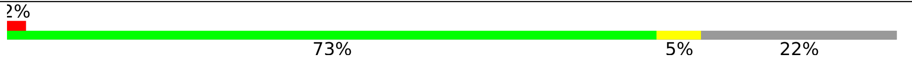
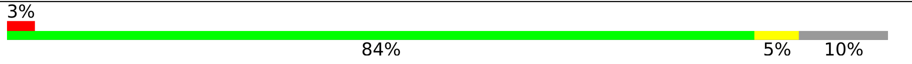
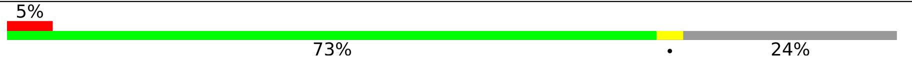
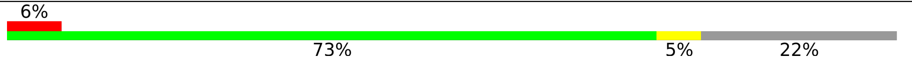
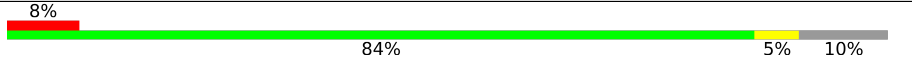
Mol	Chain	Length	Quality of chain
1	F1	242	
1	F4	242	
1	F5	242	
1	F6	242	
1	FA	242	
1	FB	242	
1	FC	242	
1	FF	242	
1	FG	242	
1	FH	242	
1	FK	242	
1	FL	242	
1	FM	242	
1	FP	242	
1	FQ	242	
1	FR	242	
1	FU	242	
1	FV	242	
1	FW	242	
1	FZ	242	
1	Fa	242	
1	Fb	242	
1	Fe	242	
1	Ff	242	
1	Fg	242	

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Mol	Chain	Length	Quality of chain
1	Fj	242	% 71% 5% 24%
1	Fk	242	3% 74% • 22%
1	Fl	242	3% 84% 5% 10%
1	Fo	242	2% 73% • 24%
1	Fp	242	74% • 22%
1	Fq	242	2% 83% 6% • 10%
1	Ft	242	71% 5% 24%
1	Fu	242	73% 5% 22%
1	Fv	242	2% 84% 5% 10%
1	Fy	242	73% • 24%
1	Fz	242	2% 74% • 22%
1	G1	242	4% 84% 5% 10%
1	G4	242	2% 73% • 24%
1	G5	242	4% 73% 5% 22%
1	G6	242	5% 84% 5% 10%
1	GA	242	73% • 24%
1	GB	242	73% 5% 22%
1	GC	242	4% 84% 5% • 10%
1	GF	242	72% 5% 24%
1	GG	242	% 73% 5% 22%
1	GH	242	2% 84% 5% 10%
1	GK	242	3% 71% 5% 24%
1	GL	242	4% 73% 5% 22%
1	GM	242	3% 84% 5% 10%
1	GP	242	72% • 24%

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Mol	Chain	Length	Quality of chain
1	GQ	242	% 73% 5% 22%
1	GR	242	2% 84% 5% 10%
1	GU	242	% 72% 5% 24%
1	GV	242	% 74% 5% 22%
1	GW	242	2% 83% 6% • 10%
1	GZ	242	71% 5% 24%
1	Ga	242	% 73% 5% 22%
1	Gb	242	4% 84% 5% 10%
1	Ge	242	2% 73% • 24%
1	Gf	242	% 73% 5% 22%
1	Gg	242	4% 83% 6% 10%
1	Gj	242	3% 71% 5% 24%
1	Gk	242	2% 74% 5% 22%
1	Gl	242	6% 84% 5% 10%
1	Go	242	6% 72% • 24%
1	Gp	242	5% 74% • 22%
1	Gq	242	4% 84% 5% 10%
1	Gt	242	% 72% 5% 24%
1	Gu	242	73% 5% 22%
1	Gv	242	2% 84% 5% • 10%
1	Gy	242	% 71% 5% 24%
1	Gz	242	% 74% • 22%
1	H1	242	4% 83% 5% • 10%
1	H4	242	5% 72% 5% 24%
1	H5	242	3% 73% 5% 22%

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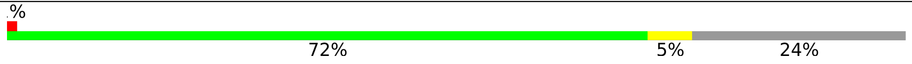
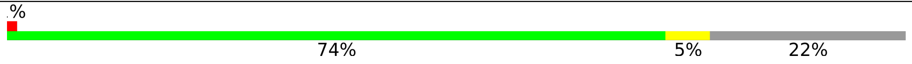
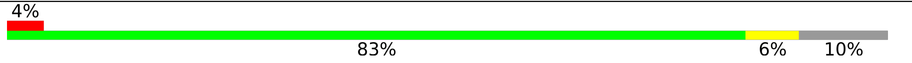
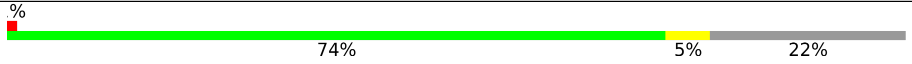
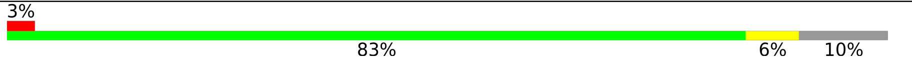
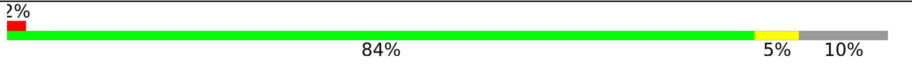
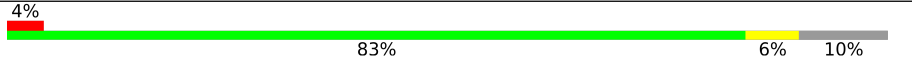
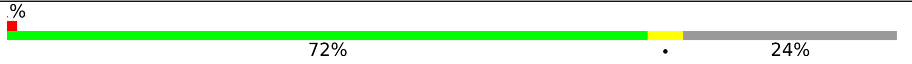
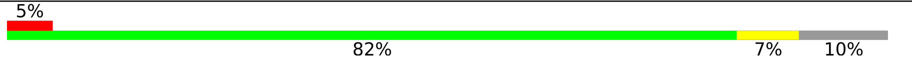
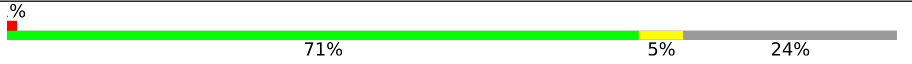
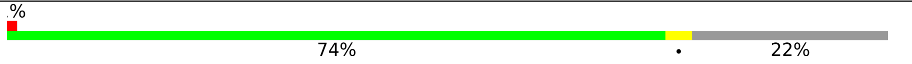
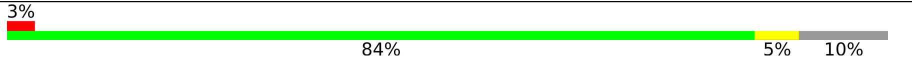
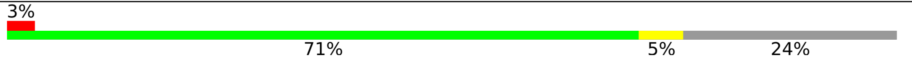
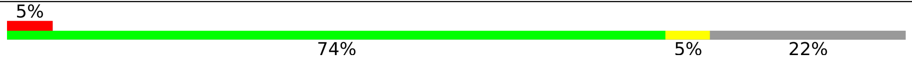
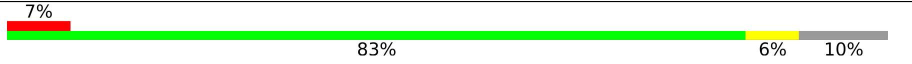
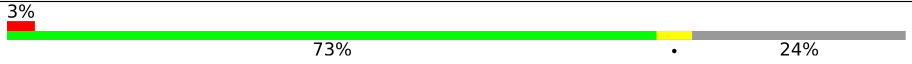
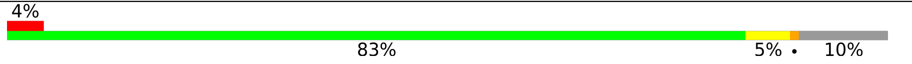
Mol	Chain	Length	Quality of chain
1	H6	242	
1	HA	242	
1	HB	242	
1	HC	242	
1	HF	242	
1	HG	242	
1	HH	242	
1	HK	242	
1	HL	242	
1	HM	242	
1	HP	242	
1	HQ	242	
1	HR	242	
1	HU	242	
1	HV	242	
1	HW	242	
1	HZ	242	
1	Ha	242	
1	Hb	242	
1	He	242	
1	Hf	242	
1	Hg	242	
1	Hj	242	
1	Hk	242	
1	Hl	242	

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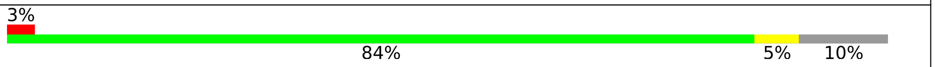
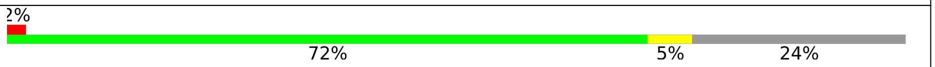
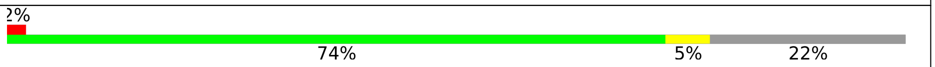
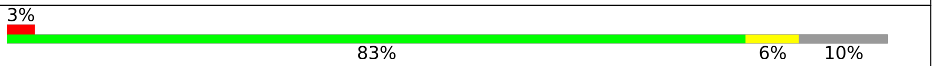
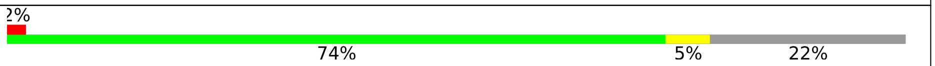
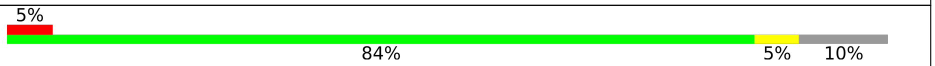
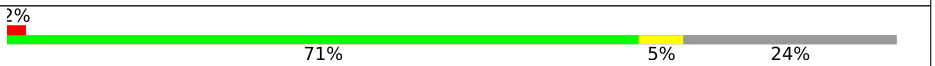
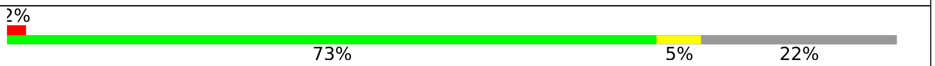
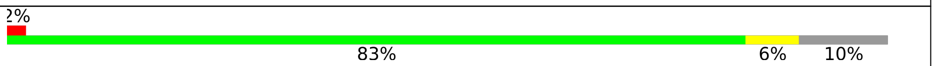
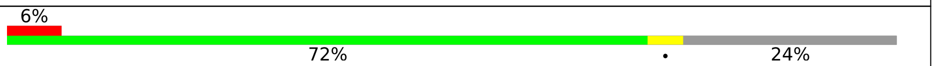
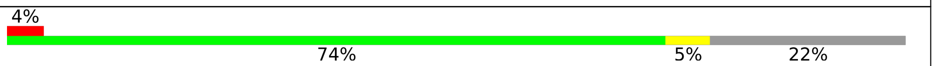
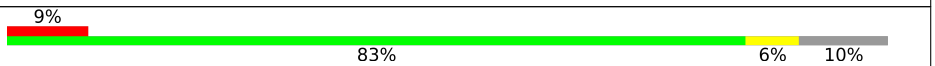
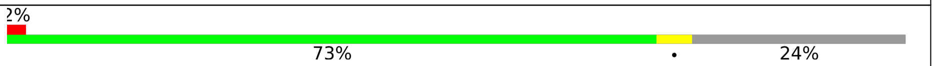
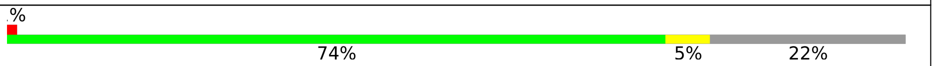
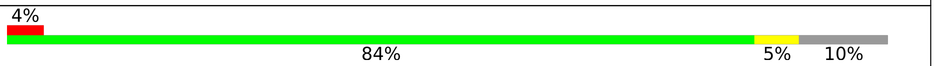
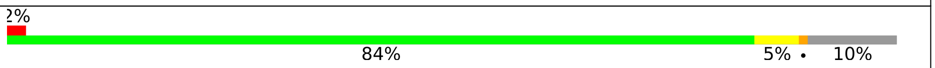
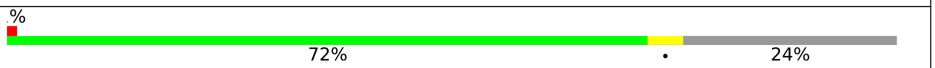
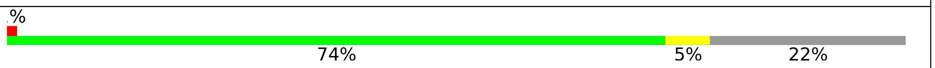
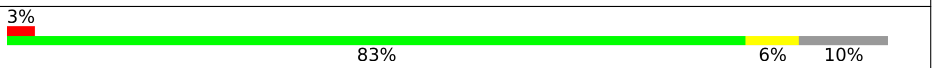
Mol	Chain	Length	Quality of chain
1	Ho	242	 72% • 24%
1	Hp	242	 74% 5% 22%
1	Hq	242	 3% 84% 5% 10%
1	Ht	242	 2% 72% 5% 24%
1	Hu	242	 2% 74% 5% 22%
1	Hv	242	 3% 83% 6% 10%
1	Hy	242	 73% • 24%
1	Hz	242	 2% 74% 5% 22%
1	I1	242	 5% 84% 5% 10%
1	I4	242	 2% 71% 5% 24%
1	I5	242	 2% 73% 5% 22%
1	I6	242	 2% 83% 6% 10%
1	IA	242	 6% 72% • 24%
1	IB	242	 4% 74% 5% 22%
1	IC	242	 9% 83% 6% 10%
1	IF	242	 2% 73% • 24%
1	IG	242	 % 74% 5% 22%
1	IH	242	 4% 84% 5% 10%
1	IK	242	 72% • 24%
1	IL	242	 73% 5% 22%
1	IM	242	 2% 84% 5% • 10%
1	IP	242	 % 72% • 24%
1	IQ	242	 % 74% 5% 22%
1	IR	242	 3% 83% 6% 10%
1	IU	242	 72% • 24%

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Mol	Chain	Length	Quality of chain
1	IV	242	73% 5% 22%
1	IW	242	2% 83% 6% 10%
1	IZ	242	72% 5% 24%
1	Ia	242	73% 5% 22%
1	Ib	242	3% 83% 6% 10%
1	Ie	242	2% 72% 5% 24%
1	If	242	% 74% • 22%
1	Ig	242	4% 84% 5% 10%
1	Ij	242	6% 72% • 24%
1	Ik	242	2% 73% 5% 22%
1	Il	242	5% 83% 6% 10%
1	Io	242	% 73% • 24%
1	Ip	242	74% • 22%
1	Iq	242	3% 84% 5% 10%
1	It	242	73% • 24%
1	Iu	242	% 74% 5% 22%
1	Iv	242	2% 83% 6% 10%
1	Iy	242	% 72% • 24%
1	Iz	242	% 73% 5% 22%
1	J1	242	2% 84% 5% 10%
1	J4	242	5% 72% • 24%
1	J5	242	2% 72% 6% 22%
1	J6	242	4% 83% 5% • 10%
1	JA	242	2% 72% • 24%
1	JB	242	% 73% 5% 22%

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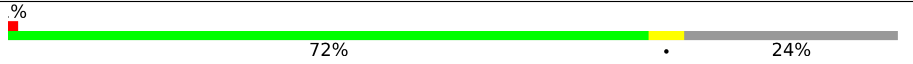
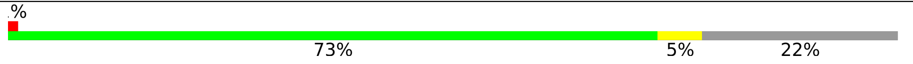
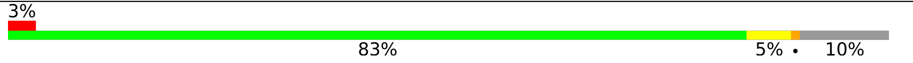
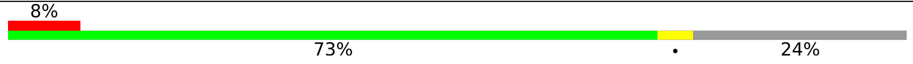
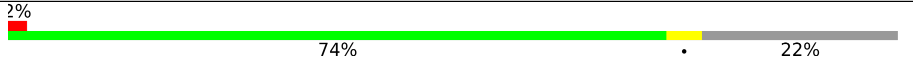
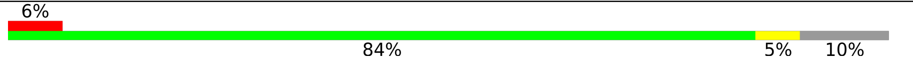
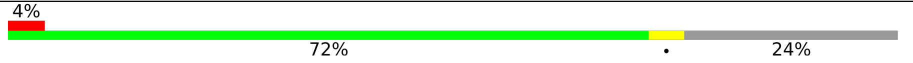
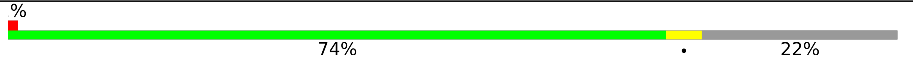
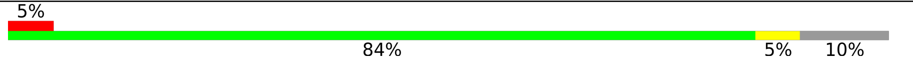
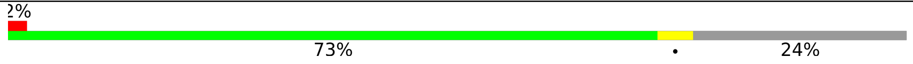
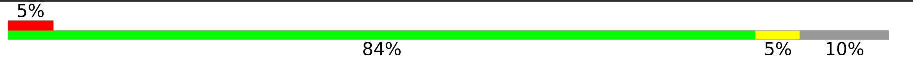
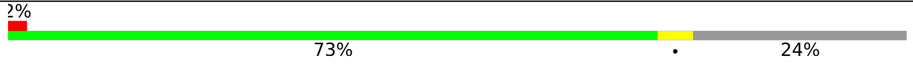
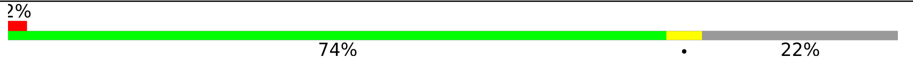
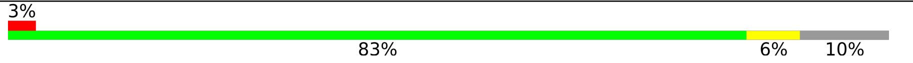
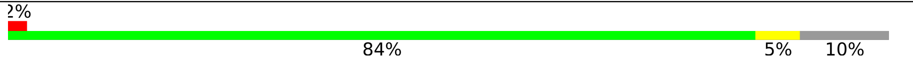
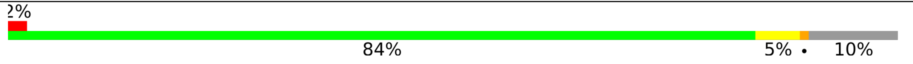
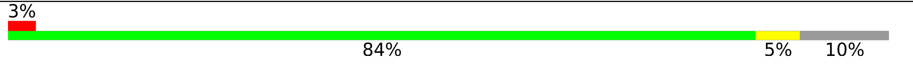
Mol	Chain	Length	Quality of chain
1	JC	242	
1	JF	242	
1	JG	242	
1	JH	242	
1	JK	242	
1	JL	242	
1	JM	242	
1	JP	242	
1	JQ	242	
1	JR	242	
1	JU	242	
1	JV	242	
1	JW	242	
1	JZ	242	
1	Ja	242	
1	Jb	242	
1	Je	242	
1	Jf	242	
1	Jg	242	
1	Jj	242	
1	Jk	242	
1	Jl	242	
1	Jo	242	
1	Jp	242	
1	Jq	242	

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Mol	Chain	Length	Quality of chain
1	Jt	242	71% 5% 24%
1	Ju	242	2% 74% • 22%
1	Jv	242	2% 84% 5% 10%
1	Jy	242	% 71% 5% 24%
1	Jz	242	2% 72% 6% 22%
2	A2	17	82% 71% 29%
2	A7	17	100% 71% 29%
2	AD	17	88% 71% 29%
2	AI	17	94% 71% 29%
2	AN	17	94% 71% 29%
2	AS	17	71% 71% 29%
2	AX	17	76% 71% 29%
2	Ac	17	88% 76% 24%
2	Ah	17	94% 76% 24%
2	Am	17	94% 76% 24%
2	Ar	17	88% 76% 24%
2	Aw	17	100% 76% 24%
2	B2	17	94% 71% 29%
2	B7	17	88% 71% 29%
2	BD	17	100% 71% 29%
2	BI	17	94% 71% 29%
2	BN	17	65% 71% 29%
2	BS	17	88% 71% 29%
2	BX	17	94% 71% 29%
2	Bc	17	82% 76% 24%

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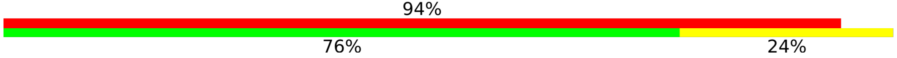
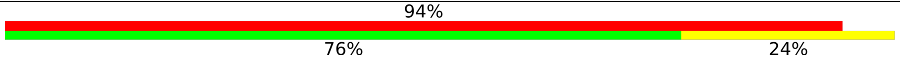
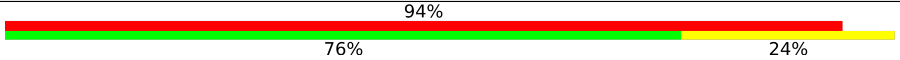
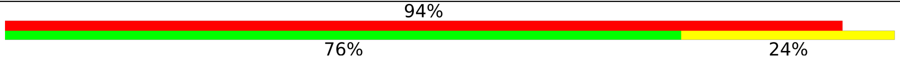
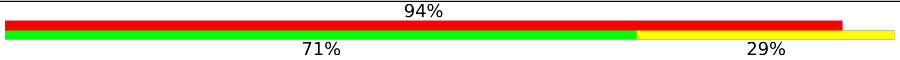
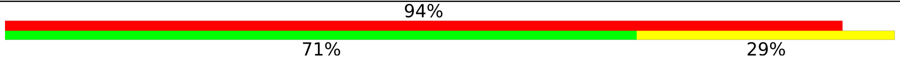
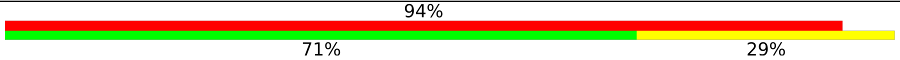
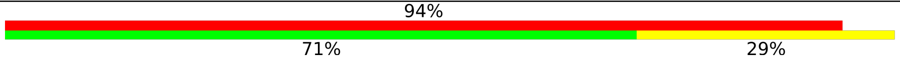
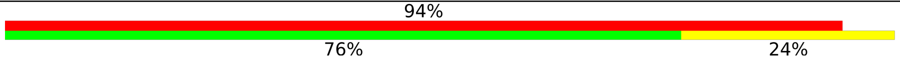
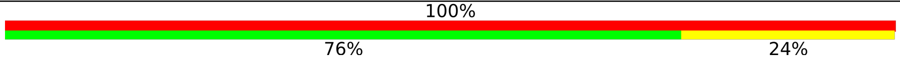
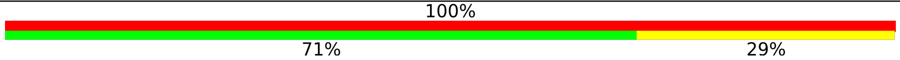
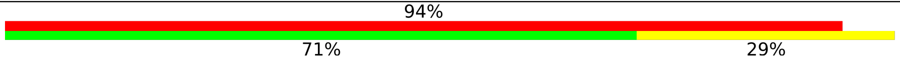
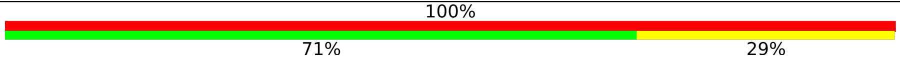
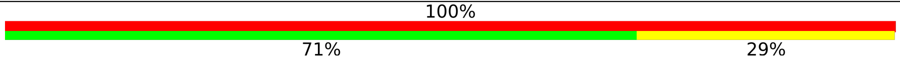
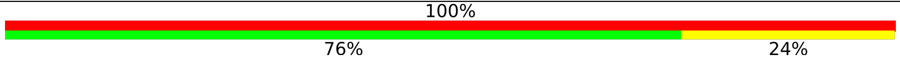
Mol	Chain	Length	Quality of chain
2	Bh	17	
2	Bm	17	
2	Br	17	
2	Bw	17	
2	C2	17	
2	C7	17	
2	CD	17	
2	CI	17	
2	CN	17	
2	CS	17	
2	CX	17	
2	Cc	17	
2	Ch	17	
2	Cm	17	
2	Cr	17	
2	Cw	17	
2	D2	17	
2	D7	17	
2	DD	17	
2	DI	17	
2	DN	17	
2	DS	17	
2	DX	17	
2	Dc	17	
2	Dh	17	

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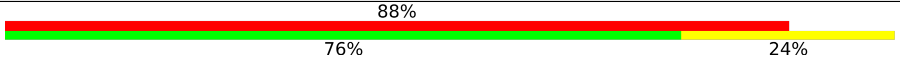
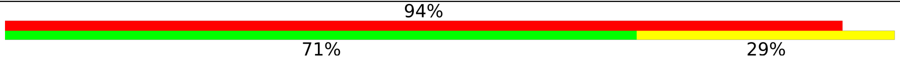
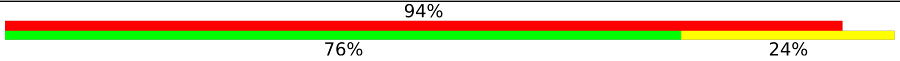
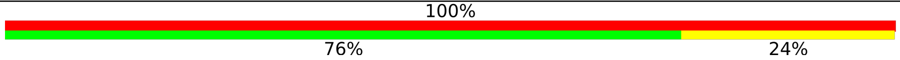
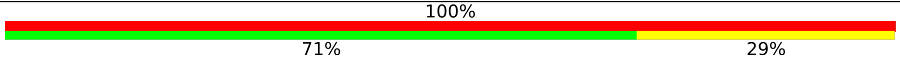
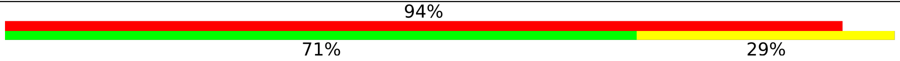
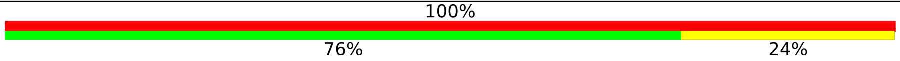
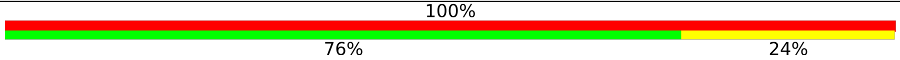
Mol	Chain	Length	Quality of chain
2	Dm	17	
2	Dr	17	
2	Dw	17	
2	E2	17	
2	E7	17	
2	ED	17	
2	EI	17	
2	EN	17	
2	ES	17	
2	EX	17	
2	Ec	17	
2	Eh	17	
2	Em	17	
2	Er	17	
2	Ew	17	
2	F2	17	
2	F7	17	
2	FD	17	
2	FI	17	
2	FN	17	
2	FS	17	
2	FX	17	
2	Fc	17	
2	Fh	17	
2	Fm	17	

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Mol	Chain	Length	Quality of chain
2	Fr	17	94% 76% 24%
2	Fw	17	88% 76% 24%
2	G2	17	94% 71% 29%
2	G7	17	88% 71% 29%
2	GD	17	100% 71% 29%
2	GI	17	100% 71% 29%
2	GN	17	100% 71% 29%
2	GS	17	100% 71% 29%
2	GX	17	71% 71% 29%
2	Gc	17	76% 76% 24%
2	Gh	17	100% 76% 24%
2	Gm	17	100% 76% 24%
2	Gr	17	82% 76% 24%
2	Gw	17	94% 76% 24%
2	H2	17	100% 71% 29%
2	H7	17	100% 71% 29%
2	HD	17	88% 71% 29%
2	HI	17	94% 71% 29%
2	HN	17	100% 71% 29%
2	HS	17	88% 71% 29%
2	HX	17	65% 71% 29%
2	Hc	17	65% 76% 24%
2	Hh	17	94% 76% 24%
2	Hm	17	88% 76% 24%
2	Hr	17	94% 76% 24%

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Mol	Chain	Length	Quality of chain
2	Hw	17	94% 76% 24%
2	I2	17	82% 71% 29%
2	I7	17	88% 71% 29%
2	ID	17	100% 71% 29%
2	II	17	100% 71% 29%
2	IN	17	82% 71% 29%
2	IS	17	100% 71% 29%
2	IX	17	94% 71% 29%
2	Ic	17	82% 76% 24%
2	Ih	17	100% 76% 24%
2	Im	17	82% 76% 24%
2	Ir	17	94% 76% 24%
2	Iw	17	94% 76% 24%
2	J2	17	100% 71% 29%
2	J7	17	100% 71% 29%
2	JD	17	71% 71% 29%
2	JI	17	94% 71% 29%
2	JN	17	88% 71% 29%
2	JS	17	94% 71% 29%
2	JX	17	100% 71% 29%
2	Jc	17	100% 76% 24%
2	Jh	17	76% 76% 24%
2	Jm	17	88% 76% 24%
2	Jr	17	100% 76% 24%
2	Jw	17	76% 76% 24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 588120 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	AA	185	Total C N O S 1426 901 248 273 4	0	0	0
1	AB	189	Total C N O S 1451 915 253 278 5	0	0	0
1	AC	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	AF	185	Total C N O S 1426 901 248 273 4	0	0	0
1	AG	189	Total C N O S 1451 915 253 278 5	0	0	0
1	AH	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	AK	185	Total C N O S 1426 901 248 273 4	0	0	0
1	AL	189	Total C N O S 1451 915 253 278 5	0	0	0
1	AM	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	AP	185	Total C N O S 1426 901 248 273 4	0	0	0
1	AQ	189	Total C N O S 1451 915 253 278 5	0	0	0
1	AR	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	AU	185	Total C N O S 1426 901 248 273 4	0	0	0
1	AV	189	Total C N O S 1451 915 253 278 5	0	0	0
1	AW	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	AZ	185	Total C N O S 1426 901 248 273 4	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	Aa	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Ab	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Ae	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Af	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Ag	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Aj	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Ak	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Al	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Ao	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Ap	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Aq	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	At	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Au	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Av	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Ay	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Az	189	Total C N O S 1451 915 253 278 5	0	0	0
1	A1	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	A4	185	Total C N O S 1426 901 248 273 4	0	0	0
1	A5	189	Total C N O S 1451 915 253 278 5	0	0	0
1	A6	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	BA	185	Total C N O S 1426 901 248 273 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BB	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	BC	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	BF	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	BG	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	BH	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	BK	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	BL	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	BM	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	BP	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	BQ	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	BR	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	BU	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	BV	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	BW	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	BZ	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Ba	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Bb	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	Be	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Bf	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Bg	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	Bj	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	Bk	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Bl	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Bo	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Bp	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Bq	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Bt	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Bu	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Bv	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	By	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Bz	189	Total C N O S 1451 915 253 278 5	0	0	0
1	B1	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	B4	185	Total C N O S 1426 901 248 273 4	0	0	0
1	B5	189	Total C N O S 1451 915 253 278 5	0	0	0
1	B6	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	CA	185	Total C N O S 1426 901 248 273 4	0	0	0
1	CB	189	Total C N O S 1451 915 253 278 5	0	0	0
1	CC	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	CF	185	Total C N O S 1426 901 248 273 4	0	0	0
1	CG	189	Total C N O S 1451 915 253 278 5	0	0	0
1	CH	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	CK	185	Total C N O S 1426 901 248 273 4	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	CL	189	Total C N O S 1451 915 253 278 5	0	0	0
1	CM	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	CP	185	Total C N O S 1426 901 248 273 4	0	0	0
1	CQ	189	Total C N O S 1451 915 253 278 5	0	0	0
1	CR	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	CU	185	Total C N O S 1426 901 248 273 4	0	0	0
1	CV	189	Total C N O S 1451 915 253 278 5	0	0	0
1	CW	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	CZ	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Ca	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Cb	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Ce	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Cf	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Cg	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Cj	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Ck	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Cl	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Co	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Cp	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Cq	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Ct	185	Total C N O S 1426 901 248 273 4	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	Cu	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Cv	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Cy	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Cz	189	Total C N O S 1451 915 253 278 5	0	0	0
1	C1	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	C4	185	Total C N O S 1426 901 248 273 4	0	0	0
1	C5	189	Total C N O S 1451 915 253 278 5	0	0	0
1	C6	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	DA	185	Total C N O S 1426 901 248 273 4	0	0	0
1	DB	189	Total C N O S 1451 915 253 278 5	0	0	0
1	DC	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	DF	185	Total C N O S 1426 901 248 273 4	0	0	0
1	DG	189	Total C N O S 1451 915 253 278 5	0	0	0
1	DH	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	DK	185	Total C N O S 1426 901 248 273 4	0	0	0
1	DL	189	Total C N O S 1451 915 253 278 5	0	0	0
1	DM	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	DP	185	Total C N O S 1426 901 248 273 4	0	0	0
1	DQ	189	Total C N O S 1451 915 253 278 5	0	0	0
1	DR	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	DU	185	Total C N O S 1426 901 248 273 4	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	DV	189	Total C N O S 1451 915 253 278 5	0	0	0
1	DW	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	DZ	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Da	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Db	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	De	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Df	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Dg	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Dj	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Dk	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Dl	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Do	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Dp	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Dq	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Dt	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Du	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Dv	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Dy	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Dz	189	Total C N O S 1451 915 253 278 5	0	0	0
1	D1	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	D4	185	Total C N O S 1426 901 248 273 4	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	D5	189	Total C N O S 1451 915 253 278 5	0	0	0
1	D6	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	EA	185	Total C N O S 1426 901 248 273 4	0	0	0
1	EB	189	Total C N O S 1451 915 253 278 5	0	0	0
1	EC	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	EF	185	Total C N O S 1426 901 248 273 4	0	0	0
1	EG	189	Total C N O S 1451 915 253 278 5	0	0	0
1	EH	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	EK	185	Total C N O S 1426 901 248 273 4	0	0	0
1	EL	189	Total C N O S 1451 915 253 278 5	0	0	0
1	EM	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	EP	185	Total C N O S 1426 901 248 273 4	0	0	0
1	EQ	189	Total C N O S 1451 915 253 278 5	0	0	0
1	ER	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	EU	185	Total C N O S 1426 901 248 273 4	0	0	0
1	EV	189	Total C N O S 1451 915 253 278 5	0	0	0
1	EW	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	EZ	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Ea	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Eb	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Ee	185	Total C N O S 1426 901 248 273 4	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	Ef	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Eg	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Ej	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Ek	189	Total C N O S 1451 915 253 278 5	0	0	0
1	El	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Eo	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Ep	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Eq	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Et	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Eu	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Ev	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Ey	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Ez	189	Total C N O S 1451 915 253 278 5	0	0	0
1	E1	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	E4	185	Total C N O S 1426 901 248 273 4	0	0	0
1	E5	189	Total C N O S 1451 915 253 278 5	0	0	0
1	E6	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	FA	185	Total C N O S 1426 901 248 273 4	0	0	0
1	FB	189	Total C N O S 1451 915 253 278 5	0	0	0
1	FC	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	FF	185	Total C N O S 1426 901 248 273 4	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	FG	189	Total C N O S 1451 915 253 278 5	0	0	0
1	FH	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	FK	185	Total C N O S 1426 901 248 273 4	0	0	0
1	FL	189	Total C N O S 1451 915 253 278 5	0	0	0
1	FM	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	FP	185	Total C N O S 1426 901 248 273 4	0	0	0
1	FQ	189	Total C N O S 1451 915 253 278 5	0	0	0
1	FR	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	FU	185	Total C N O S 1426 901 248 273 4	0	0	0
1	FV	189	Total C N O S 1451 915 253 278 5	0	0	0
1	FW	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	FZ	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Fa	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Fb	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Fe	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Ff	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Fg	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Fj	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Fk	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Fl	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Fo	185	Total C N O S 1426 901 248 273 4	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	Fp	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Fq	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Ft	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Fu	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Fv	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Fy	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Fz	189	Total C N O S 1451 915 253 278 5	0	0	0
1	F1	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	F4	185	Total C N O S 1426 901 248 273 4	0	0	0
1	F5	189	Total C N O S 1451 915 253 278 5	0	0	0
1	F6	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	GA	185	Total C N O S 1426 901 248 273 4	0	0	0
1	GB	189	Total C N O S 1451 915 253 278 5	0	0	0
1	GC	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	GF	185	Total C N O S 1426 901 248 273 4	0	0	0
1	GG	189	Total C N O S 1451 915 253 278 5	0	0	0
1	GH	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	GK	185	Total C N O S 1426 901 248 273 4	0	0	0
1	GL	189	Total C N O S 1451 915 253 278 5	0	0	0
1	GM	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	GP	185	Total C N O S 1426 901 248 273 4	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	GQ	189	Total C N O S 1451 915 253 278 5	0	0	0
1	GR	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	GU	185	Total C N O S 1426 901 248 273 4	0	0	0
1	GV	189	Total C N O S 1451 915 253 278 5	0	0	0
1	GW	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	GZ	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Ga	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Gb	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Ge	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Gf	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Gg	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Gj	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Gk	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Gl	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Go	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Gp	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Gq	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Gt	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Gu	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Gv	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Gy	185	Total C N O S 1426 901 248 273 4	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	Gz	189	Total C N O S 1451 915 253 278 5	0	0	0
1	G1	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	G4	185	Total C N O S 1426 901 248 273 4	0	0	0
1	G5	189	Total C N O S 1451 915 253 278 5	0	0	0
1	G6	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	HA	185	Total C N O S 1426 901 248 273 4	0	0	0
1	HB	189	Total C N O S 1451 915 253 278 5	0	0	0
1	HC	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	HF	185	Total C N O S 1426 901 248 273 4	0	0	0
1	HG	189	Total C N O S 1451 915 253 278 5	0	0	0
1	HH	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	HK	185	Total C N O S 1426 901 248 273 4	0	0	0
1	HL	189	Total C N O S 1451 915 253 278 5	0	0	0
1	HM	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	HP	185	Total C N O S 1426 901 248 273 4	0	0	0
1	HQ	189	Total C N O S 1451 915 253 278 5	0	0	0
1	HR	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	HU	185	Total C N O S 1426 901 248 273 4	0	0	0
1	HV	189	Total C N O S 1451 915 253 278 5	0	0	0
1	HW	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	HZ	185	Total C N O S 1426 901 248 273 4	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	Ha	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Hb	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	He	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Hf	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Hg	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Hj	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Hk	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Hl	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Ho	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Hp	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Hq	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Ht	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Hu	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Hv	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Hy	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Hz	189	Total C N O S 1451 915 253 278 5	0	0	0
1	H1	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	H4	185	Total C N O S 1426 901 248 273 4	0	0	0
1	H5	189	Total C N O S 1451 915 253 278 5	0	0	0
1	H6	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	IA	185	Total C N O S 1426 901 248 273 4	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	IB	189	Total C N O S 1451 915 253 278 5	0	0	0
1	IC	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	IF	185	Total C N O S 1426 901 248 273 4	0	0	0
1	IG	189	Total C N O S 1451 915 253 278 5	0	0	0
1	IH	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	IK	185	Total C N O S 1426 901 248 273 4	0	0	0
1	IL	189	Total C N O S 1451 915 253 278 5	0	0	0
1	IM	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	IP	185	Total C N O S 1426 901 248 273 4	0	0	0
1	IQ	189	Total C N O S 1451 915 253 278 5	0	0	0
1	IR	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	IU	185	Total C N O S 1426 901 248 273 4	0	0	0
1	IV	189	Total C N O S 1451 915 253 278 5	0	0	0
1	IW	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	IZ	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Ia	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Ib	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Ie	185	Total C N O S 1426 901 248 273 4	0	0	0
1	If	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Ig	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Ij	185	Total C N O S 1426 901 248 273 4	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	Ik	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Il	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Io	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Ip	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Iq	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	It	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Iu	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Iv	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Iy	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Iz	189	Total C N O S 1451 915 253 278 5	0	0	0
1	I1	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	I4	185	Total C N O S 1426 901 248 273 4	0	0	0
1	I5	189	Total C N O S 1451 915 253 278 5	0	0	0
1	I6	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	JA	185	Total C N O S 1426 901 248 273 4	0	0	0
1	JB	189	Total C N O S 1451 915 253 278 5	0	0	0
1	JC	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	JF	185	Total C N O S 1426 901 248 273 4	0	0	0
1	JG	189	Total C N O S 1451 915 253 278 5	0	0	0
1	JH	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	JK	185	Total C N O S 1426 901 248 273 4	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	JL	189	Total C N O S 1451 915 253 278 5	0	0	0
1	JM	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	JP	185	Total C N O S 1426 901 248 273 4	0	0	0
1	JQ	189	Total C N O S 1451 915 253 278 5	0	0	0
1	JR	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	JU	185	Total C N O S 1426 901 248 273 4	0	0	0
1	JV	189	Total C N O S 1451 915 253 278 5	0	0	0
1	JW	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	JZ	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Ja	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Jb	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Je	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Jf	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Jg	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Jj	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Jk	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Jl	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Jo	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Jp	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Jq	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Jt	185	Total C N O S 1426 901 248 273 4	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	Ju	189	Total C N O S 1451 915 253 278 5	0	0	0
1	Jv	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	Jy	185	Total C N O S 1426 901 248 273 4	0	0	0
1	Jz	189	Total C N O S 1451 915 253 278 5	0	0	0
1	J1	217	Total C N O S 1674 1049 304 316 5	0	0	0
1	J4	185	Total C N O S 1426 901 248 273 4	0	0	0
1	J5	189	Total C N O S 1451 915 253 278 5	0	0	0
1	J6	217	Total C N O S 1674 1049 304 316 5	0	0	0

- Molecule 2 is a RNA chain called 5'-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	AD	17	Total C N O P 349 157 46 129 17	0	0	0
2	AI	17	Total C N O P 349 157 46 129 17	0	0	0
2	AN	17	Total C N O P 349 157 46 129 17	0	0	0
2	AS	17	Total C N O P 349 157 46 129 17	0	0	0
2	AX	17	Total C N O P 349 157 46 129 17	0	0	0
2	Ac	17	Total C N O P 349 157 46 129 17	0	0	0
2	Ah	17	Total C N O P 349 157 46 129 17	0	0	0
2	Am	17	Total C N O P 349 157 46 129 17	0	0	0
2	Ar	17	Total C N O P 349 157 46 129 17	0	0	0
2	Aw	17	Total C N O P 349 157 46 129 17	0	0	0
2	A2	17	Total C N O P 349 157 46 129 17	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	A7	17	Total C N O P 349 157 46 129 17	0	0	0
2	BD	17	Total C N O P 349 157 46 129 17	0	0	0
2	BI	17	Total C N O P 349 157 46 129 17	0	0	0
2	BN	17	Total C N O P 349 157 46 129 17	0	0	0
2	BS	17	Total C N O P 349 157 46 129 17	0	0	0
2	BX	17	Total C N O P 349 157 46 129 17	0	0	0
2	Bc	17	Total C N O P 349 157 46 129 17	0	0	0
2	Bh	17	Total C N O P 349 157 46 129 17	0	0	0
2	Bm	17	Total C N O P 349 157 46 129 17	0	0	0
2	Br	17	Total C N O P 349 157 46 129 17	0	0	0
2	Bw	17	Total C N O P 349 157 46 129 17	0	0	0
2	B2	17	Total C N O P 349 157 46 129 17	0	0	0
2	B7	17	Total C N O P 349 157 46 129 17	0	0	0
2	CD	17	Total C N O P 349 157 46 129 17	0	0	0
2	CI	17	Total C N O P 349 157 46 129 17	0	0	0
2	CN	17	Total C N O P 349 157 46 129 17	0	0	0
2	CS	17	Total C N O P 349 157 46 129 17	0	0	0
2	CX	17	Total C N O P 349 157 46 129 17	0	0	0
2	Cc	17	Total C N O P 349 157 46 129 17	0	0	0
2	Ch	17	Total C N O P 349 157 46 129 17	0	0	0
2	Cm	17	Total C N O P 349 157 46 129 17	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	Cr	17	Total C N O P 349 157 46 129 17	0	0	0
2	Cw	17	Total C N O P 349 157 46 129 17	0	0	0
2	C2	17	Total C N O P 349 157 46 129 17	0	0	0
2	C7	17	Total C N O P 349 157 46 129 17	0	0	0
2	DD	17	Total C N O P 349 157 46 129 17	0	0	0
2	DI	17	Total C N O P 349 157 46 129 17	0	0	0
2	DN	17	Total C N O P 349 157 46 129 17	0	0	0
2	DS	17	Total C N O P 349 157 46 129 17	0	0	0
2	DX	17	Total C N O P 349 157 46 129 17	0	0	0
2	Dc	17	Total C N O P 349 157 46 129 17	0	0	0
2	Dh	17	Total C N O P 349 157 46 129 17	0	0	0
2	Dm	17	Total C N O P 349 157 46 129 17	0	0	0
2	Dr	17	Total C N O P 349 157 46 129 17	0	0	0
2	Dw	17	Total C N O P 349 157 46 129 17	0	0	0
2	D2	17	Total C N O P 349 157 46 129 17	0	0	0
2	D7	17	Total C N O P 349 157 46 129 17	0	0	0
2	ED	17	Total C N O P 349 157 46 129 17	0	0	0
2	EI	17	Total C N O P 349 157 46 129 17	0	0	0
2	EN	17	Total C N O P 349 157 46 129 17	0	0	0
2	ES	17	Total C N O P 349 157 46 129 17	0	0	0
2	EX	17	Total C N O P 349 157 46 129 17	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	Ec	17	Total C N O P 349 157 46 129 17	0	0	0
2	Eh	17	Total C N O P 349 157 46 129 17	0	0	0
2	Em	17	Total C N O P 349 157 46 129 17	0	0	0
2	Er	17	Total C N O P 349 157 46 129 17	0	0	0
2	Ew	17	Total C N O P 349 157 46 129 17	0	0	0
2	E2	17	Total C N O P 349 157 46 129 17	0	0	0
2	E7	17	Total C N O P 349 157 46 129 17	0	0	0
2	FD	17	Total C N O P 349 157 46 129 17	0	0	0
2	FI	17	Total C N O P 349 157 46 129 17	0	0	0
2	FN	17	Total C N O P 349 157 46 129 17	0	0	0
2	FS	17	Total C N O P 349 157 46 129 17	0	0	0
2	FX	17	Total C N O P 349 157 46 129 17	0	0	0
2	Fc	17	Total C N O P 349 157 46 129 17	0	0	0
2	Fh	17	Total C N O P 349 157 46 129 17	0	0	0
2	Fm	17	Total C N O P 349 157 46 129 17	0	0	0
2	Fr	17	Total C N O P 349 157 46 129 17	0	0	0
2	Fw	17	Total C N O P 349 157 46 129 17	0	0	0
2	F2	17	Total C N O P 349 157 46 129 17	0	0	0
2	F7	17	Total C N O P 349 157 46 129 17	0	0	0
2	GD	17	Total C N O P 349 157 46 129 17	0	0	0
2	GI	17	Total C N O P 349 157 46 129 17	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	GN	17	Total C N O P 349 157 46 129 17	0	0	0
2	GS	17	Total C N O P 349 157 46 129 17	0	0	0
2	GX	17	Total C N O P 349 157 46 129 17	0	0	0
2	Gc	17	Total C N O P 349 157 46 129 17	0	0	0
2	Gh	17	Total C N O P 349 157 46 129 17	0	0	0
2	Gm	17	Total C N O P 349 157 46 129 17	0	0	0
2	Gr	17	Total C N O P 349 157 46 129 17	0	0	0
2	Gw	17	Total C N O P 349 157 46 129 17	0	0	0
2	G2	17	Total C N O P 349 157 46 129 17	0	0	0
2	G7	17	Total C N O P 349 157 46 129 17	0	0	0
2	HD	17	Total C N O P 349 157 46 129 17	0	0	0
2	HI	17	Total C N O P 349 157 46 129 17	0	0	0
2	HN	17	Total C N O P 349 157 46 129 17	0	0	0
2	HS	17	Total C N O P 349 157 46 129 17	0	0	0
2	HX	17	Total C N O P 349 157 46 129 17	0	0	0
2	Hc	17	Total C N O P 349 157 46 129 17	0	0	0
2	Hh	17	Total C N O P 349 157 46 129 17	0	0	0
2	Hm	17	Total C N O P 349 157 46 129 17	0	0	0
2	Hr	17	Total C N O P 349 157 46 129 17	0	0	0
2	Hw	17	Total C N O P 349 157 46 129 17	0	0	0
2	H2	17	Total C N O P 349 157 46 129 17	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	H7	17	Total C N O P 349 157 46 129 17	0	0	0
2	ID	17	Total C N O P 349 157 46 129 17	0	0	0
2	II	17	Total C N O P 349 157 46 129 17	0	0	0
2	IN	17	Total C N O P 349 157 46 129 17	0	0	0
2	IS	17	Total C N O P 349 157 46 129 17	0	0	0
2	IX	17	Total C N O P 349 157 46 129 17	0	0	0
2	Ic	17	Total C N O P 349 157 46 129 17	0	0	0
2	Ih	17	Total C N O P 349 157 46 129 17	0	0	0
2	Im	17	Total C N O P 349 157 46 129 17	0	0	0
2	Ir	17	Total C N O P 349 157 46 129 17	0	0	0
2	Iw	17	Total C N O P 349 157 46 129 17	0	0	0
2	I2	17	Total C N O P 349 157 46 129 17	0	0	0
2	I7	17	Total C N O P 349 157 46 129 17	0	0	0
2	JD	17	Total C N O P 349 157 46 129 17	0	0	0
2	JI	17	Total C N O P 349 157 46 129 17	0	0	0
2	JN	17	Total C N O P 349 157 46 129 17	0	0	0
2	JS	17	Total C N O P 349 157 46 129 17	0	0	0
2	JX	17	Total C N O P 349 157 46 129 17	0	0	0
2	Jc	17	Total C N O P 349 157 46 129 17	0	0	0
2	Jh	17	Total C N O P 349 157 46 129 17	0	0	0
2	Jm	17	Total C N O P 349 157 46 129 17	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Jr	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Jw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	J2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	J7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AA	1	Total 1	Ca 1	0	0
3	AF	1	Total 1	Ca 1	0	0
3	AL	1	Total 1	Ca 1	0	0
3	AP	1	Total 1	Ca 1	0	0
3	AU	1	Total 1	Ca 1	0	0
3	AZ	1	Total 1	Ca 1	0	0
3	Af	1	Total 1	Ca 1	0	0
3	Aj	1	Total 1	Ca 1	0	0
3	Ao	1	Total 1	Ca 1	0	0
3	At	1	Total 1	Ca 1	0	0
3	A1	1	Total 1	Ca 1	0	0
3	A4	1	Total 1	Ca 1	0	0
3	BB	1	Total 1	Ca 1	0	0
3	BF	1	Total 1	Ca 1	0	0
3	BK	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	BQ	1	Total Ca 1 1	0	0
3	BU	1	Total Ca 1 1	0	0
3	BZ	1	Total Ca 1 1	0	0
3	Be	1	Total Ca 1 1	0	0
3	Bk	1	Total Ca 1 1	0	0
3	Bo	1	Total Ca 1 1	0	0
3	Bt	1	Total Ca 1 1	0	0
3	By	1	Total Ca 1 1	0	0
3	B5	1	Total Ca 1 1	0	0
3	CA	1	Total Ca 1 1	0	0
3	CG	1	Total Ca 1 1	0	0
3	CK	1	Total Ca 1 1	0	0
3	CP	1	Total Ca 1 1	0	0
3	CU	1	Total Ca 1 1	0	0
3	CZ	1	Total Ca 1 1	0	0
3	Ce	1	Total Ca 1 1	0	0
3	Cj	1	Total Ca 1 1	0	0
3	Co	1	Total Ca 1 1	0	0
3	Ct	1	Total Ca 1 1	0	0
3	Cy	1	Total Ca 1 1	0	0
3	C4	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	DA	1	Total Ca 1 1	0	0
3	DF	1	Total Ca 1 1	0	0
3	DK	1	Total Ca 1 1	0	0
3	DP	1	Total Ca 1 1	0	0
3	DU	1	Total Ca 1 1	0	0
3	DZ	1	Total Ca 1 1	0	0
3	Df	1	Total Ca 1 1	0	0
3	Dj	1	Total Ca 1 1	0	0
3	Do	1	Total Ca 1 1	0	0
3	Dt	1	Total Ca 1 1	0	0
3	Dy	1	Total Ca 1 1	0	0
3	D4	1	Total Ca 1 1	0	0
3	EC	1	Total Ca 1 1	0	0
3	EF	1	Total Ca 1 1	0	0
3	EK	1	Total Ca 1 1	0	0
3	EP	1	Total Ca 1 1	0	0
3	EU	1	Total Ca 1 1	0	0
3	EZ	1	Total Ca 1 1	0	0
3	Ee	1	Total Ca 1 1	0	0
3	Ek	1	Total Ca 1 1	0	0
3	Eo	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Et	1	Total Ca 1 1	0	0
3	Ey	1	Total Ca 1 1	0	0
3	E4	1	Total Ca 1 1	0	0
3	FA	1	Total Ca 1 1	0	0
3	FF	1	Total Ca 1 1	0	0
3	FK	1	Total Ca 1 1	0	0
3	FP	1	Total Ca 1 1	0	0
3	FU	1	Total Ca 1 1	0	0
3	FZ	1	Total Ca 1 1	0	0
3	Fe	1	Total Ca 1 1	0	0
3	Fk	1	Total Ca 1 1	0	0
3	Fo	1	Total Ca 1 1	0	0
3	Ft	1	Total Ca 1 1	0	0
3	F1	1	Total Ca 1 1	0	0
3	F4	1	Total Ca 1 1	0	0
3	GA	1	Total Ca 1 1	0	0
3	GF	1	Total Ca 1 1	0	0
3	GK	1	Total Ca 1 1	0	0
3	GP	1	Total Ca 1 1	0	0
3	GU	1	Total Ca 1 1	0	0
3	GZ	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Ge	1	Total Ca 1 1	0	0
3	Gj	1	Total Ca 1 1	0	0
3	Go	1	Total Ca 1 1	0	0
3	Gt	1	Total Ca 1 1	0	0
3	G1	1	Total Ca 1 1	0	0
3	G4	1	Total Ca 1 1	0	0
3	HA	1	Total Ca 1 1	0	0
3	HF	1	Total Ca 1 1	0	0
3	HK	1	Total Ca 1 1	0	0
3	HP	1	Total Ca 1 1	0	0
3	HU	1	Total Ca 1 1	0	0
3	HZ	1	Total Ca 1 1	0	0
3	Hg	1	Total Ca 1 1	0	0
3	Hj	1	Total Ca 1 1	0	0
3	Ho	1	Total Ca 1 1	0	0
3	Ht	1	Total Ca 1 1	0	0
3	Hy	1	Total Ca 1 1	0	0
3	H4	1	Total Ca 1 1	0	0
3	IA	1	Total Ca 1 1	0	0
3	IF	1	Total Ca 1 1	0	0
3	IK	1	Total Ca 1 1	0	0

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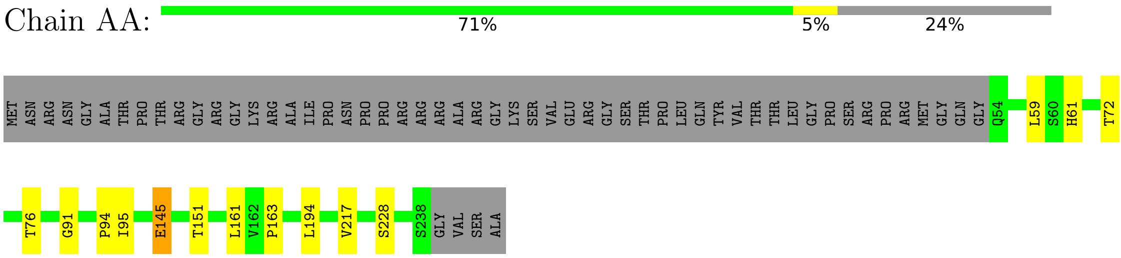
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	IR	1	Total Ca 1 1	0	0
3	IU	1	Total Ca 1 1	0	0
3	IZ	1	Total Ca 1 1	0	0
3	If	1	Total Ca 1 1	0	0
3	Ij	1	Total Ca 1 1	0	0
3	Io	1	Total Ca 1 1	0	0
3	It	1	Total Ca 1 1	0	0
3	I1	1	Total Ca 1 1	0	0
3	I4	1	Total Ca 1 1	0	0
3	JA	1	Total Ca 1 1	0	0
3	JF	1	Total Ca 1 1	0	0
3	JL	1	Total Ca 1 1	0	0
3	JP	1	Total Ca 1 1	0	0
3	JU	1	Total Ca 1 1	0	0
3	JZ	1	Total Ca 1 1	0	0
3	Je	1	Total Ca 1 1	0	0
3	Jj	1	Total Ca 1 1	0	0
3	Jo	1	Total Ca 1 1	0	0
3	Jt	1	Total Ca 1 1	0	0
3	Jy	1	Total Ca 1 1	0	0
3	J4	1	Total Ca 1 1	0	0

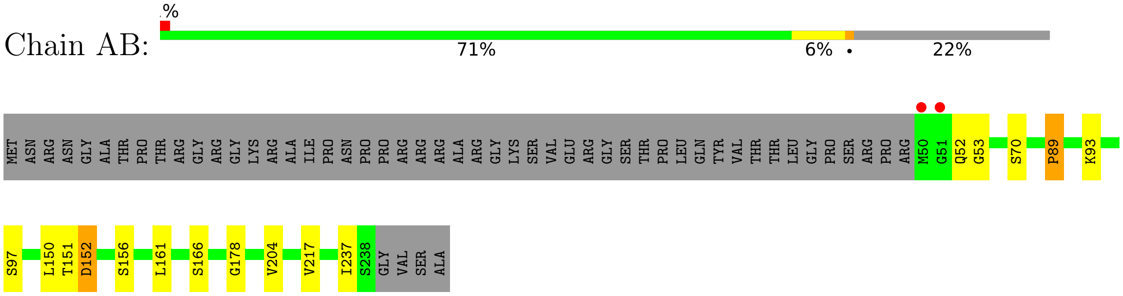
3 Residue-property plots ⓘ

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

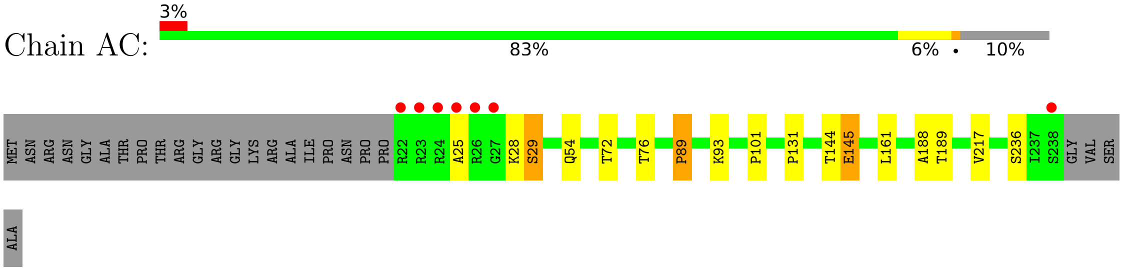
- Molecule 1: Capsid protein



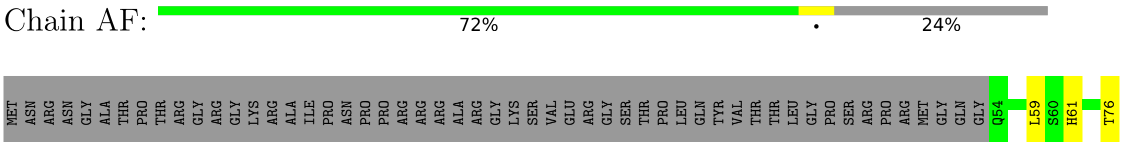
- Molecule 1: Capsid protein

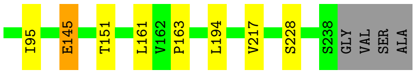


- Molecule 1: Capsid protein



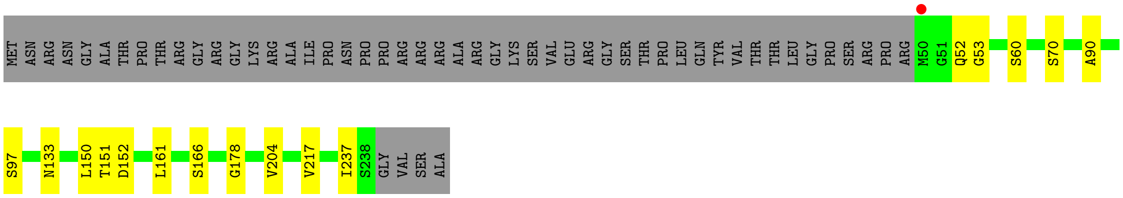
- Molecule 1: Capsid protein





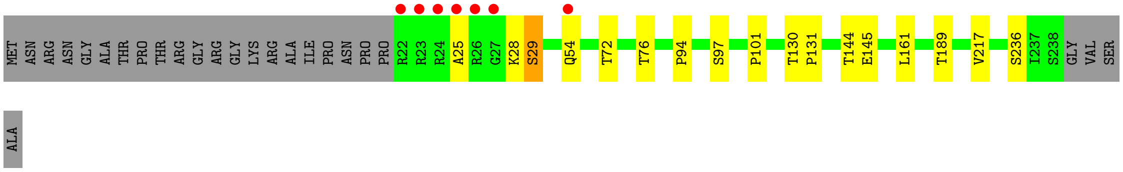
- Molecule 1: Capsid protein

Chain AG:



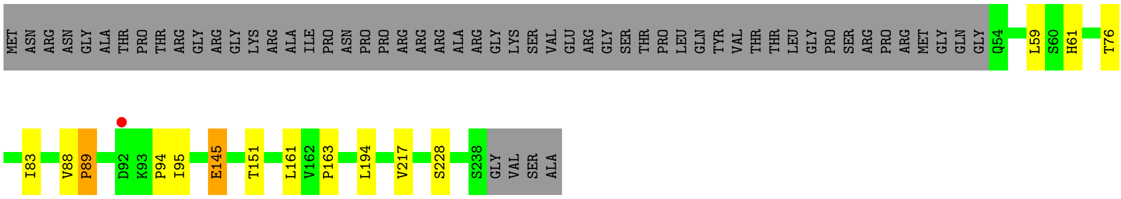
- Molecule 1: Capsid protein

Chain AH:



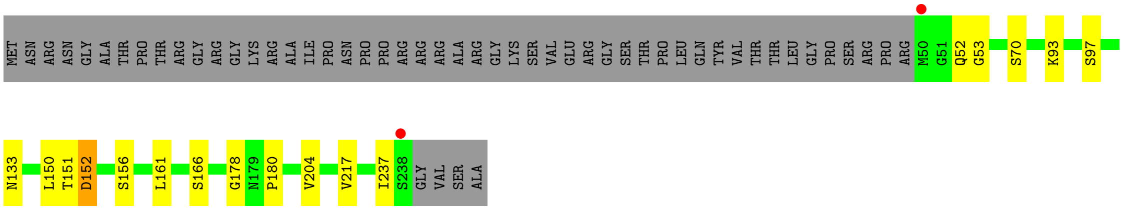
- Molecule 1: Capsid protein

Chain AK:



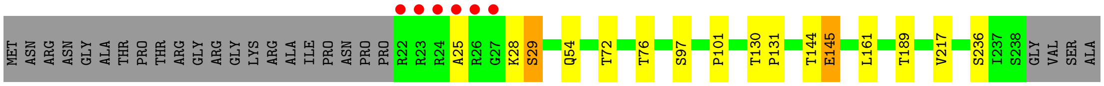
- Molecule 1: Capsid protein

Chain AL:



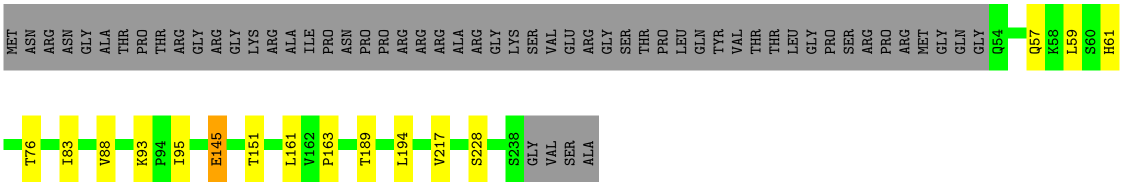
- Molecule 1: Capsid protein

Chain AM:



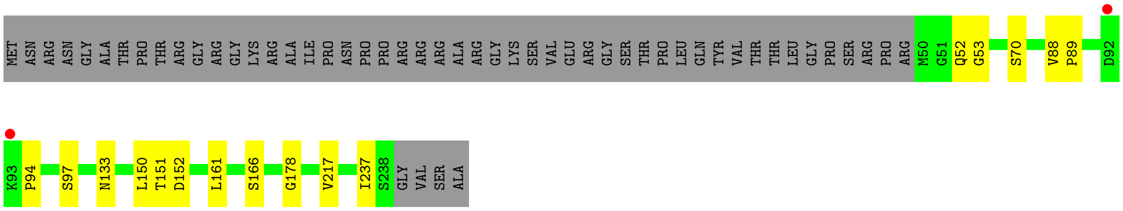
- Molecule 1: Capsid protein

Chain AP:



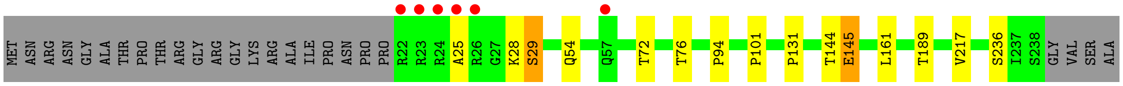
- Molecule 1: Capsid protein

Chain AQ:



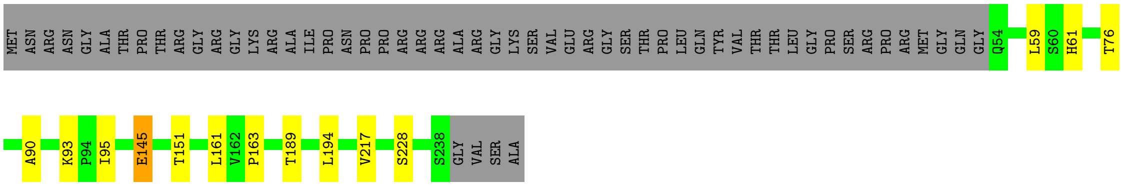
- Molecule 1: Capsid protein

Chain AR:



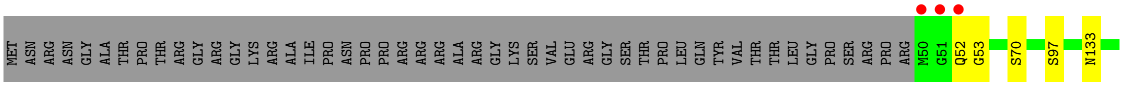
- Molecule 1: Capsid protein

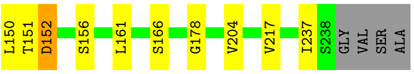
Chain AU:



- Molecule 1: Capsid protein

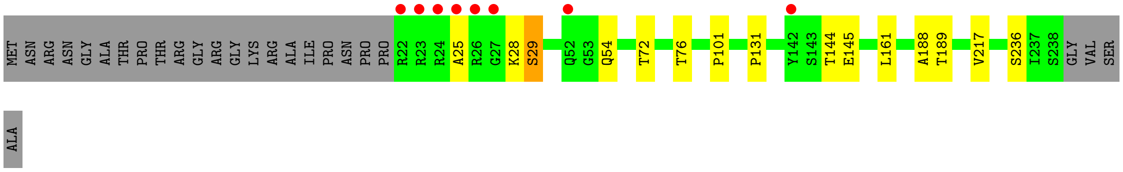
Chain AV:





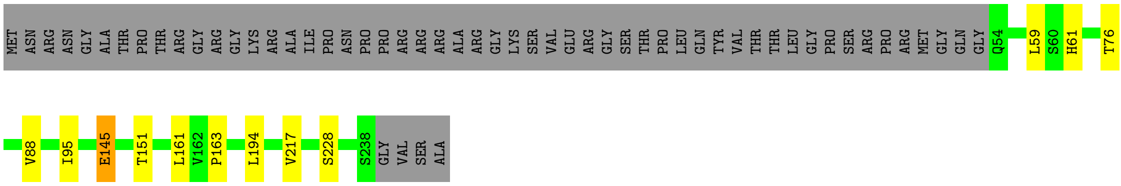
- Molecule 1: Capsid protein

Chain AW:



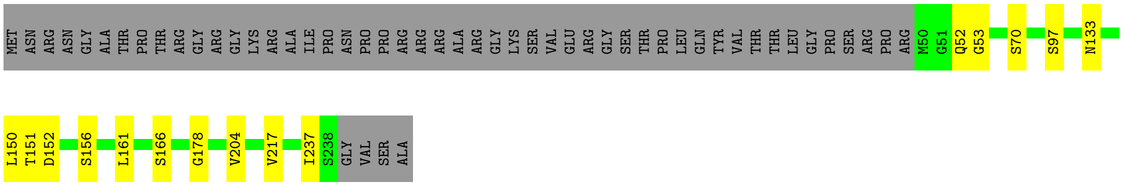
- Molecule 1: Capsid protein

Chain AZ:



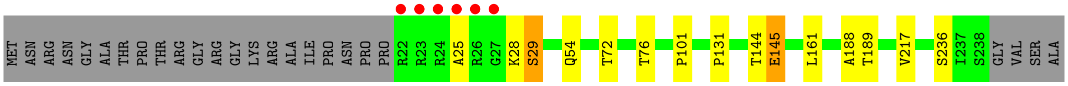
- Molecule 1: Capsid protein

Chain Aa:



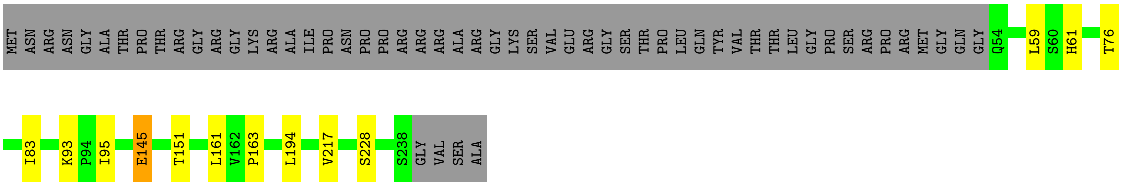
- Molecule 1: Capsid protein

Chain Ab:



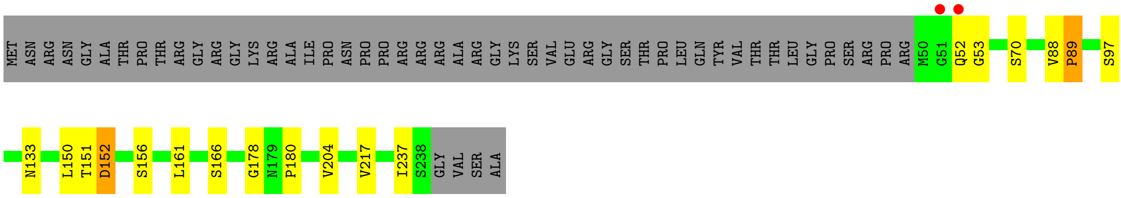
- Molecule 1: Capsid protein

Chain Ae:



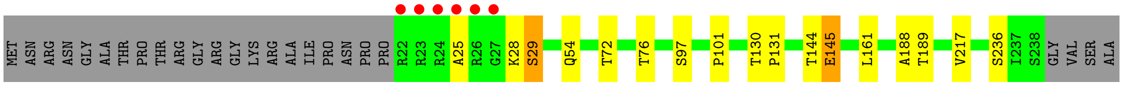
• Molecule 1: Capsid protein

Chain Af:



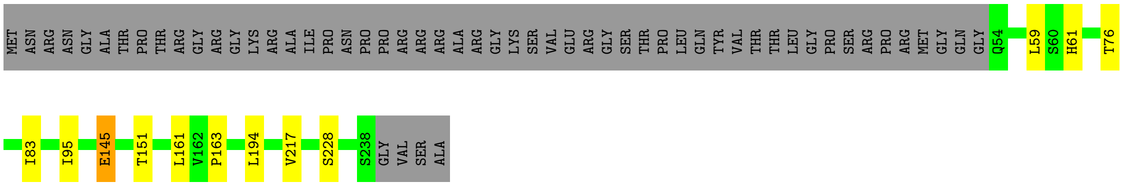
• Molecule 1: Capsid protein

Chain Ag:



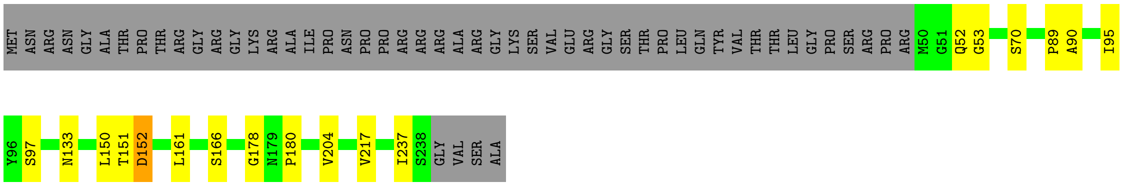
• Molecule 1: Capsid protein

Chain Aj:



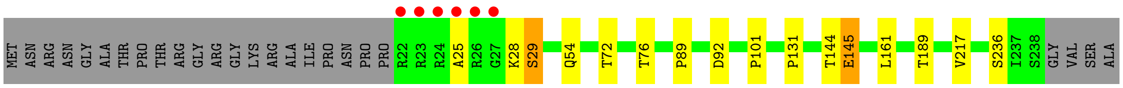
• Molecule 1: Capsid protein

Chain Ak:



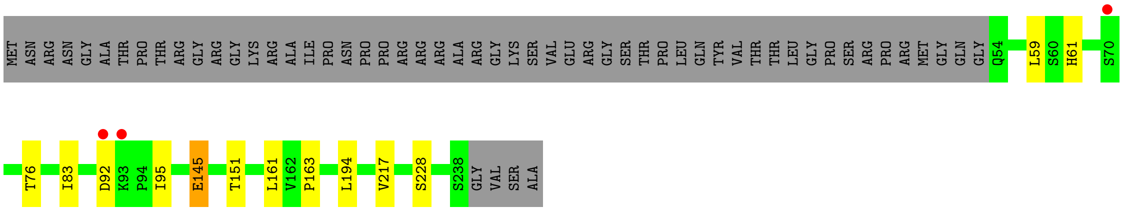
• Molecule 1: Capsid protein

Chain Al:



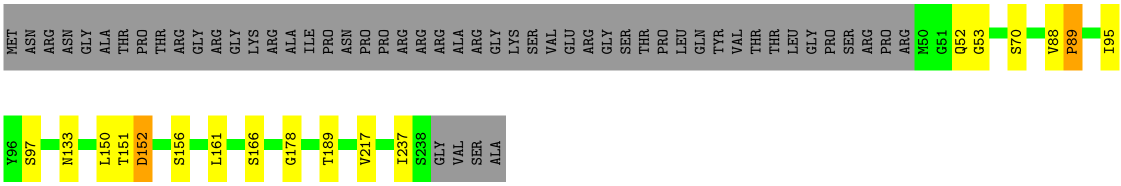
• Molecule 1: Capsid protein

Chain Ao:



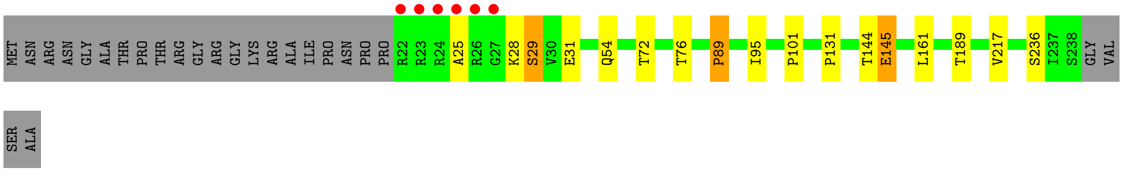
- Molecule 1: Capsid protein

Chain Ap:



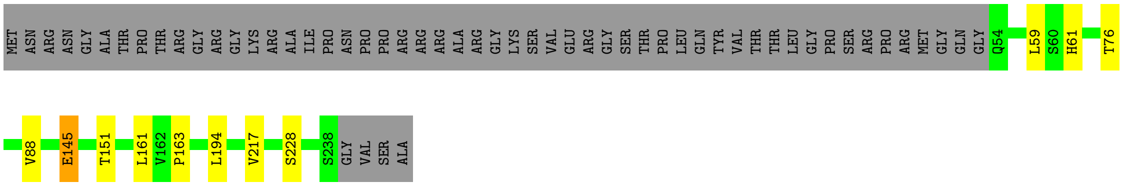
- Molecule 1: Capsid protein

Chain Aq:



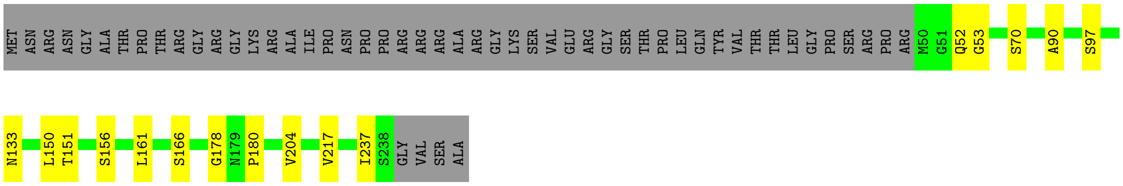
- Molecule 1: Capsid protein

Chain At:

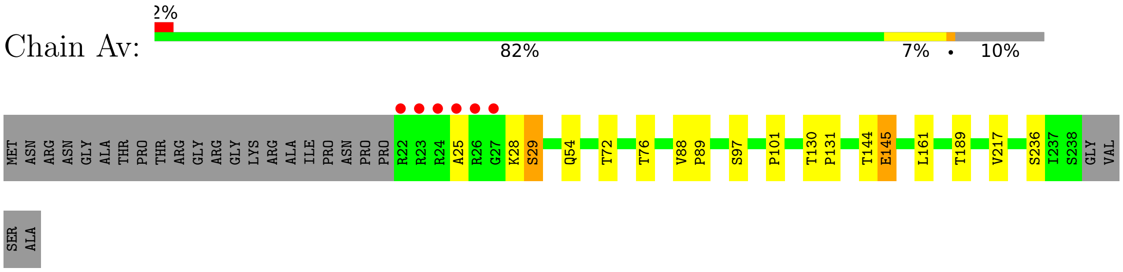


- Molecule 1: Capsid protein

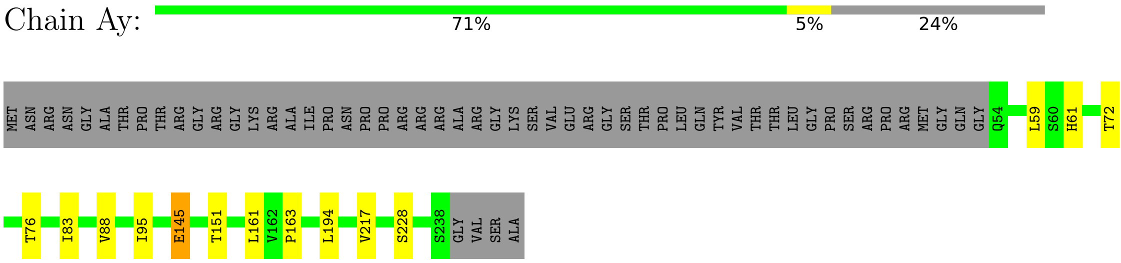
Chain Au:



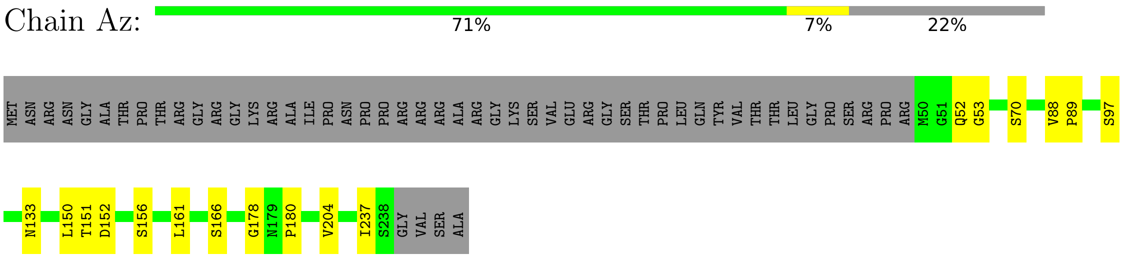
- Molecule 1: Capsid protein



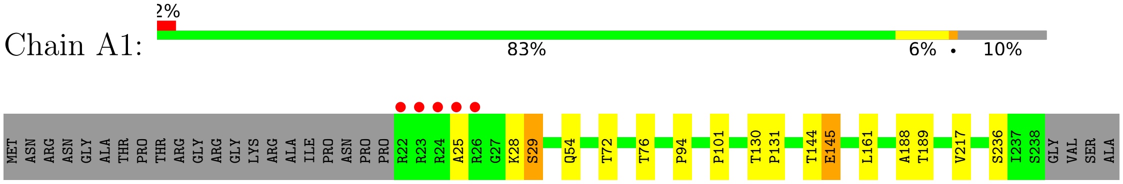
- Molecule 1: Capsid protein



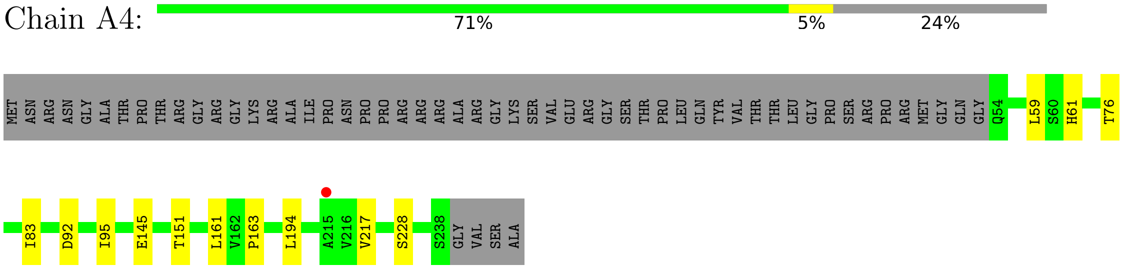
- Molecule 1: Capsid protein



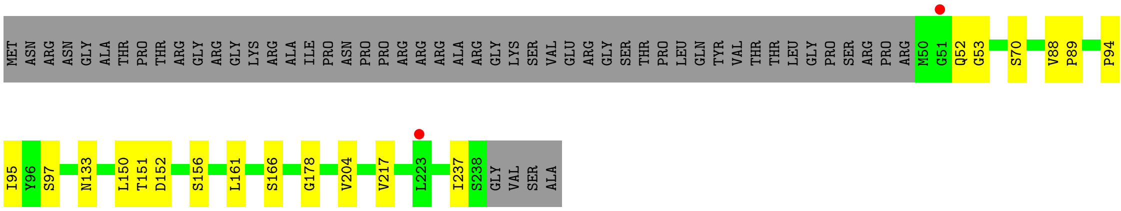
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

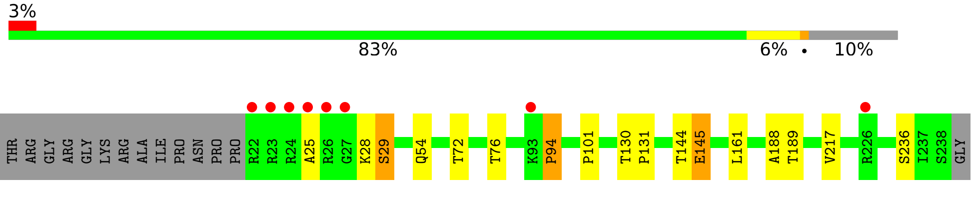


- Molecule 1: Capsid protein



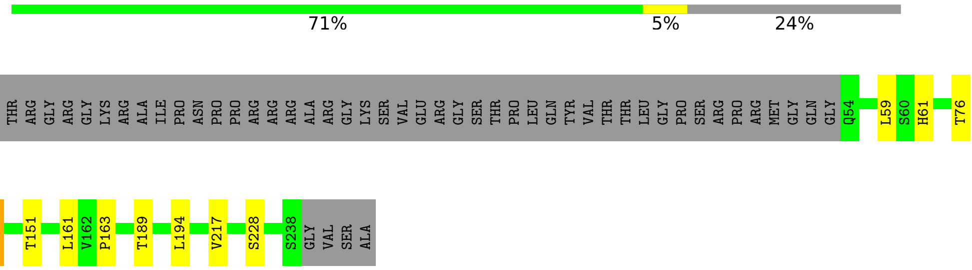
- Molecule 1: Capsid protein

Chain A6:



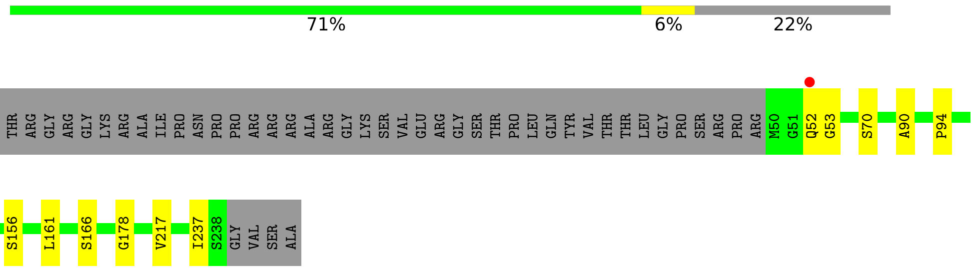
- Molecule 1: Capsid protein

Chain BA:



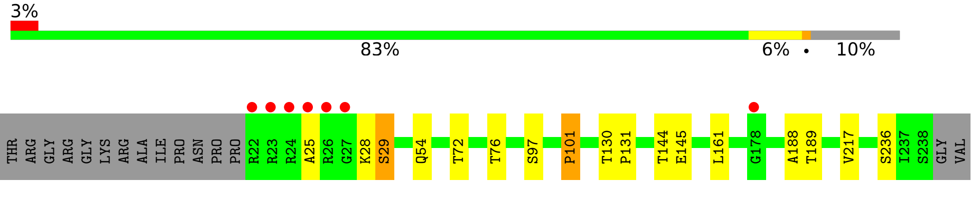
- Molecule 1: Capsid protein

Chain BB:

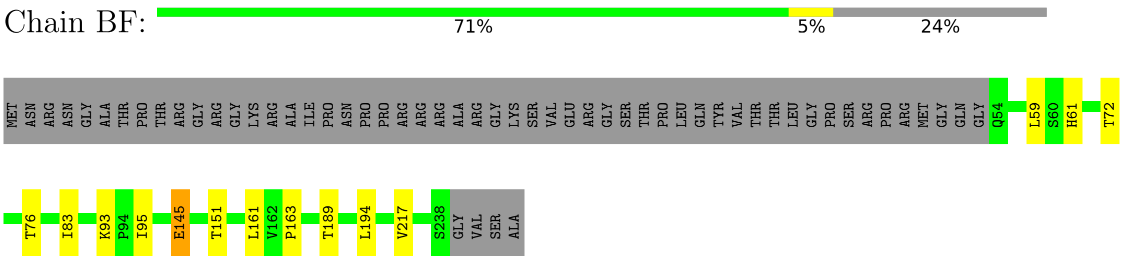


- Molecule 1: Capsid protein

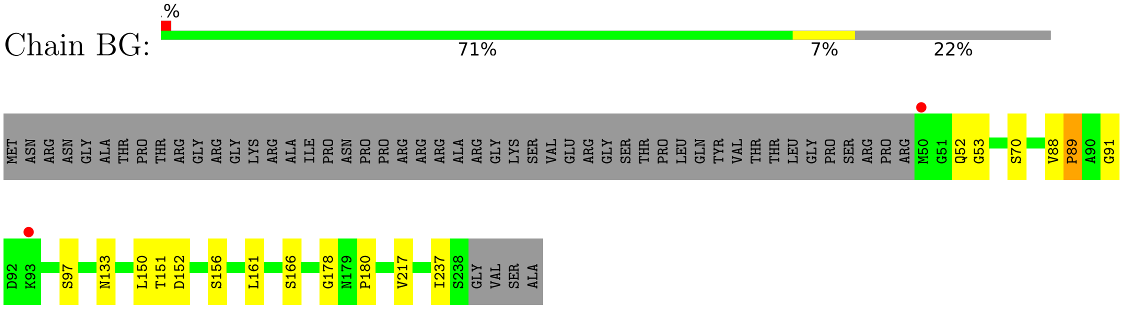
Chain BC:



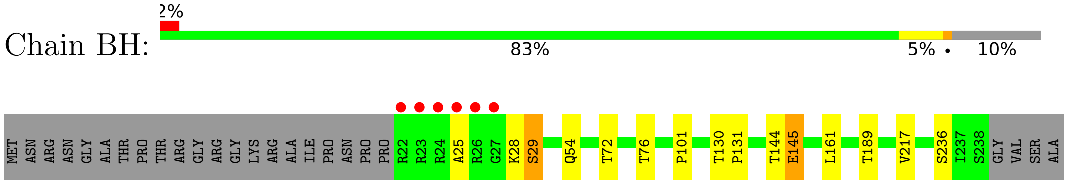
- Molecule 1: Capsid protein



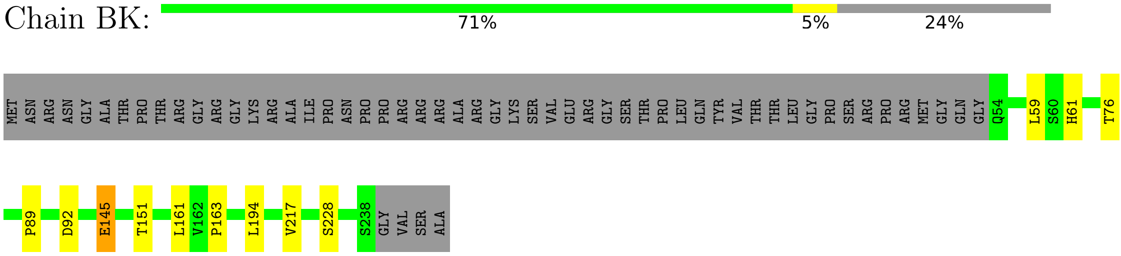
- Molecule 1: Capsid protein



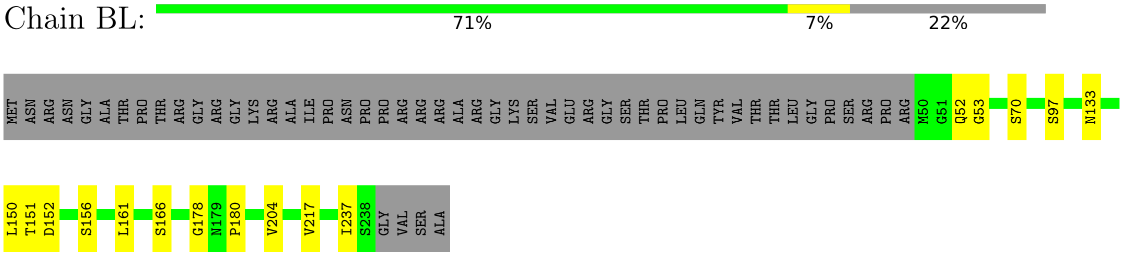
- Molecule 1: Capsid protein



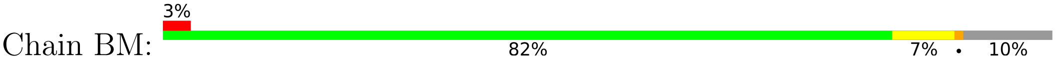
- Molecule 1: Capsid protein

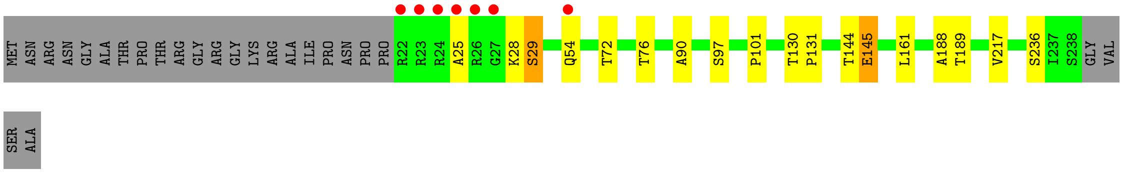


- Molecule 1: Capsid protein



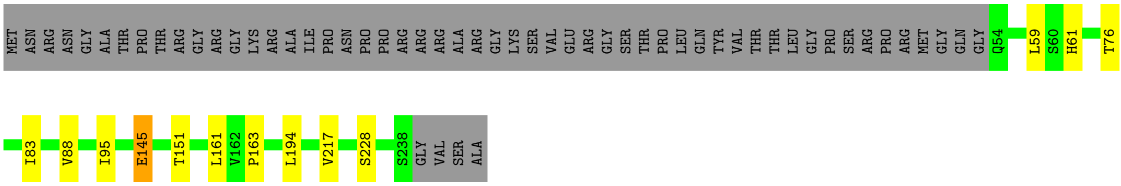
- Molecule 1: Capsid protein





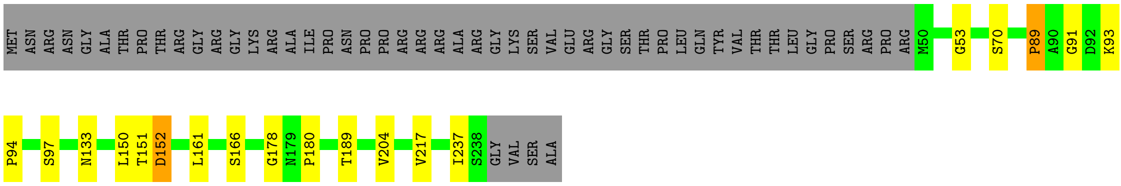
- Molecule 1: Capsid protein

Chain BP:



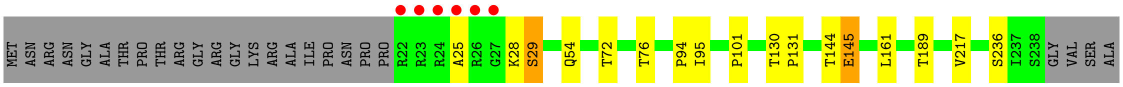
- Molecule 1: Capsid protein

Chain BQ:



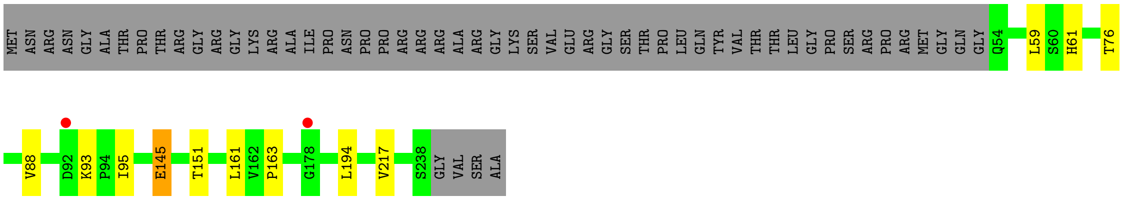
- Molecule 1: Capsid protein

Chain BR:



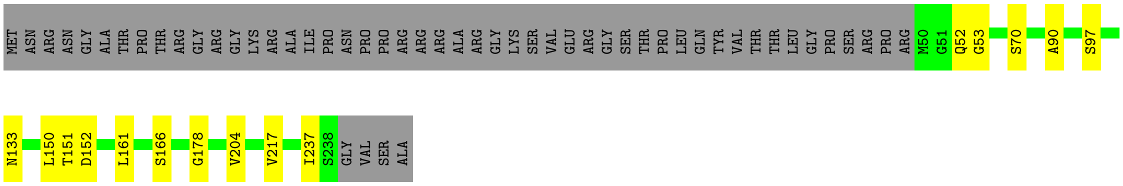
- Molecule 1: Capsid protein

Chain BU:



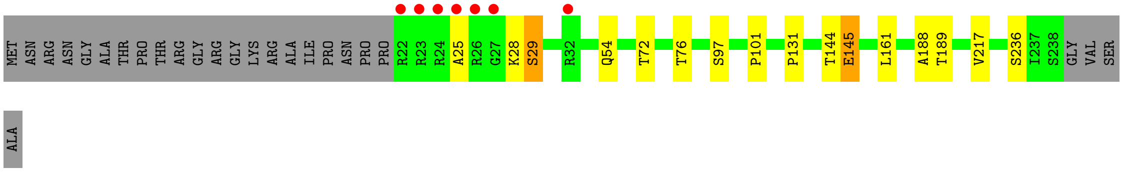
- Molecule 1: Capsid protein

Chain BV:



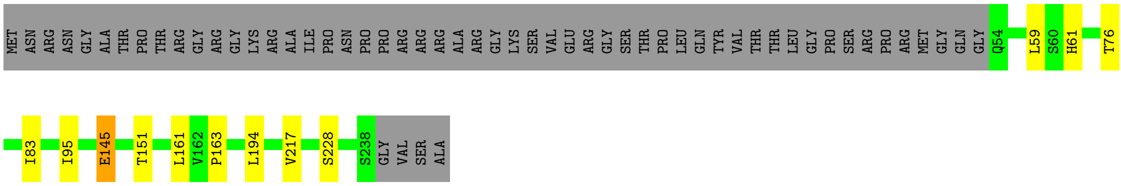
- Molecule 1: Capsid protein

Chain BW:



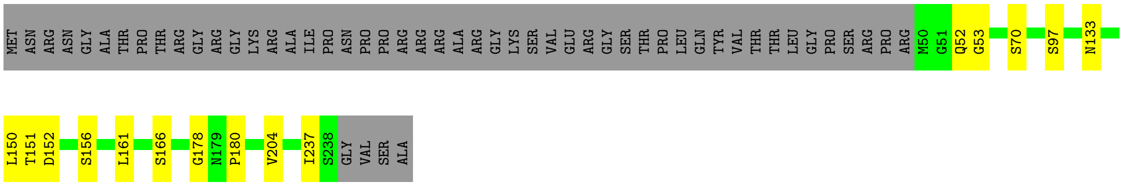
- Molecule 1: Capsid protein

Chain BZ:



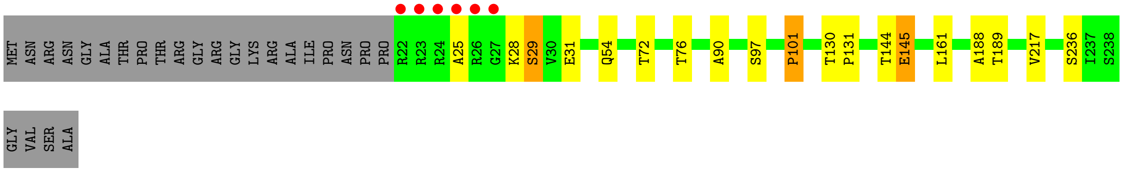
- Molecule 1: Capsid protein

Chain Ba:



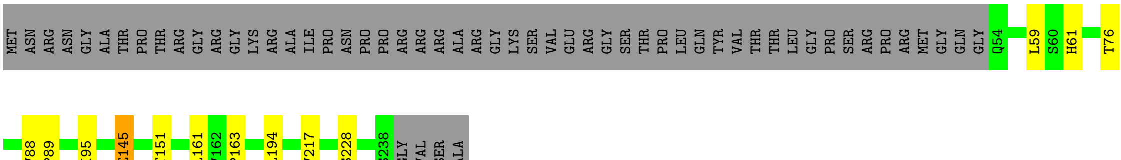
- Molecule 1: Capsid protein

Chain Bb:



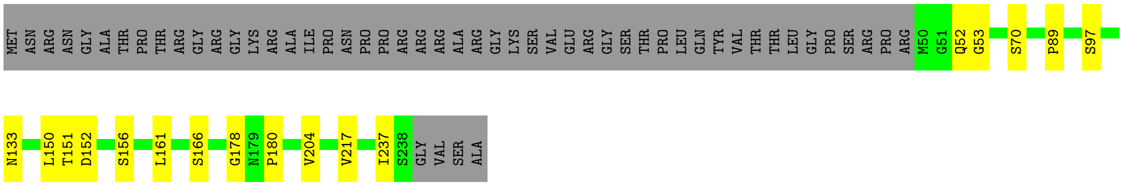
- Molecule 1: Capsid protein

Chain Be:



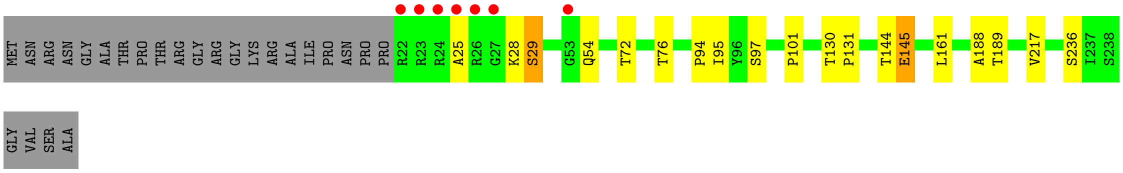
- Molecule 1: Capsid protein

Chain Bf:



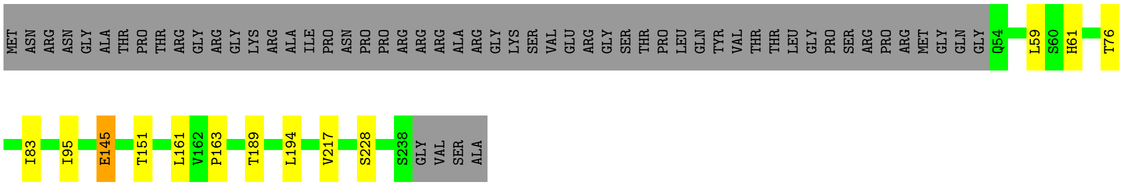
- Molecule 1: Capsid protein

Chain Bg:



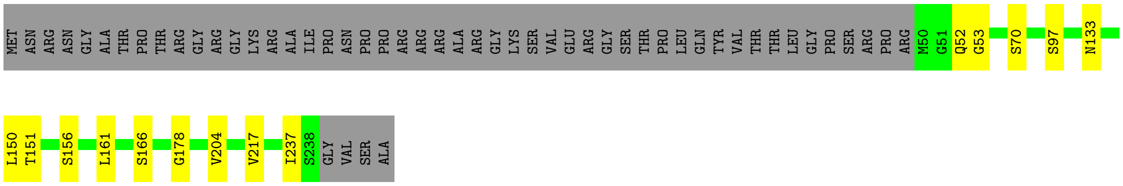
- Molecule 1: Capsid protein

Chain Bj:



- Molecule 1: Capsid protein

Chain Bk:



- Molecule 1: Capsid protein

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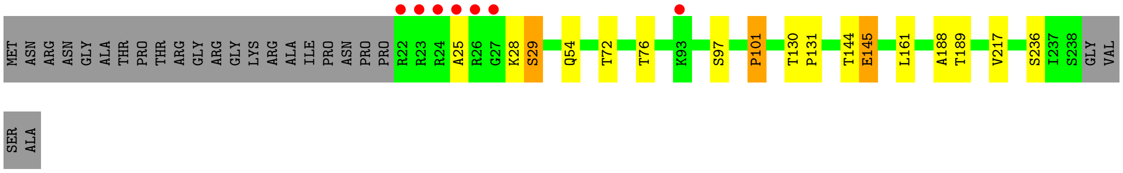
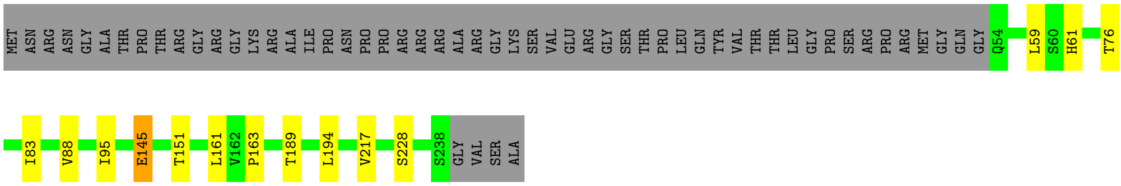


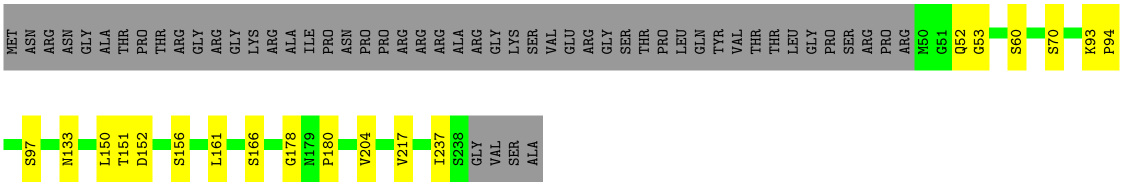
- Molecule 1: Capsid protein

Chain Bo:



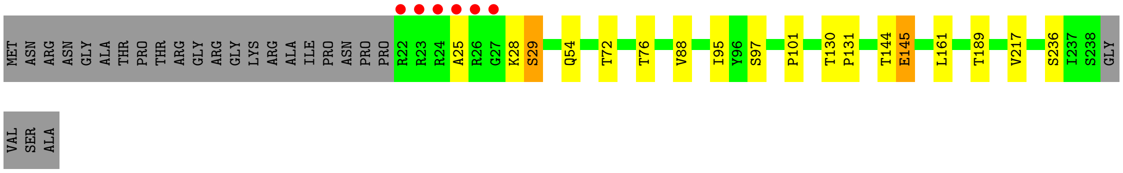
- Molecule 1: Capsid protein

Chain Bp:



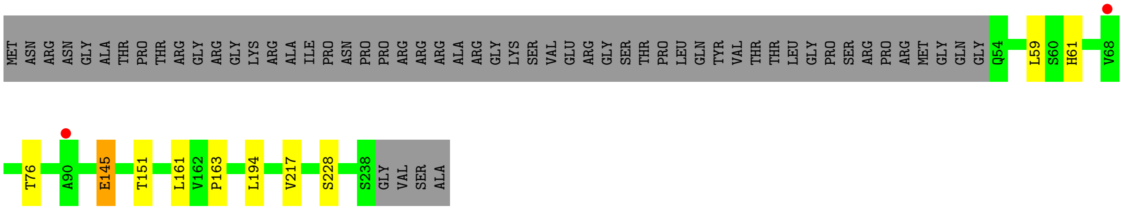
- Molecule 1: Capsid protein

Chain Bq:



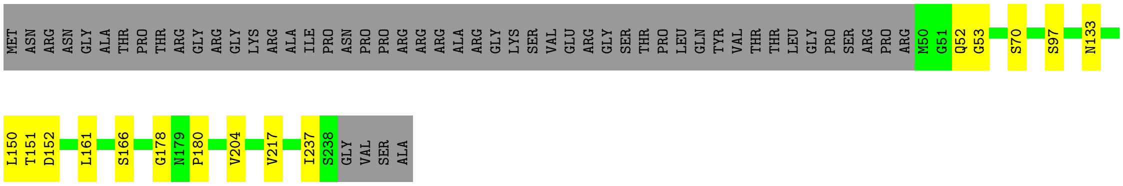
- Molecule 1: Capsid protein

Chain Bt:



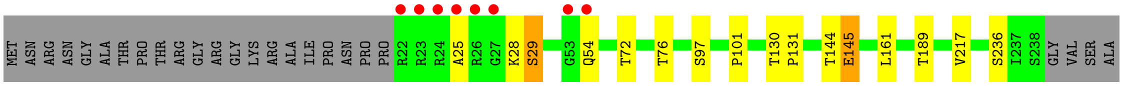
- Molecule 1: Capsid protein

Chain Bu:



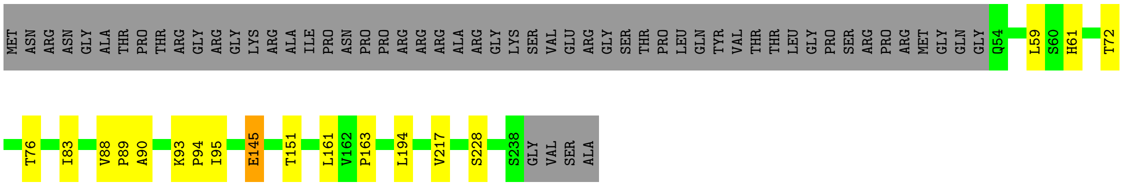
- Molecule 1: Capsid protein

Chain Bv:



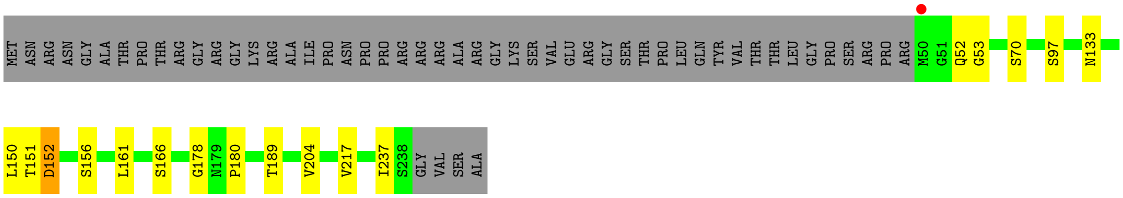
- Molecule 1: Capsid protein

Chain By:



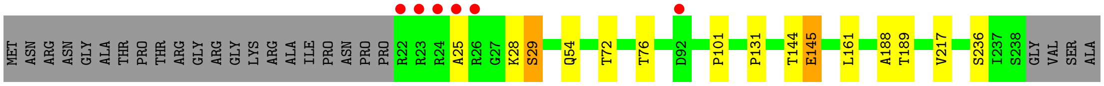
- Molecule 1: Capsid protein

Chain Bz:



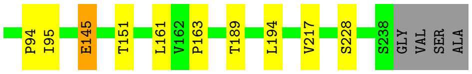
- Molecule 1: Capsid protein

Chain B1:



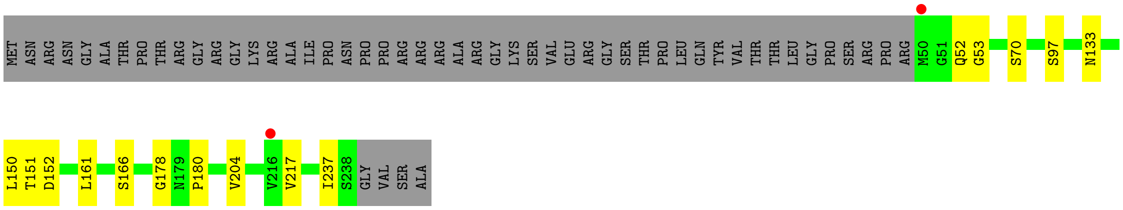
- Molecule 1: Capsid protein

Chain B4:



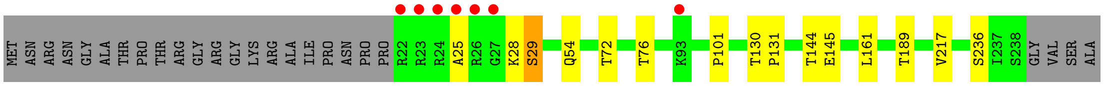
- Molecule 1: Capsid protein

Chain B5:



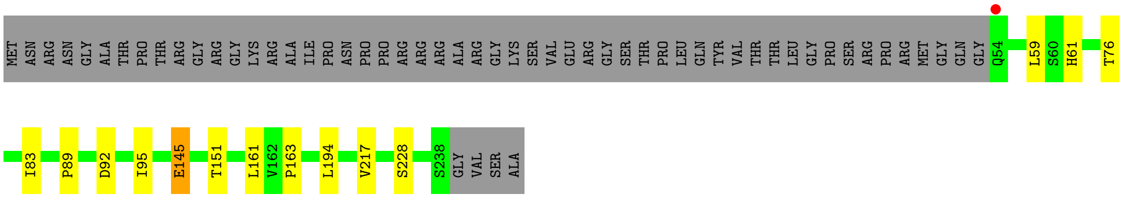
- Molecule 1: Capsid protein

Chain B6:



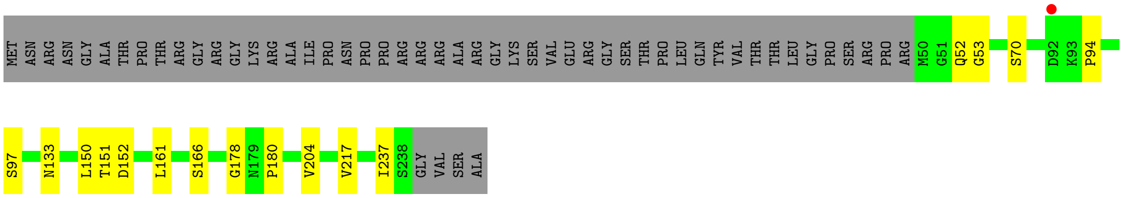
- Molecule 1: Capsid protein

Chain CA:



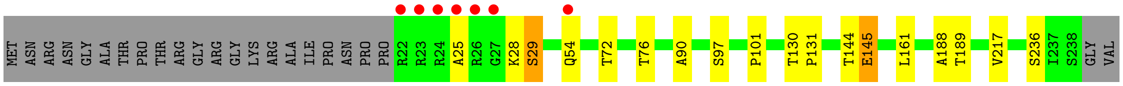
- Molecule 1: Capsid protein

Chain CB:

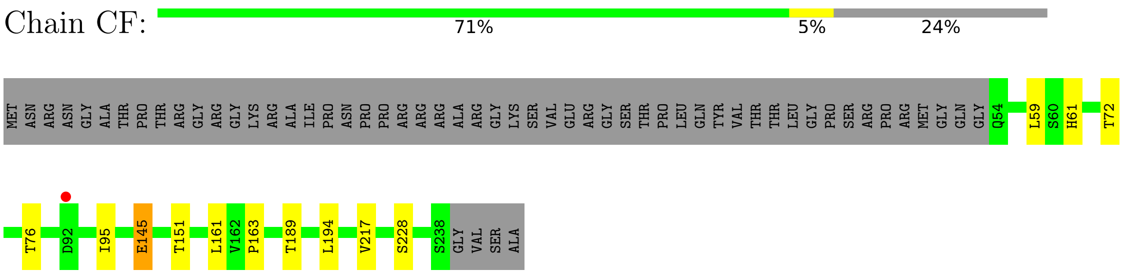


- Molecule 1: Capsid protein

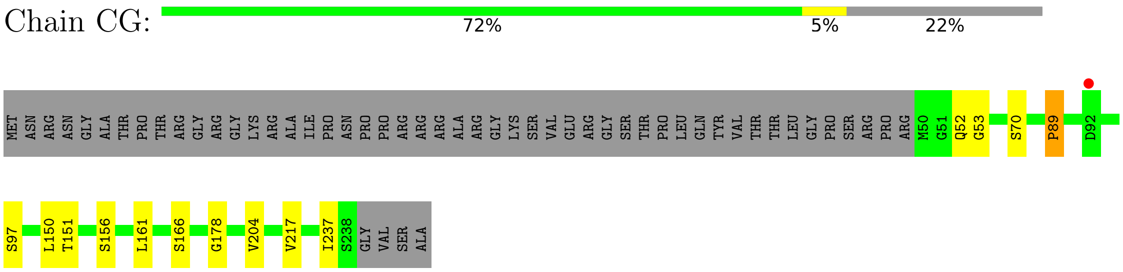
Chain CC:



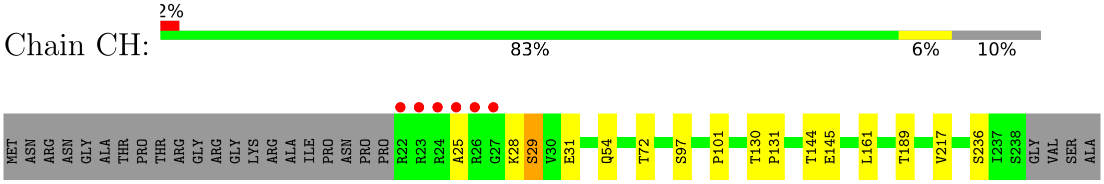
- Molecule 1: Capsid protein



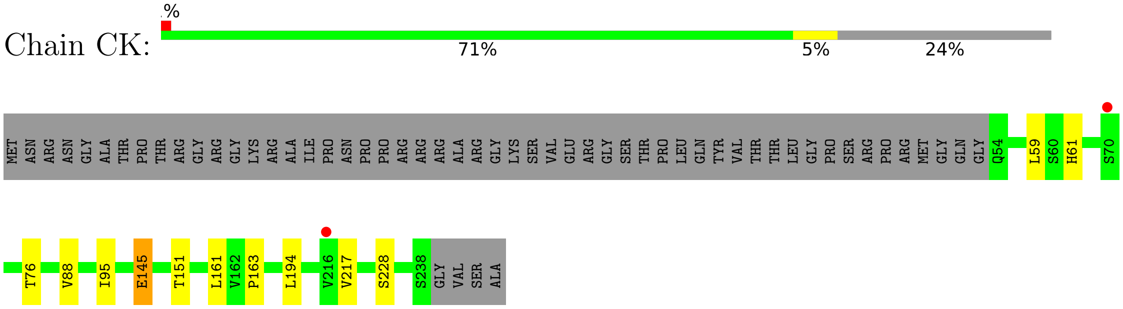
- Molecule 1: Capsid protein



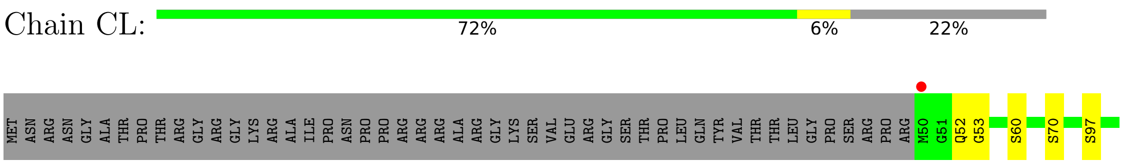
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

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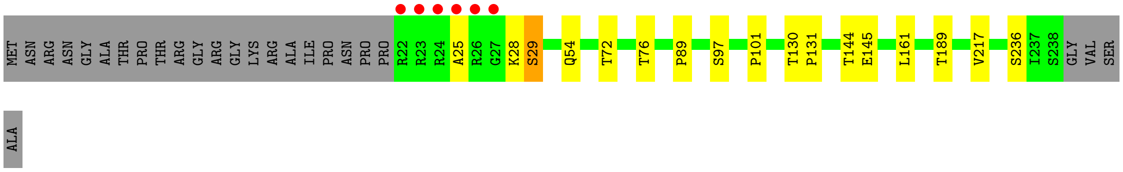
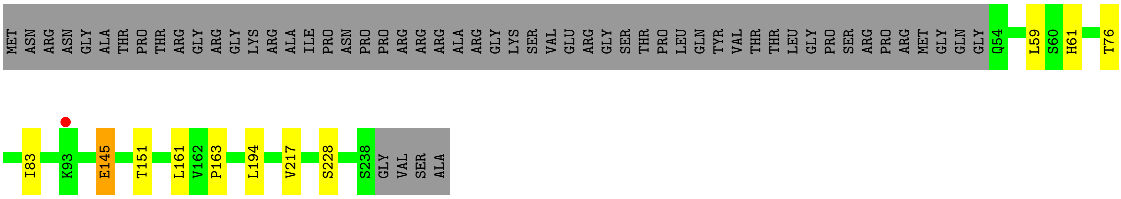


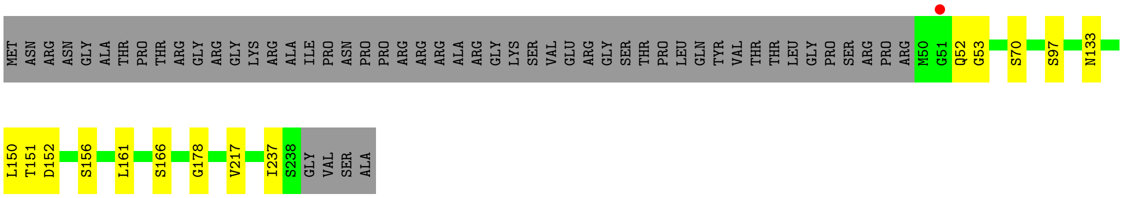
- Molecule 1: Capsid protein

Chain CP:



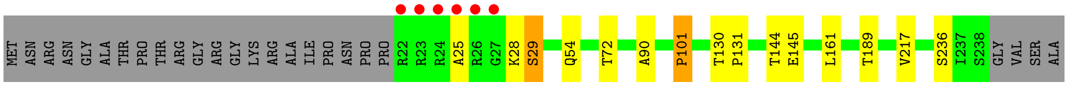
- Molecule 1: Capsid protein

Chain CQ:



- Molecule 1: Capsid protein

Chain CR:

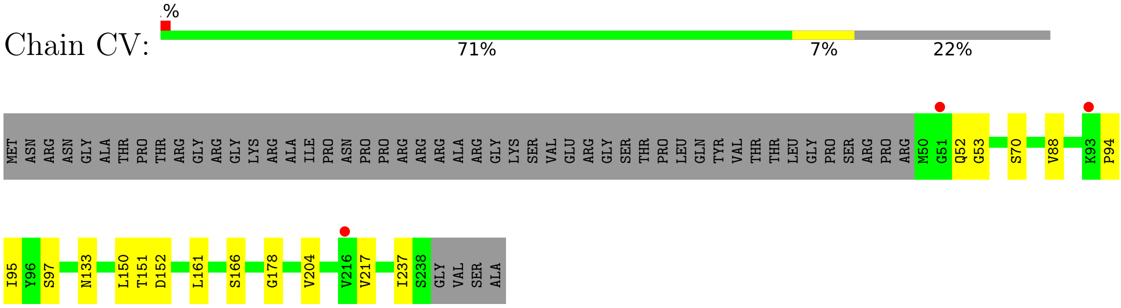


- Molecule 1: Capsid protein

Chain CU:

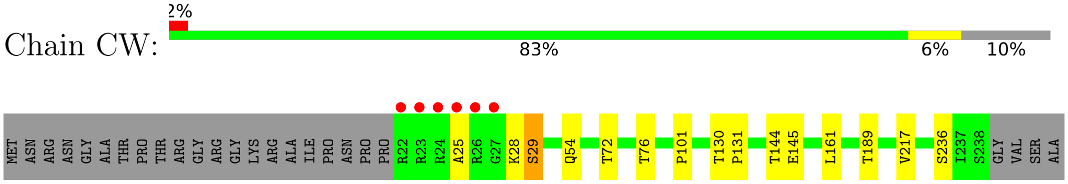
- Molecule 1: Capsid protein

Chain CV:



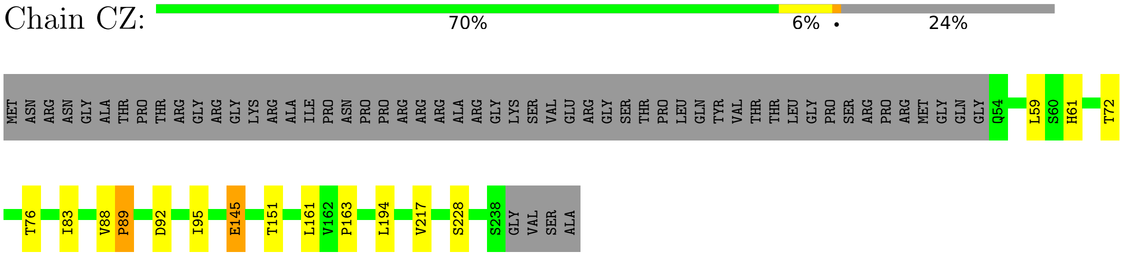
- Molecule 1: Capsid protein

Chain CW:



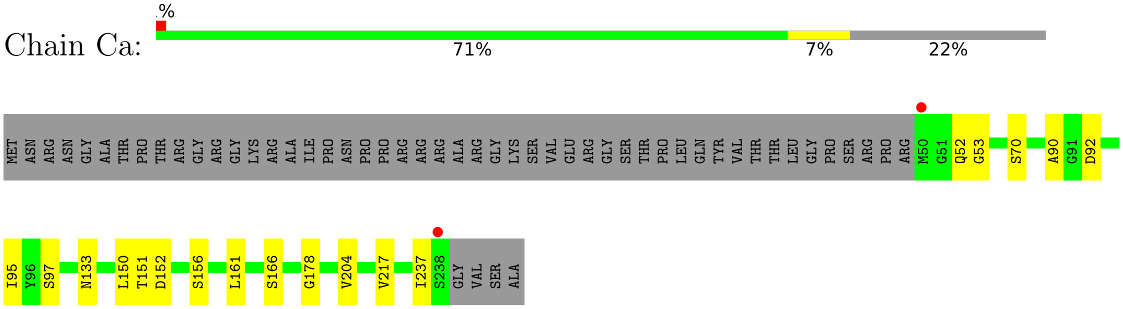
- Molecule 1: Capsid protein

Chain CZ:



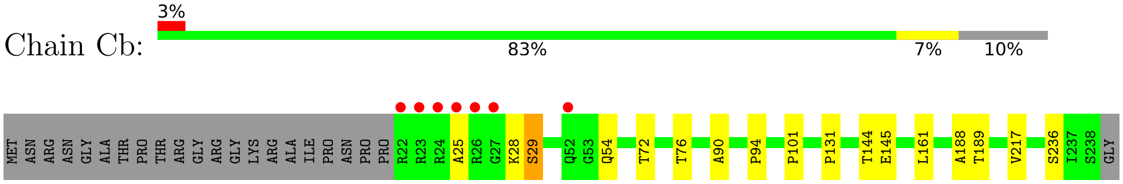
- Molecule 1: Capsid protein

Chain Ca:

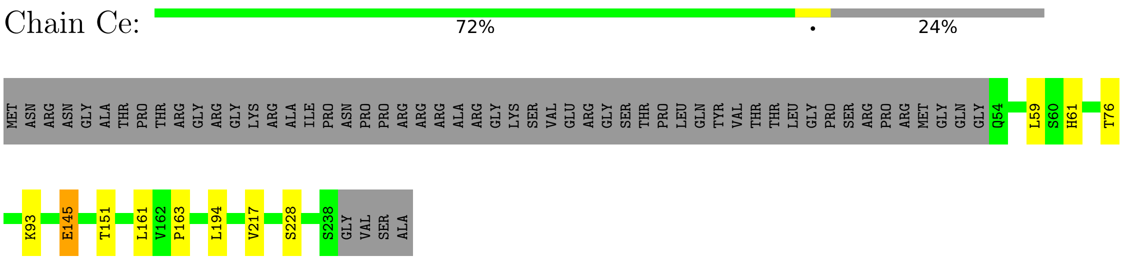


- Molecule 1: Capsid protein

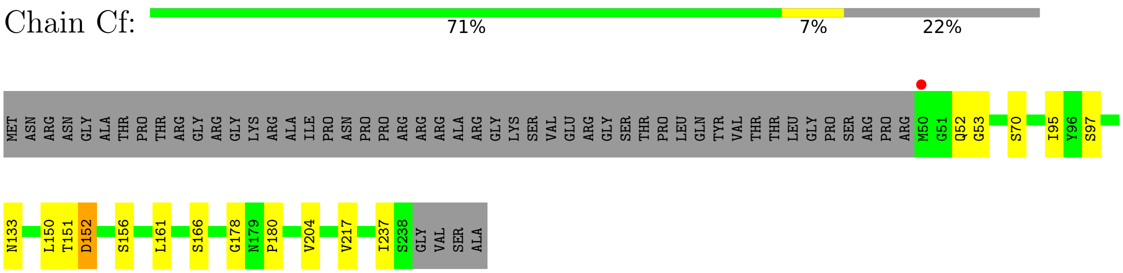
Chain Cb:



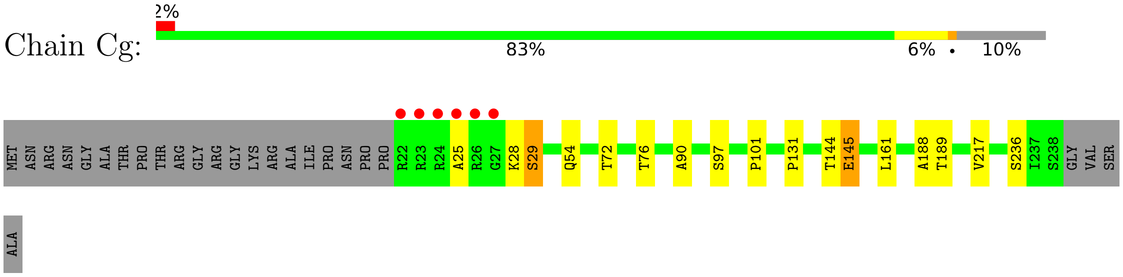
- Molecule 1: Capsid protein



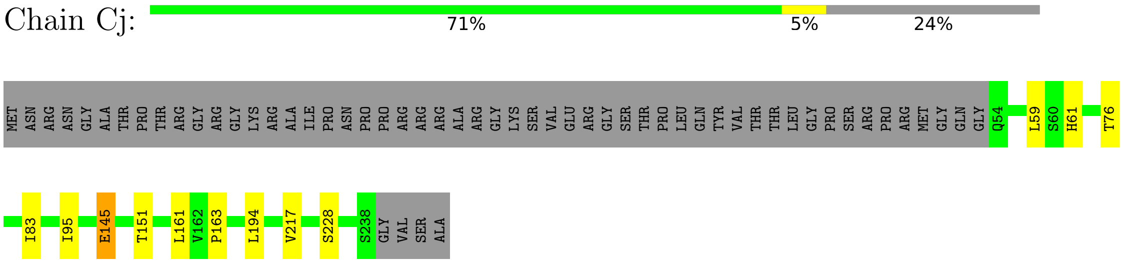
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



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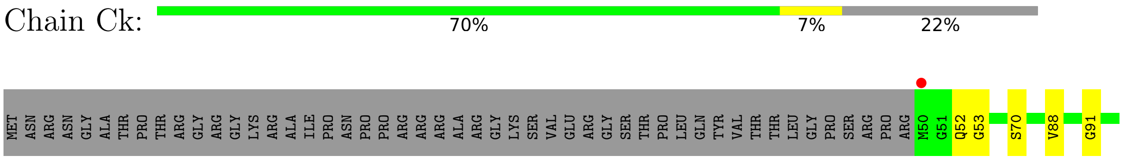
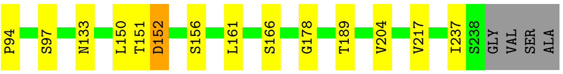
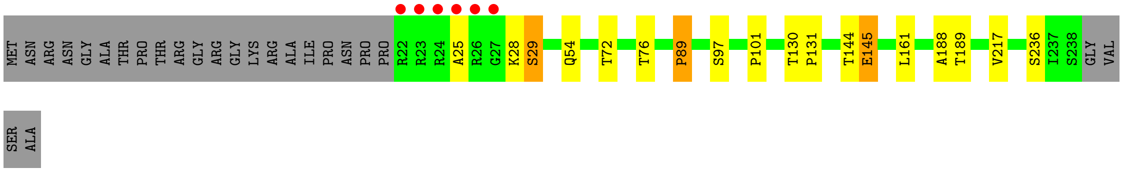




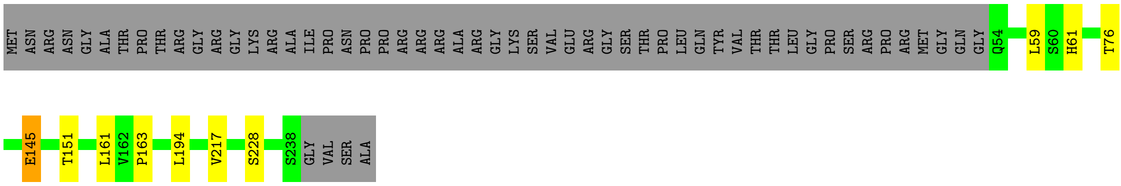
• Molecule 1: Capsid protein

Chain Cl:



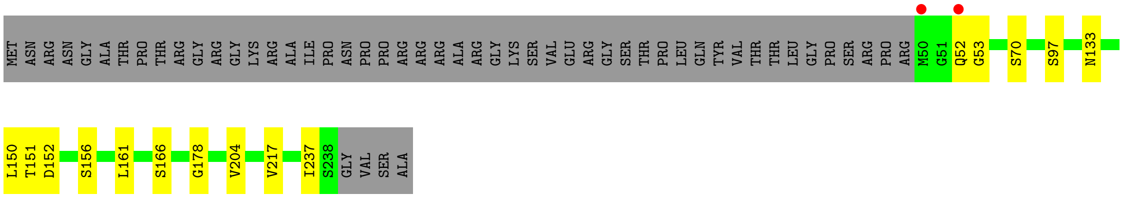
• Molecule 1: Capsid protein

Chain Co:



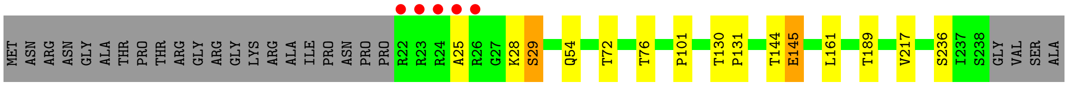
• Molecule 1: Capsid protein

Chain Cp:



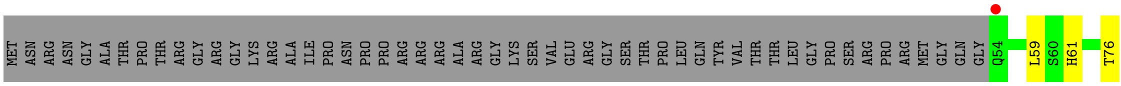
• Molecule 1: Capsid protein

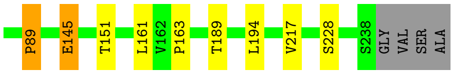
Chain Cq:



• Molecule 1: Capsid protein

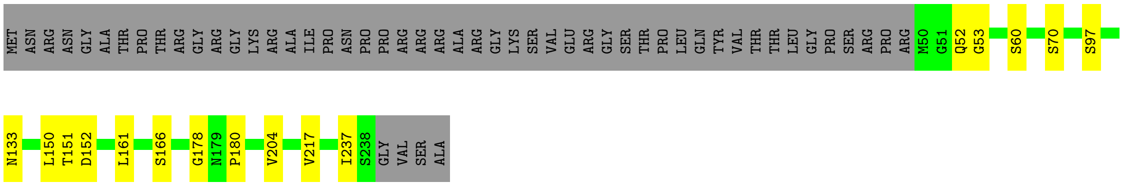
Chain Ct:





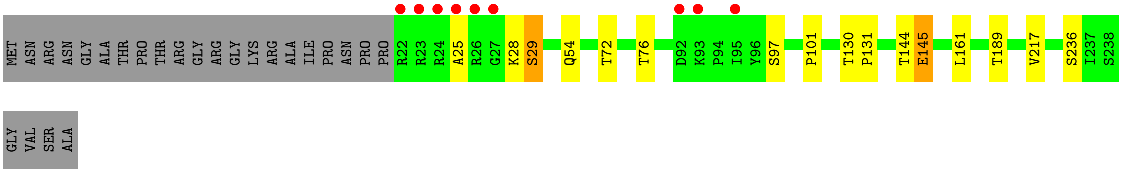
- Molecule 1: Capsid protein

Chain Cu:



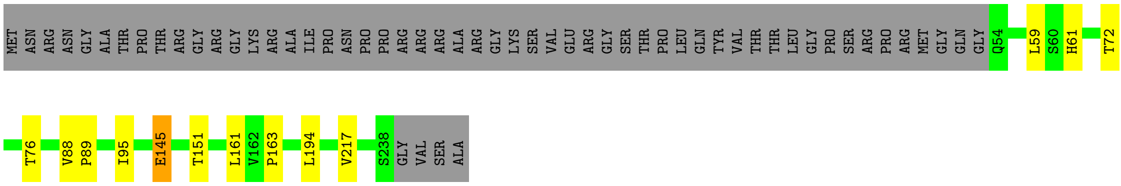
- Molecule 1: Capsid protein

Chain Cv:



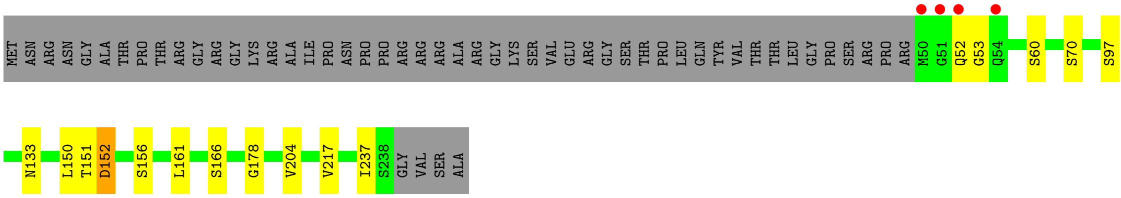
- Molecule 1: Capsid protein

Chain Cy:



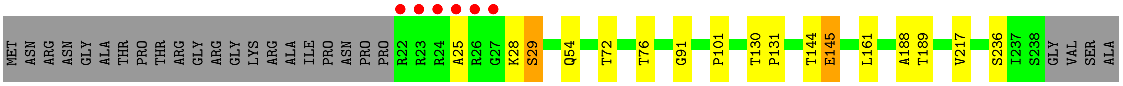
- Molecule 1: Capsid protein

Chain Cz:



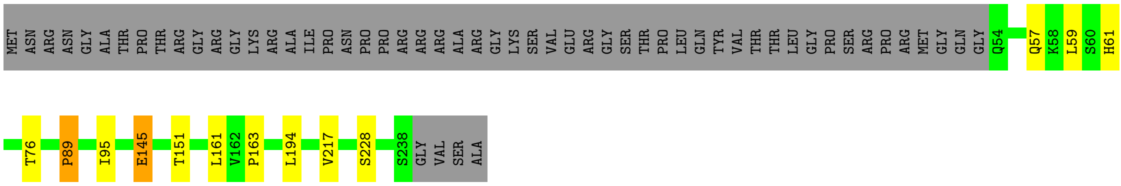
- Molecule 1: Capsid protein

Chain C1:



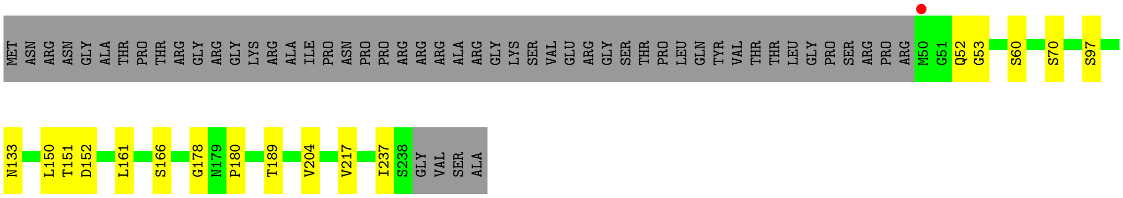
- Molecule 1: Capsid protein

Chain C4:



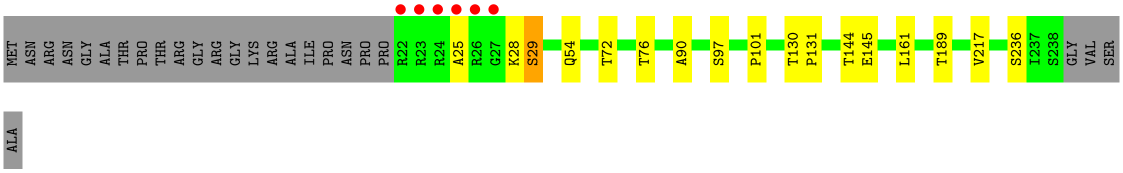
- Molecule 1: Capsid protein

Chain C5:



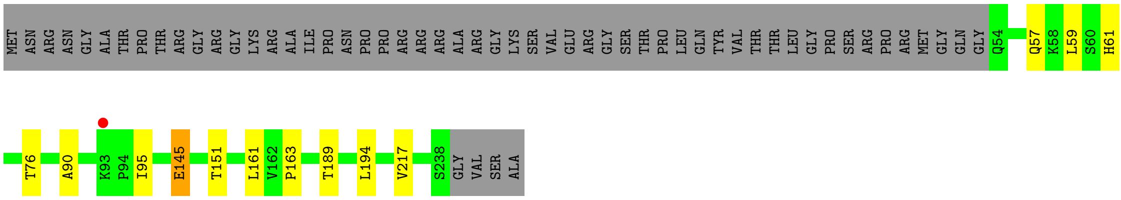
- Molecule 1: Capsid protein

Chain C6:



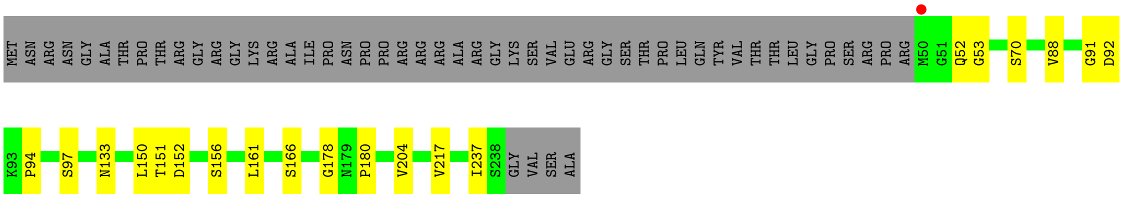
- Molecule 1: Capsid protein

Chain DA:



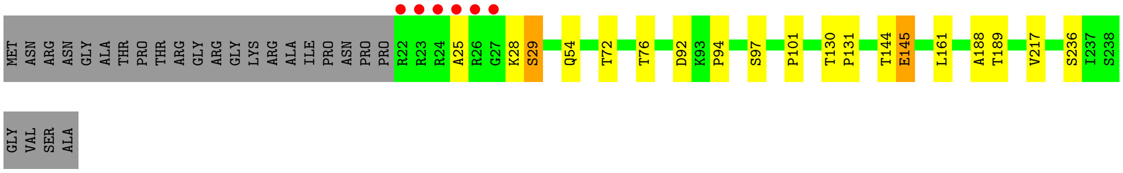
- Molecule 1: Capsid protein

Chain DB:



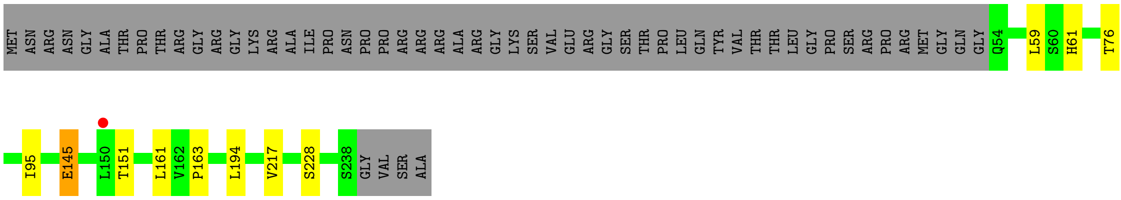
- Molecule 1: Capsid protein

Chain DC:

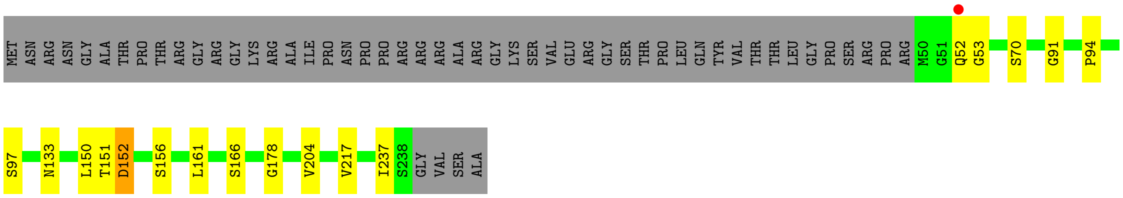
- Molecule 1: Capsid protein

Chain DF:

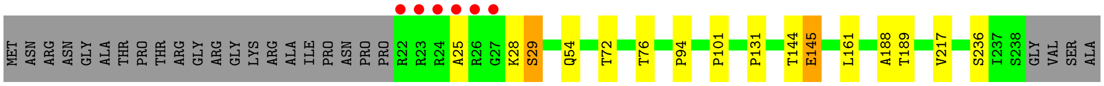
- Molecule 1: Capsid protein

Chain DG:

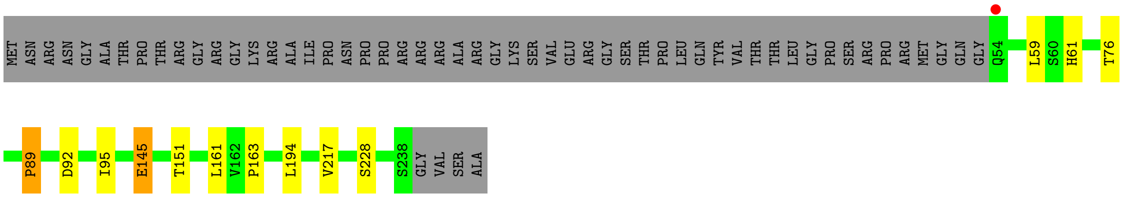
- Molecule 1: Capsid protein

Chain DH:

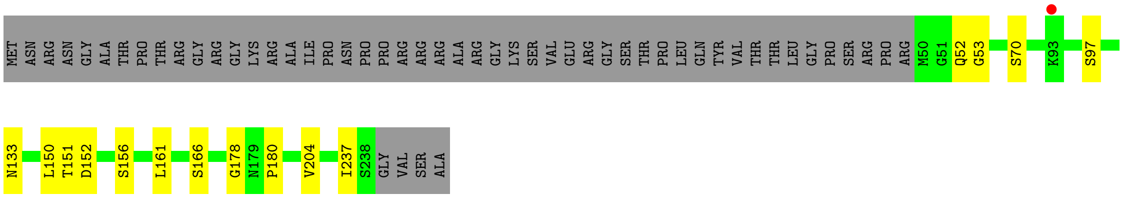
- Molecule 1: Capsid protein

Chain DK:

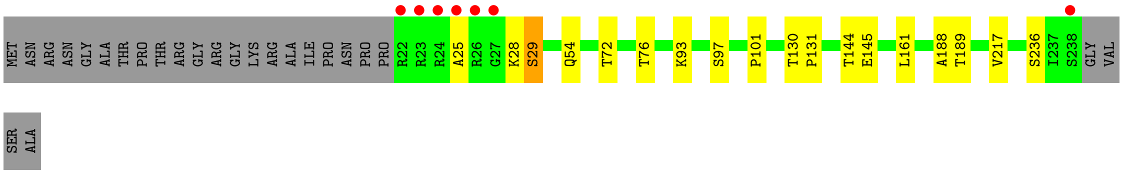
- Molecule 1: Capsid protein

Chain DL:



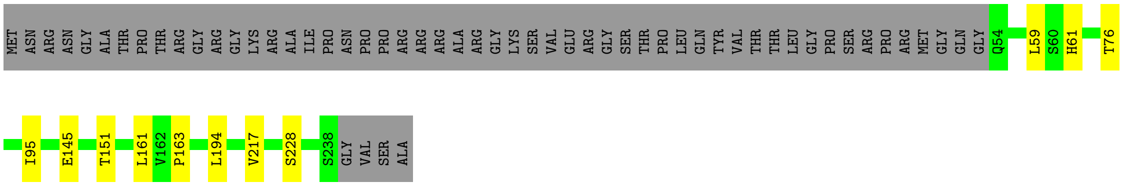
- Molecule 1: Capsid protein

Chain DM:



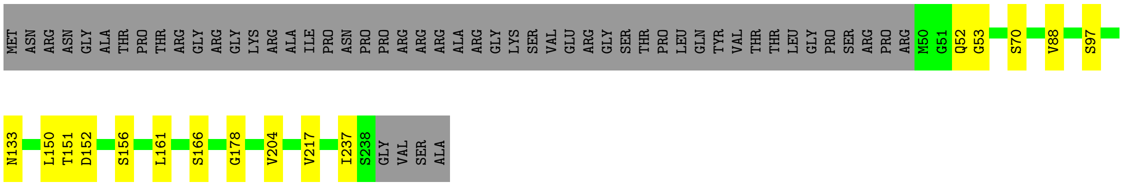
- Molecule 1: Capsid protein

Chain DP:



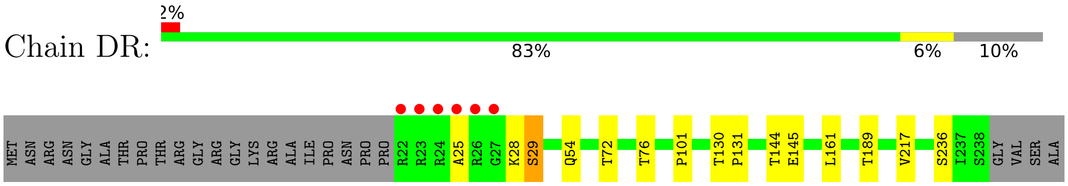
- Molecule 1: Capsid protein

Chain DQ:



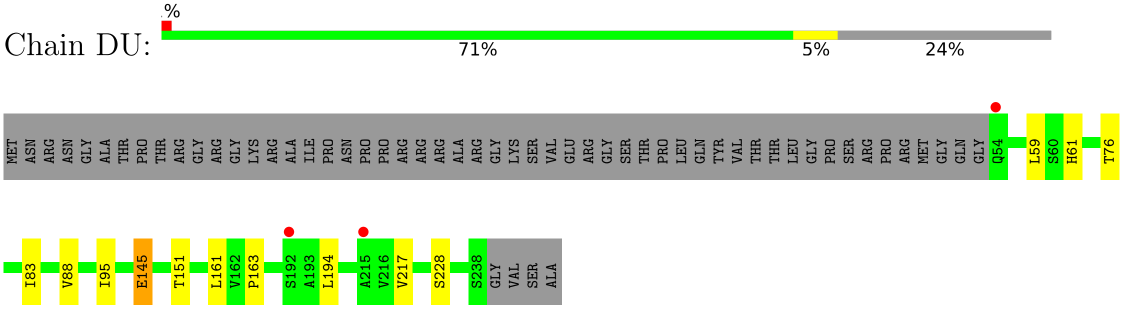
- Molecule 1: Capsid protein

Chain DR:



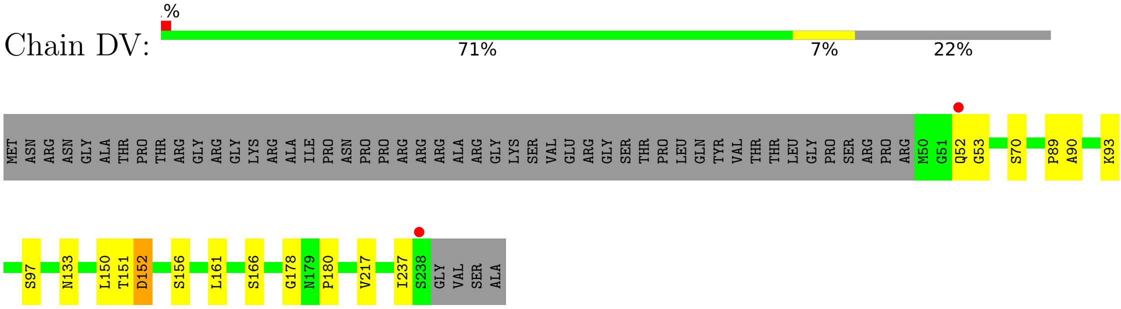
- Molecule 1: Capsid protein

Chain DU:



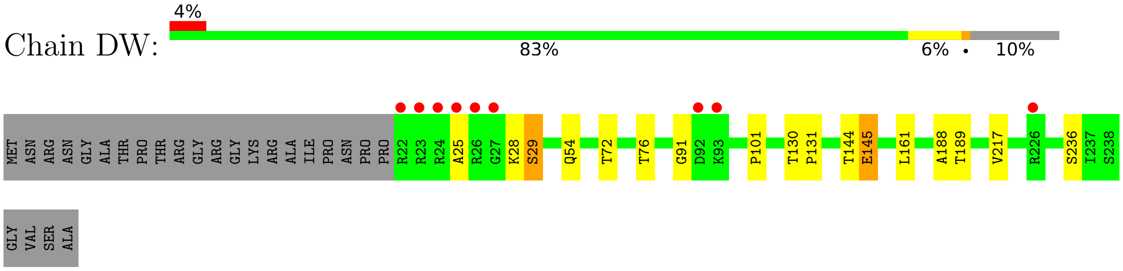
- Molecule 1: Capsid protein

Chain DV:



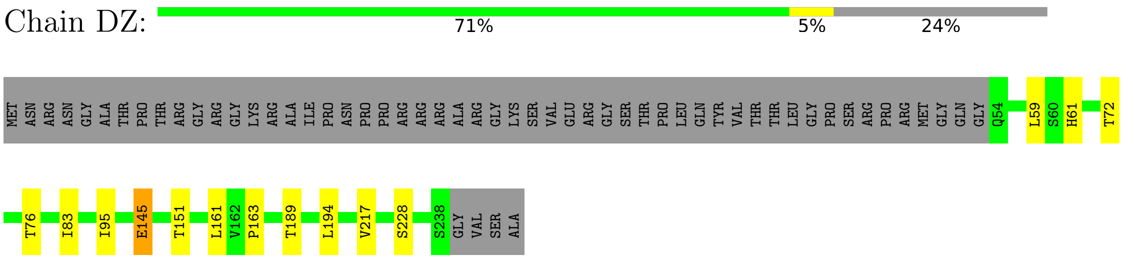
- Molecule 1: Capsid protein

Chain DW:



- Molecule 1: Capsid protein

Chain DZ:



- Molecule 1: Capsid protein

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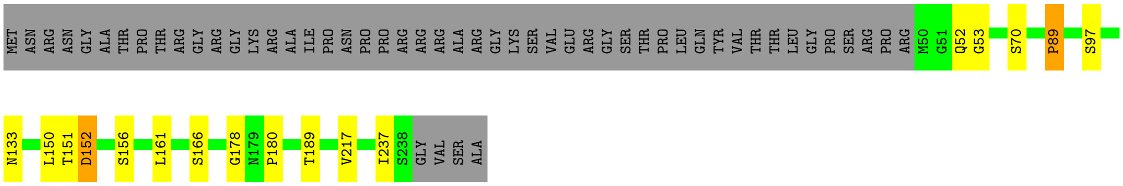
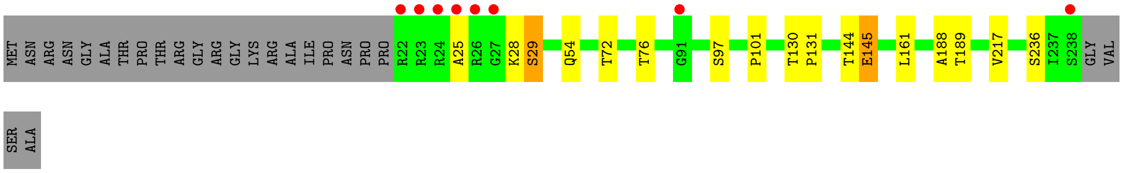


- Molecule 1: Capsid protein

Chain Db:



- Molecule 1: Capsid protein

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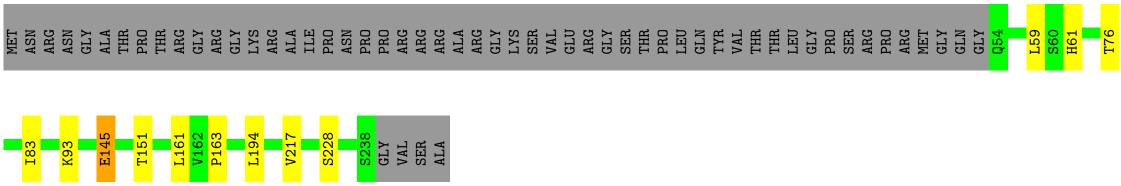
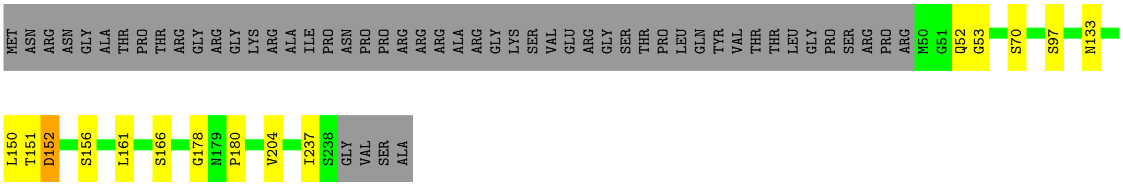


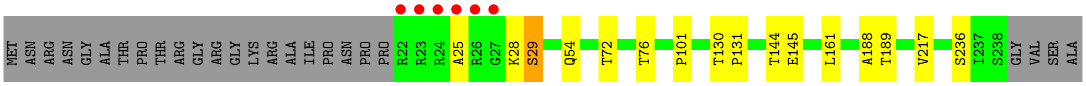
- Molecule 1: Capsid protein

Chain Df:



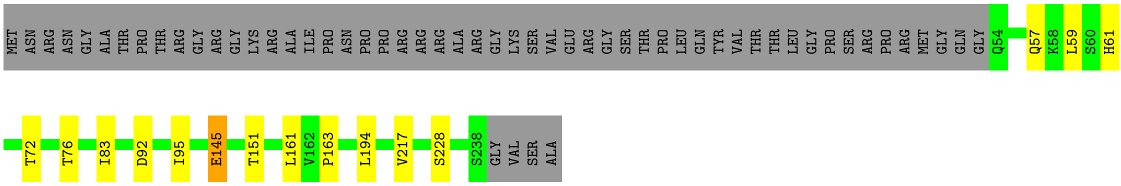
- Molecule 1: Capsid protein

Chain Dg:



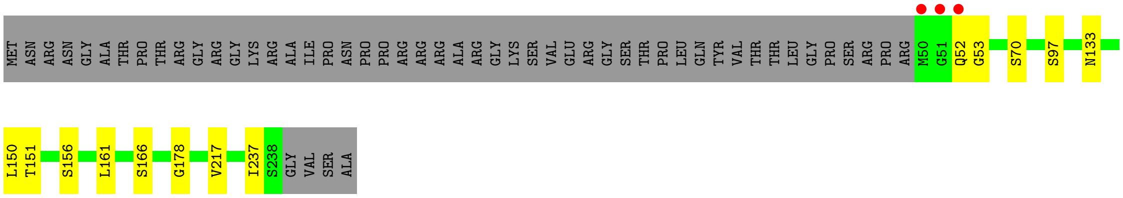
- Molecule 1: Capsid protein

Chain Dj:



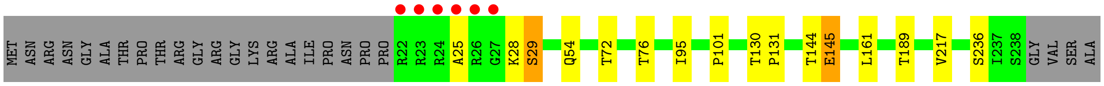
- Molecule 1: Capsid protein

Chain Dk:



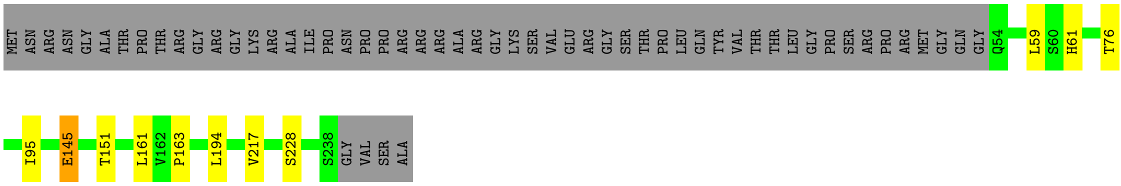
- Molecule 1: Capsid protein

Chain Dl:



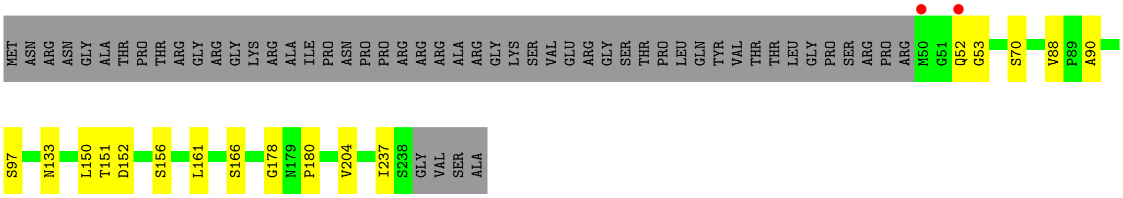
- Molecule 1: Capsid protein

Chain Do:



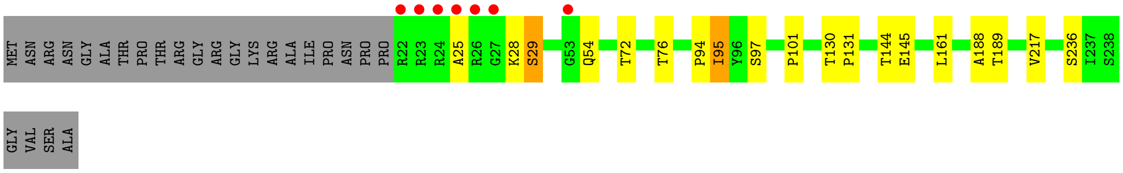
- Molecule 1: Capsid protein

Chain Dp:



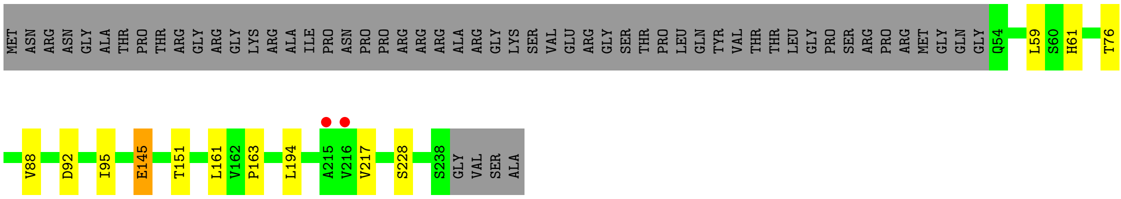
- Molecule 1: Capsid protein

Chain Dq:



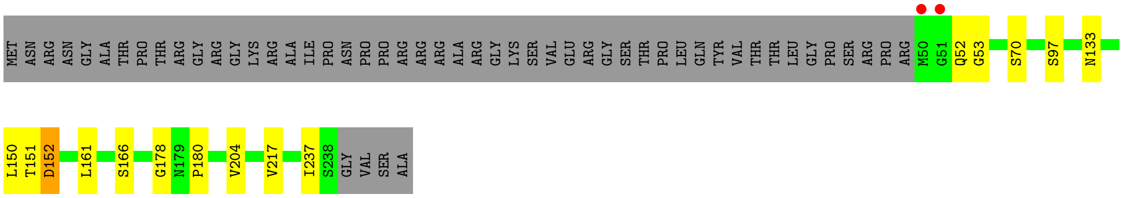
- Molecule 1: Capsid protein

Chain Dt:



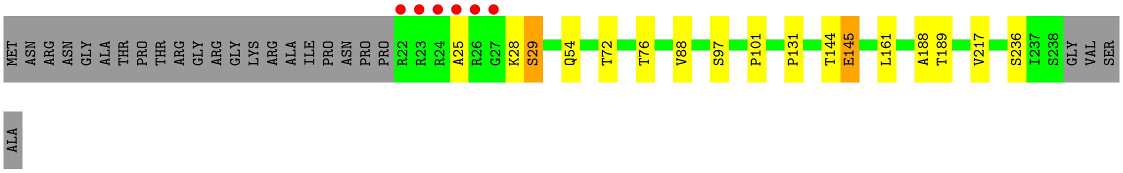
- Molecule 1: Capsid protein

Chain Du:



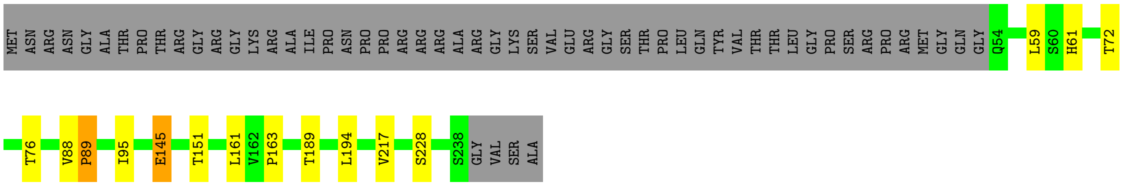
- Molecule 1: Capsid protein

Chain Dv:



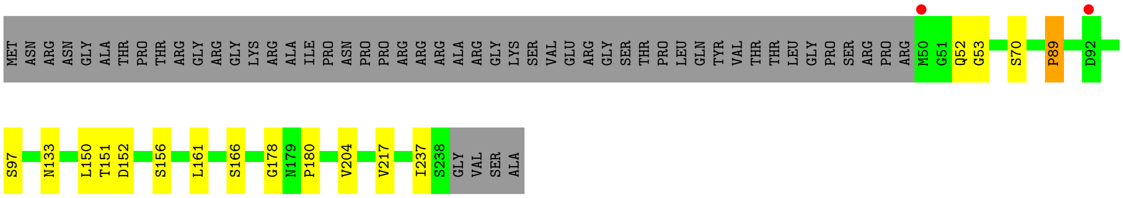
- Molecule 1: Capsid protein

Chain Dy:



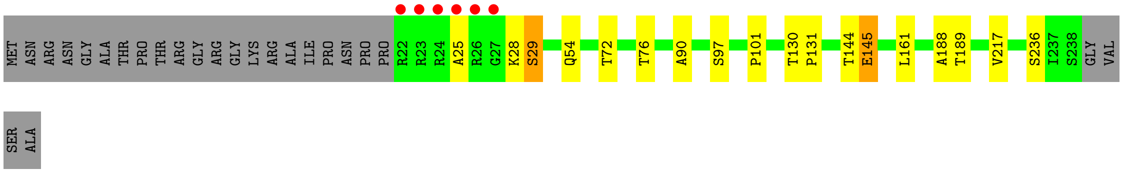
- Molecule 1: Capsid protein

Chain Dz:



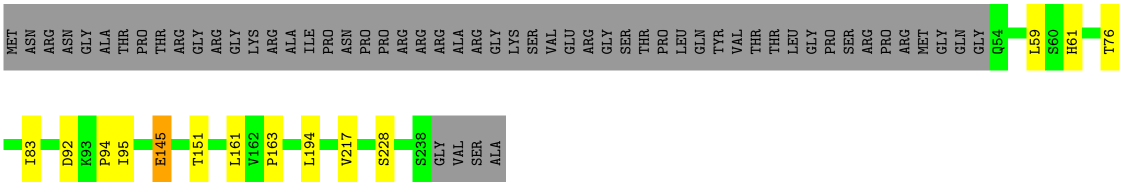
- Molecule 1: Capsid protein

Chain D1:



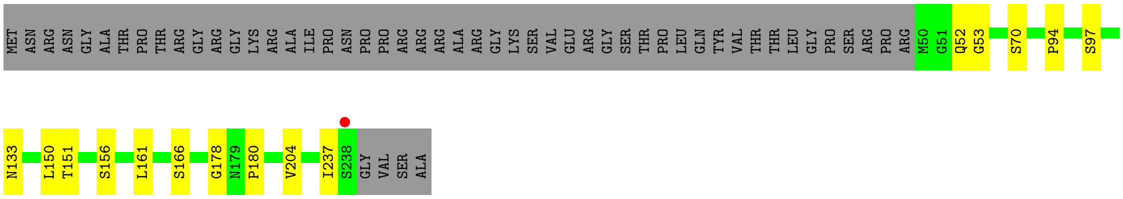
- Molecule 1: Capsid protein

Chain D4:



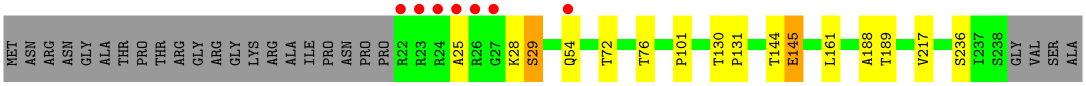
- Molecule 1: Capsid protein

Chain D5:



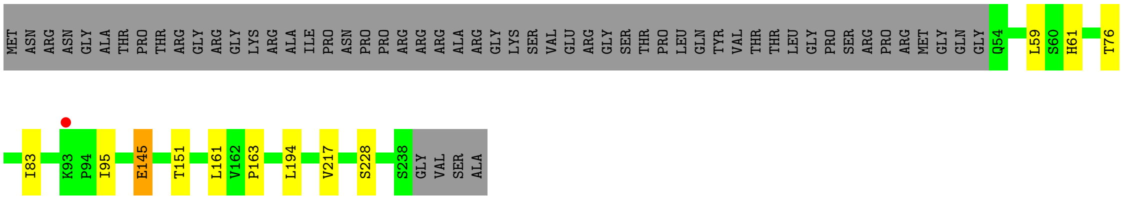
- Molecule 1: Capsid protein

Chain D6:



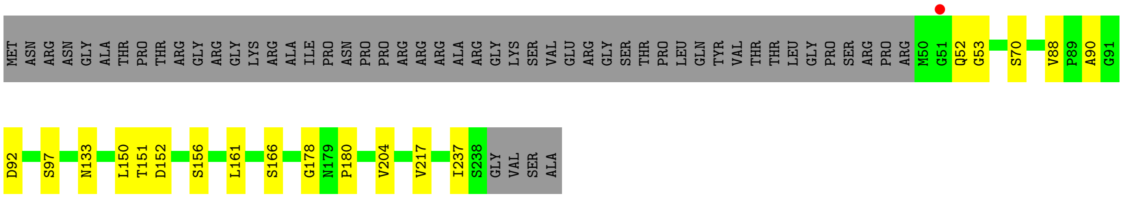
- Molecule 1: Capsid protein

Chain EA:



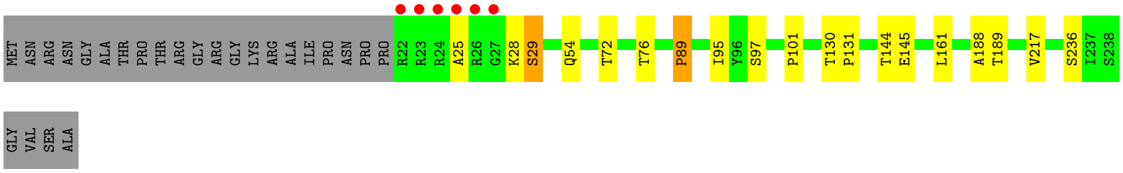
- Molecule 1: Capsid protein

Chain EB:



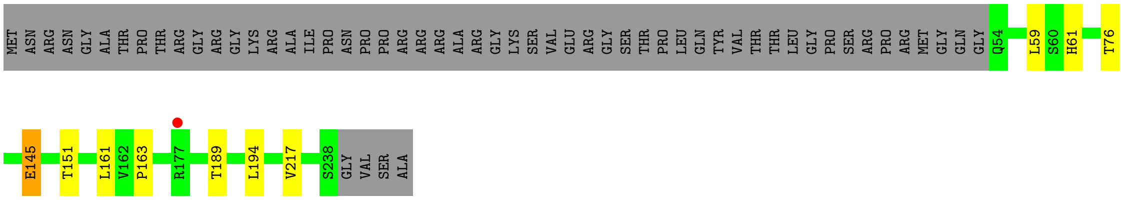
- Molecule 1: Capsid protein

Chain EC:



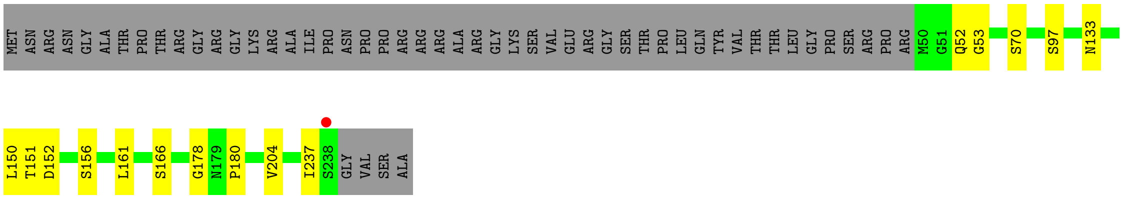
- Molecule 1: Capsid protein

Chain EF:

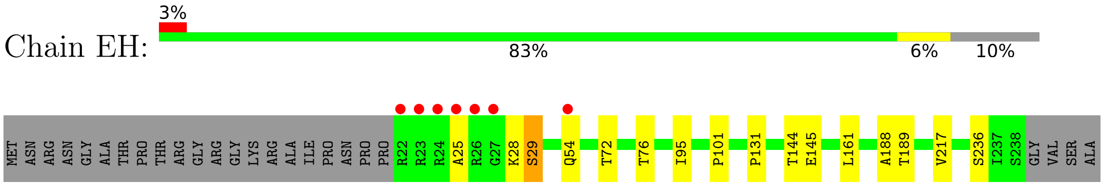


- Molecule 1: Capsid protein

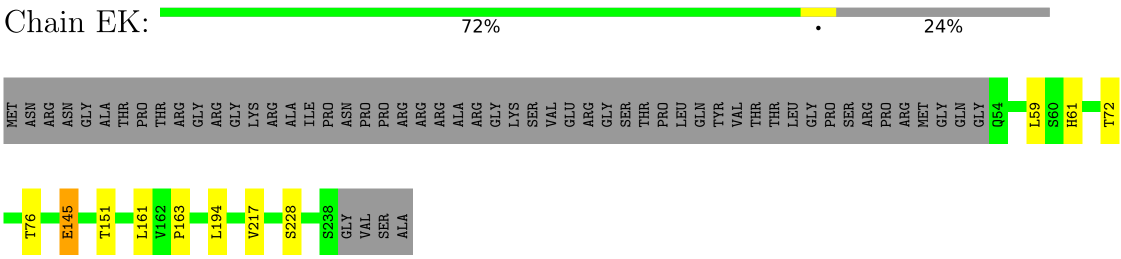
Chain EG:



- Molecule 1: Capsid protein



• Molecule 1: Capsid protein



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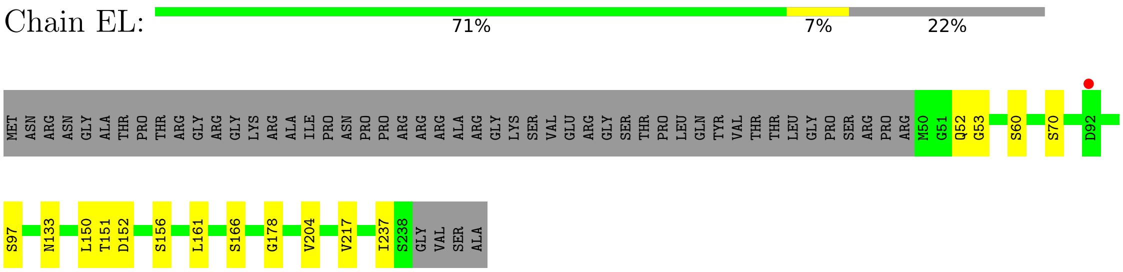

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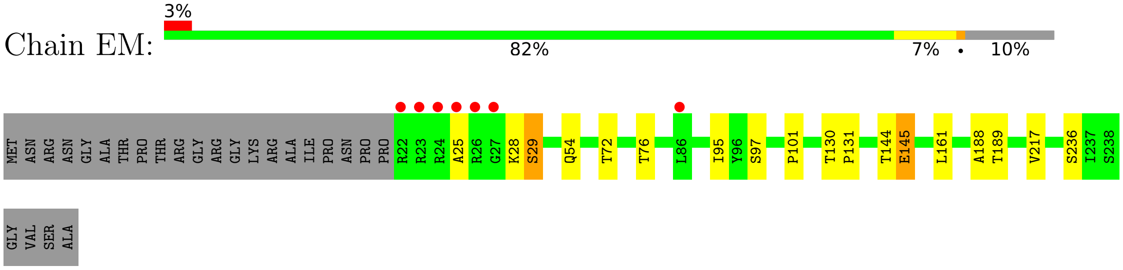

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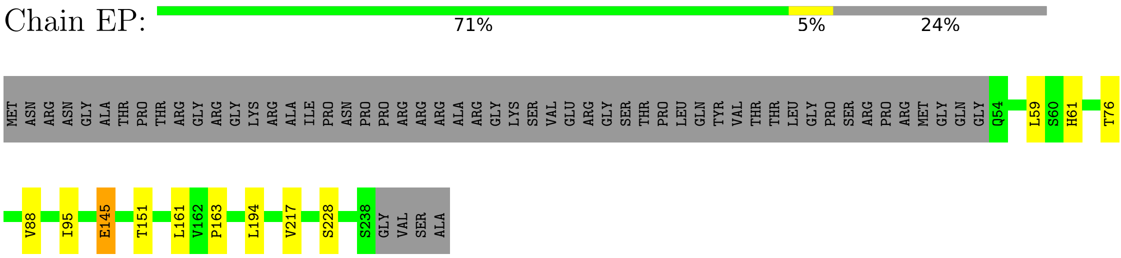

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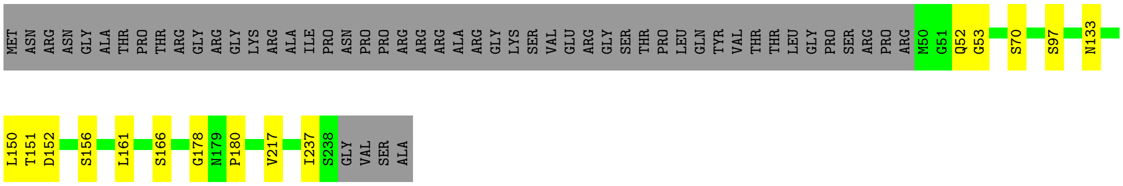

- Molecule 1: Capsid protein

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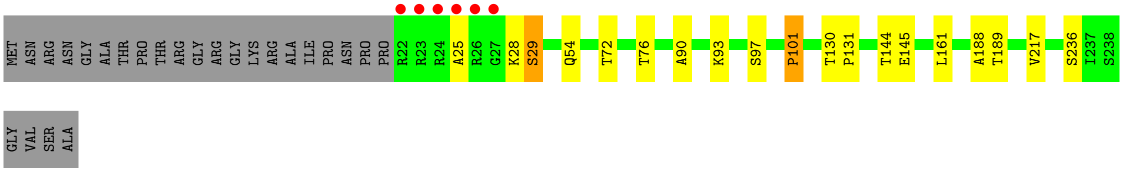
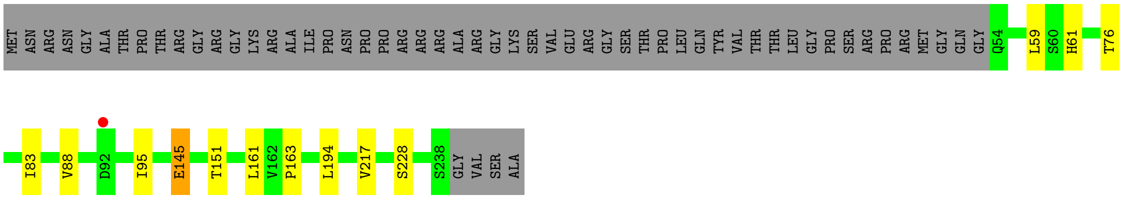


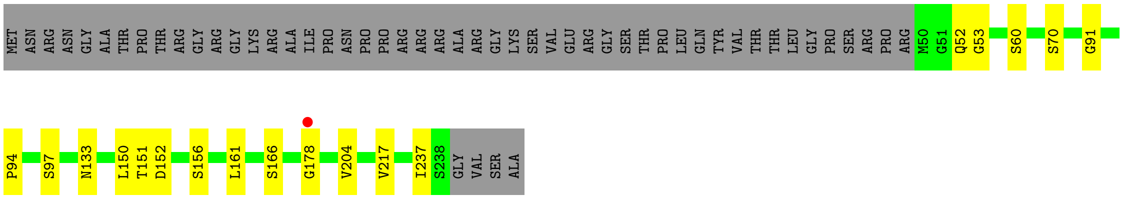
- Molecule 1: Capsid protein

Chain EU:



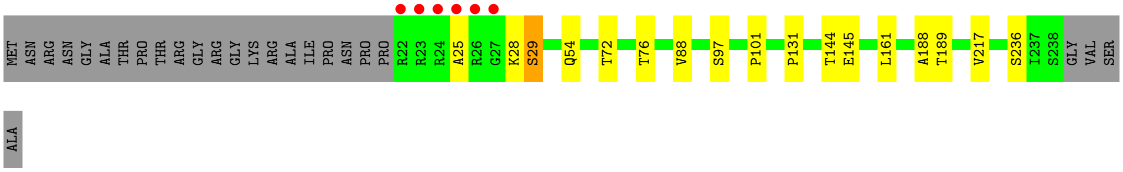
- Molecule 1: Capsid protein

Chain EV:



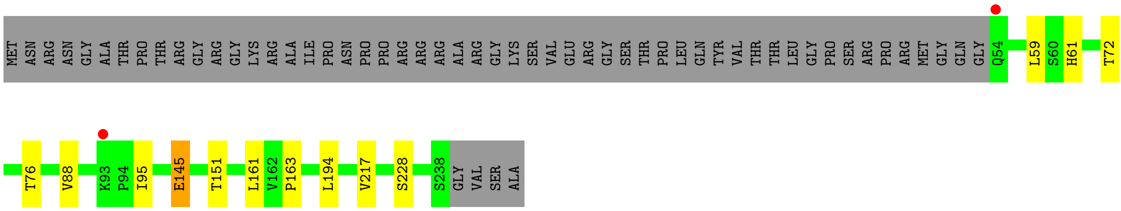
- Molecule 1: Capsid protein

Chain EW:



- Molecule 1: Capsid protein

Chain EZ:



- Molecule 1: Capsid protein

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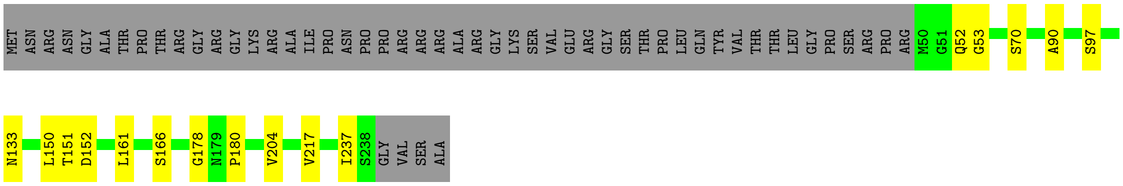

- Molecule 1: Capsid protein

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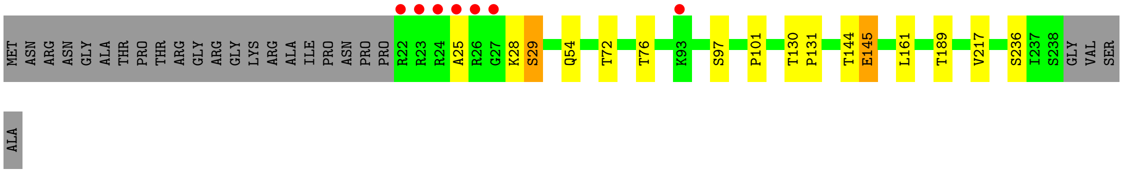
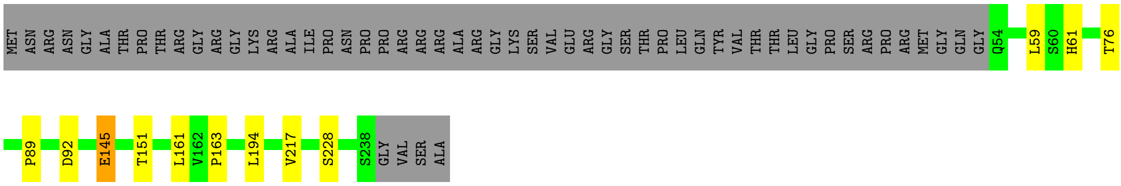


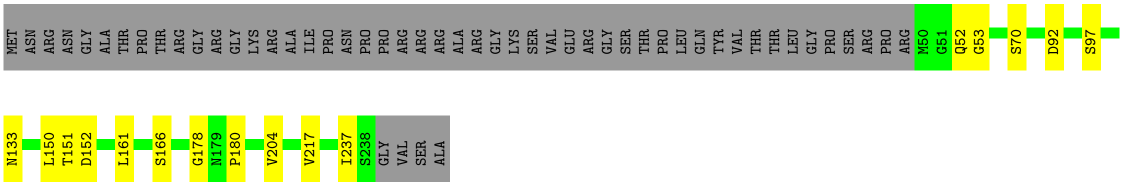
- Molecule 1: Capsid protein

Chain Ee:



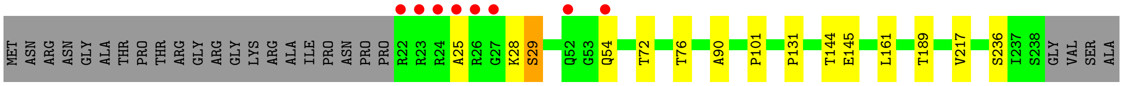
- Molecule 1: Capsid protein

Chain Ef:



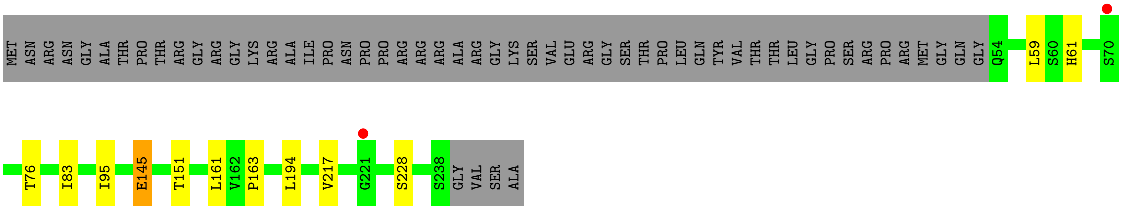
- Molecule 1: Capsid protein

Chain Eg:



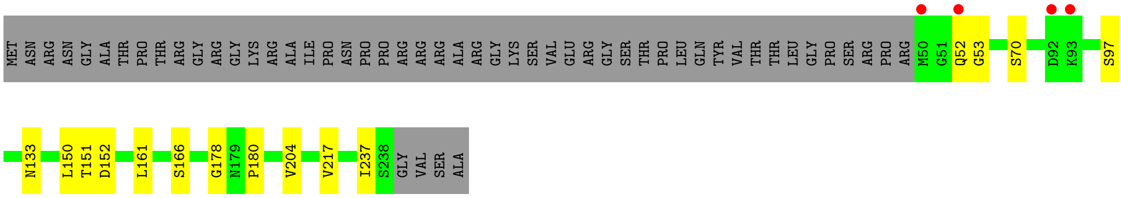
• Molecule 1: Capsid protein

Chain Ej:



• Molecule 1: Capsid protein

Chain Ek:



• Molecule 1: Capsid protein

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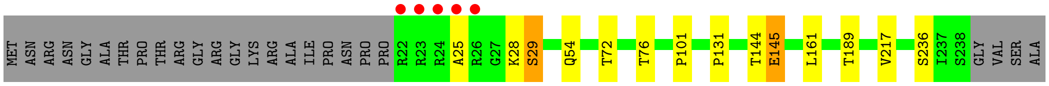

• Molecule 1: Capsid protein

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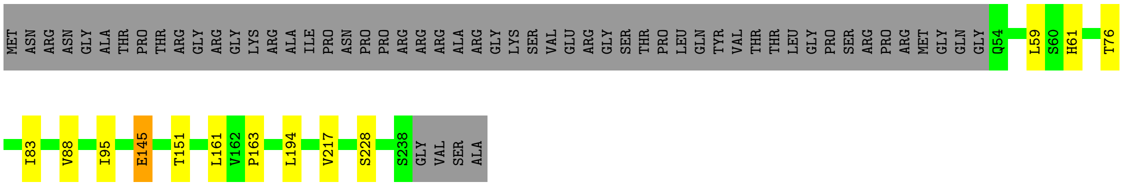

• Molecule 1: Capsid protein

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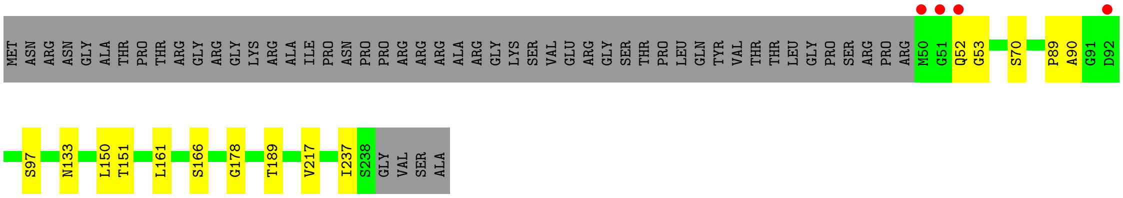

- Molecule 1: Capsid protein

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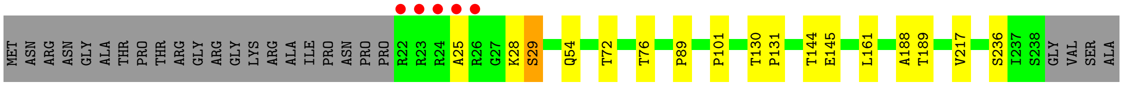

- Molecule 1: Capsid protein

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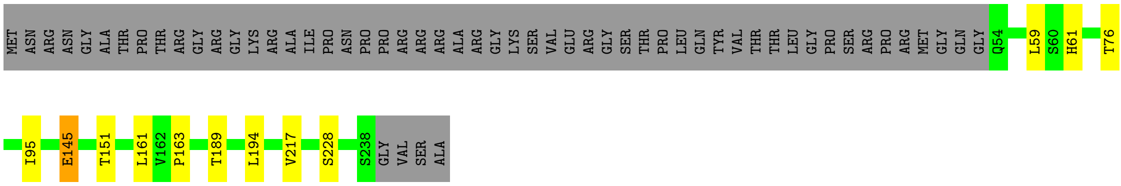

- Molecule 1: Capsid protein

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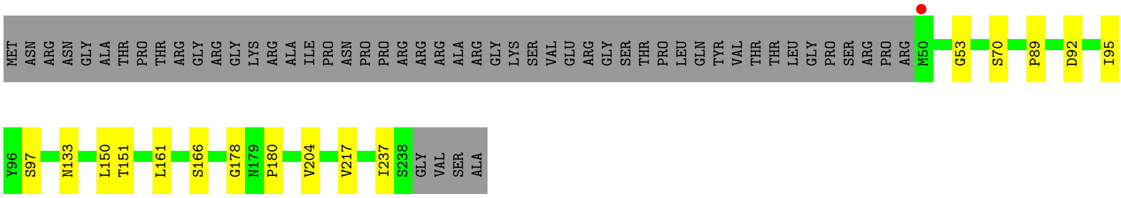

- Molecule 1: Capsid protein

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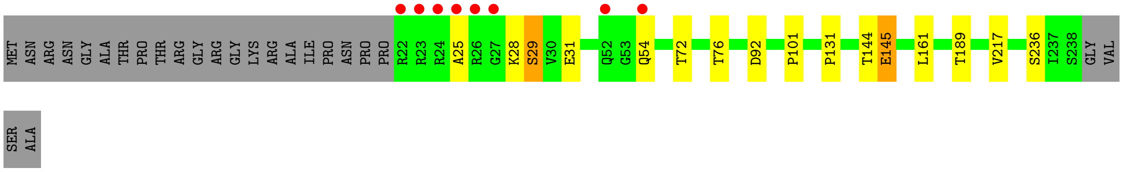
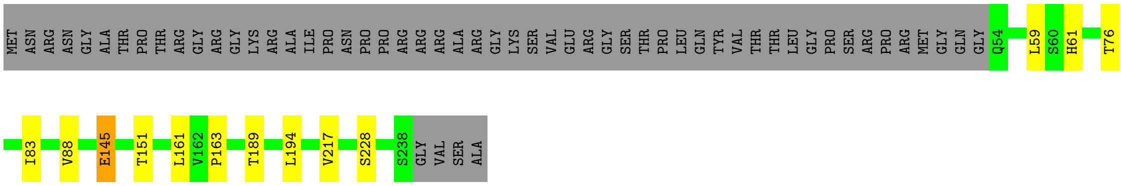


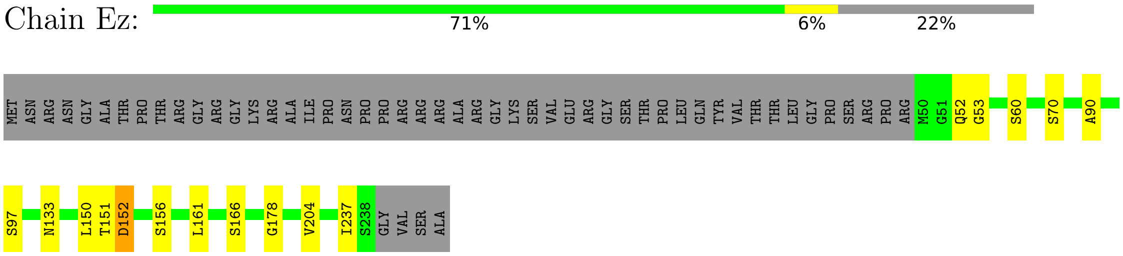
- Molecule 1: Capsid protein

Chain Ey:



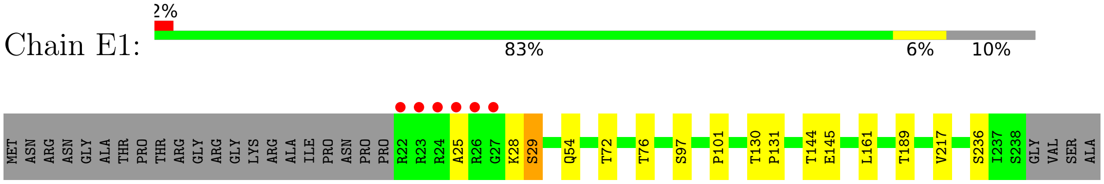
- Molecule 1: Capsid protein

Chain Ez:



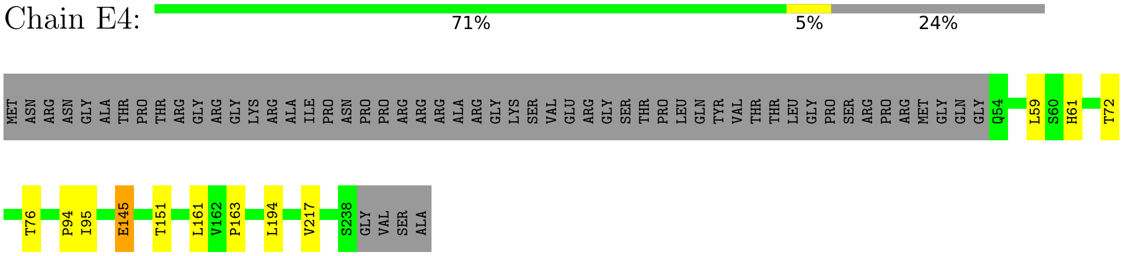
- Molecule 1: Capsid protein

Chain E1:



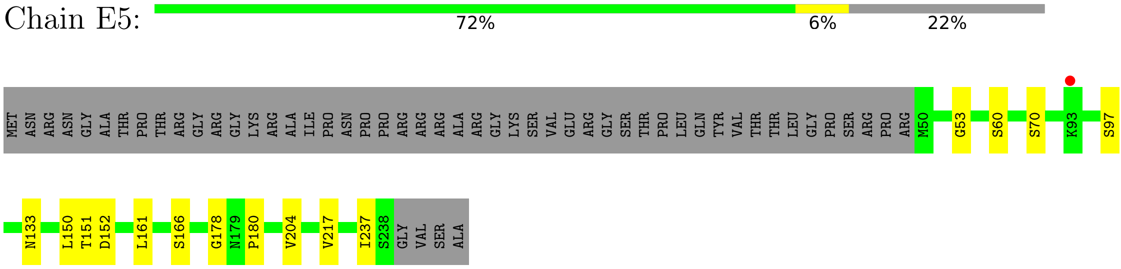
- Molecule 1: Capsid protein

Chain E4:



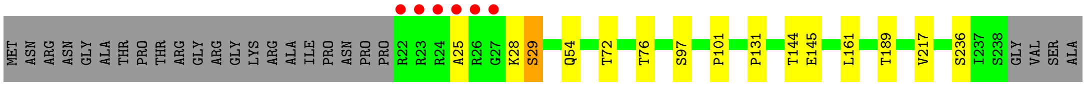
- Molecule 1: Capsid protein

Chain E5:

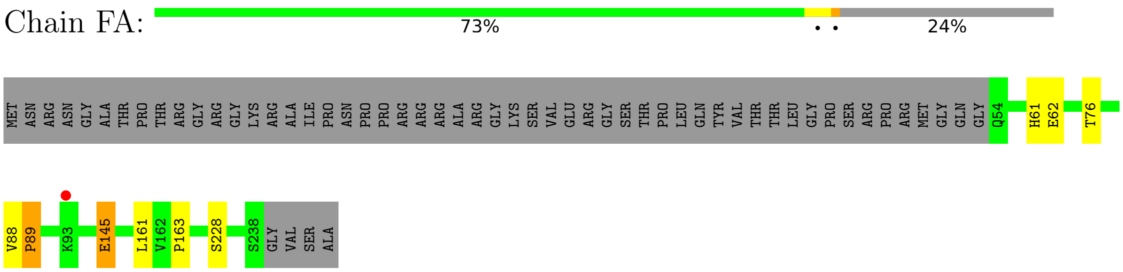


- Molecule 1: Capsid protein

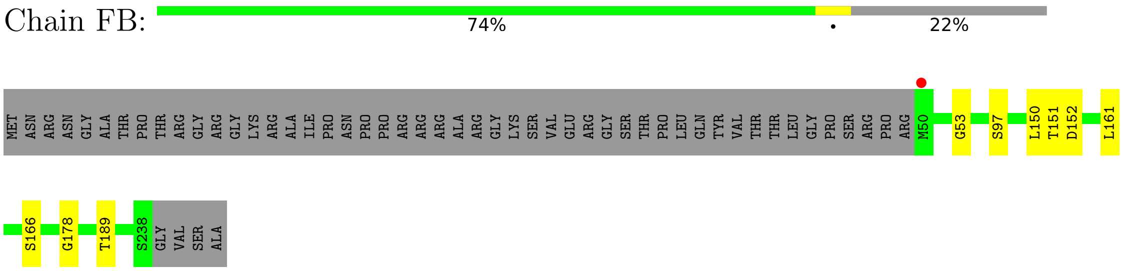
Chain E6:



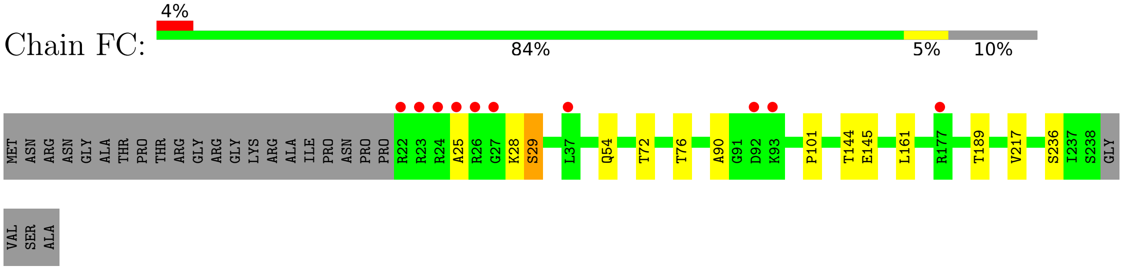
- Molecule 1: Capsid protein



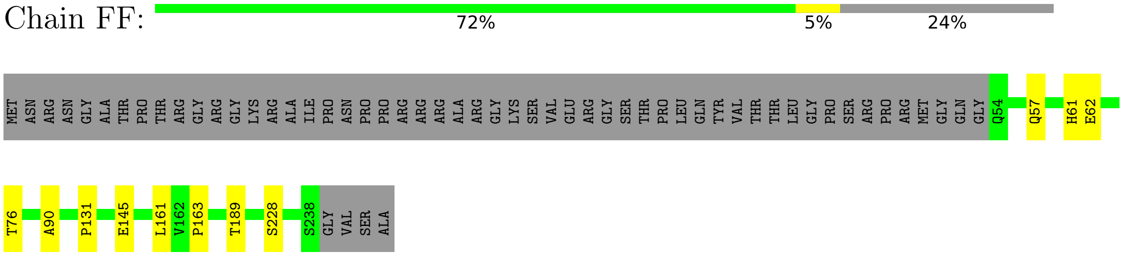
- Molecule 1: Capsid protein



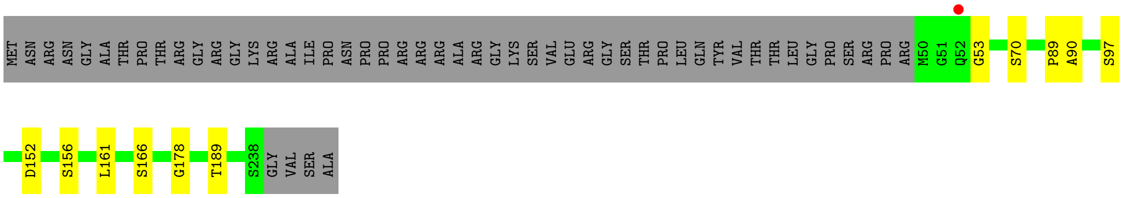
- Molecule 1: Capsid protein



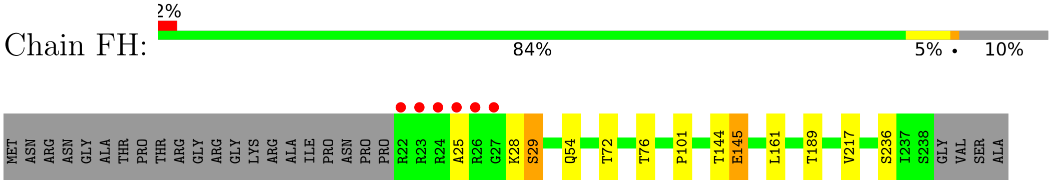
- Molecule 1: Capsid protein



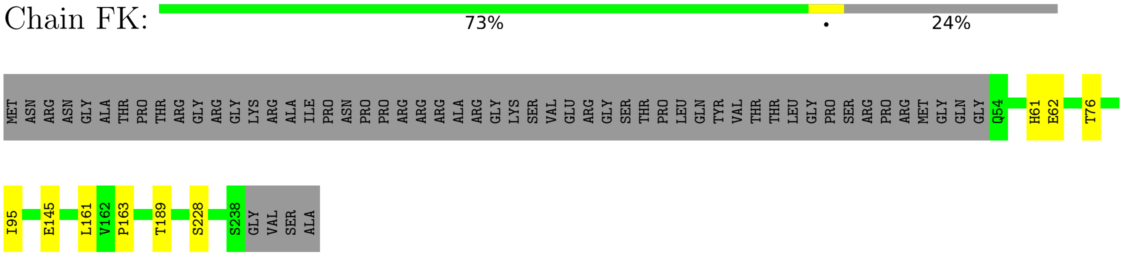
- Molecule 1: Capsid protein



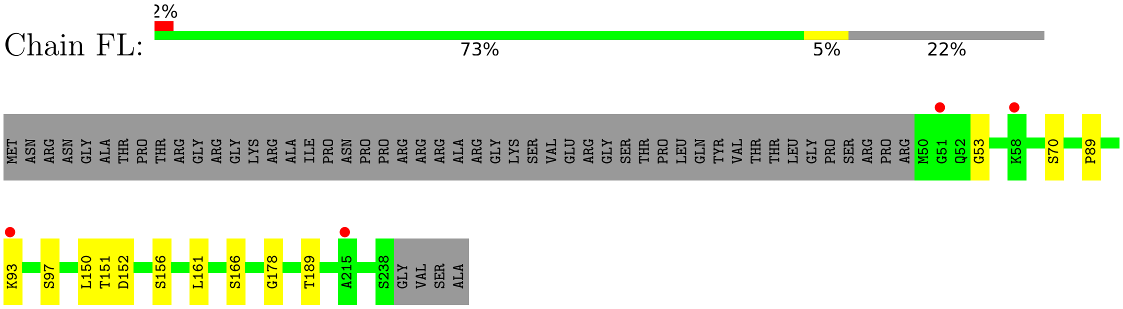
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



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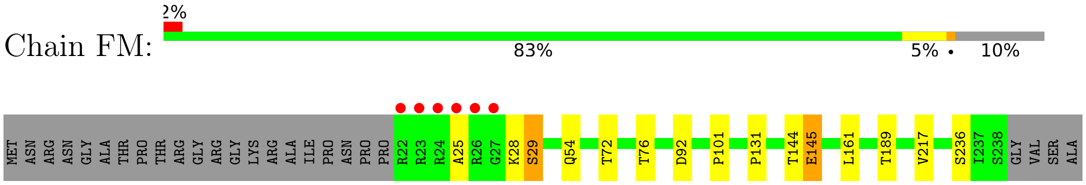

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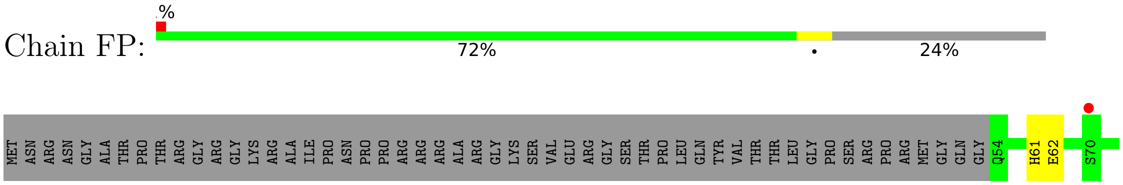
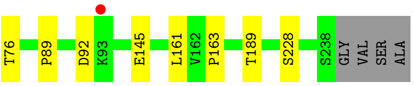
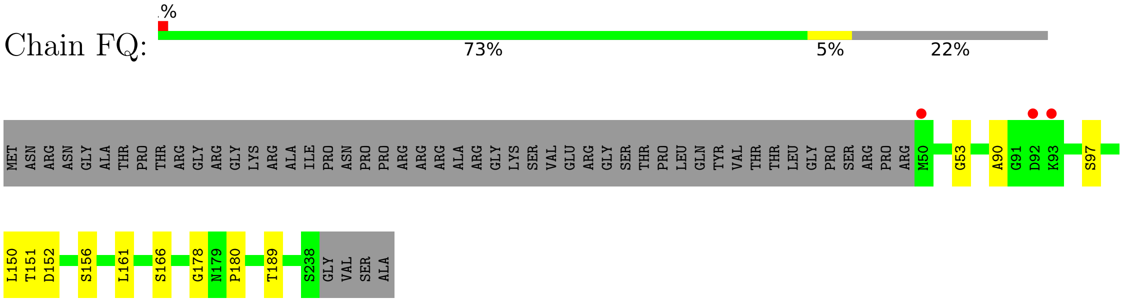




- Molecule 1: Capsid protein



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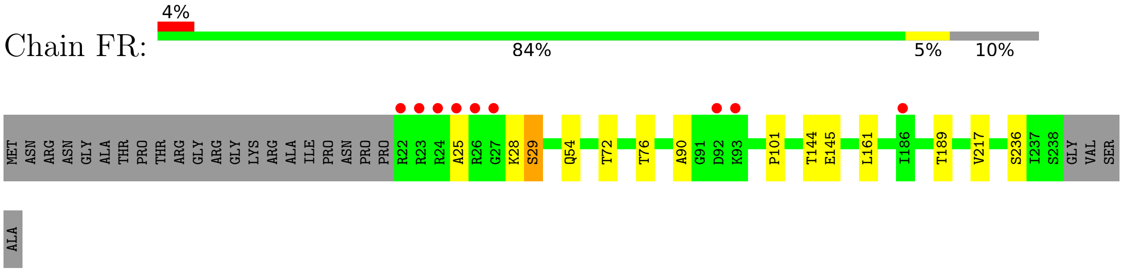

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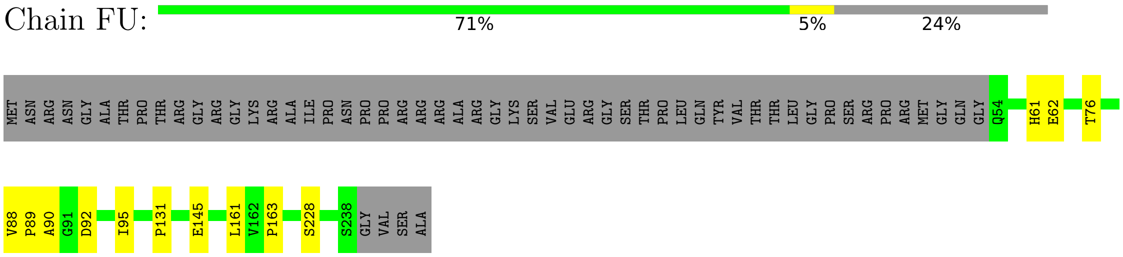
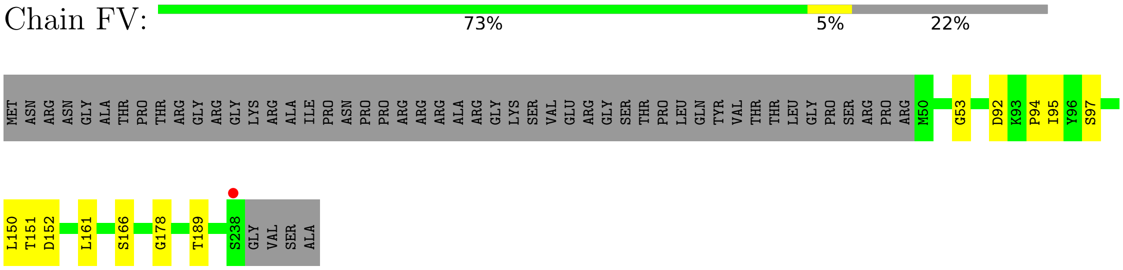
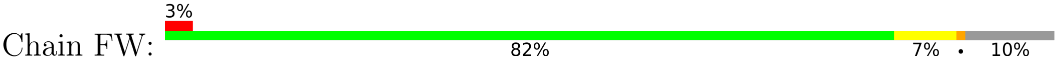
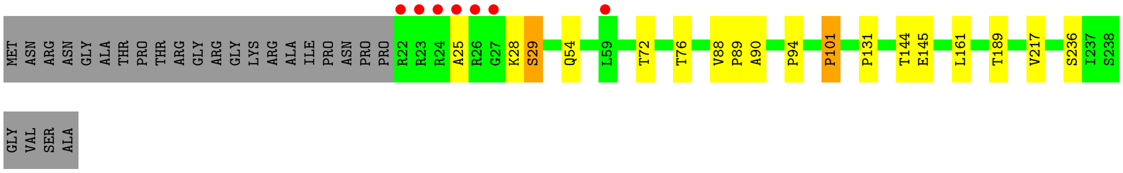


- Molecule 1: Capsid protein



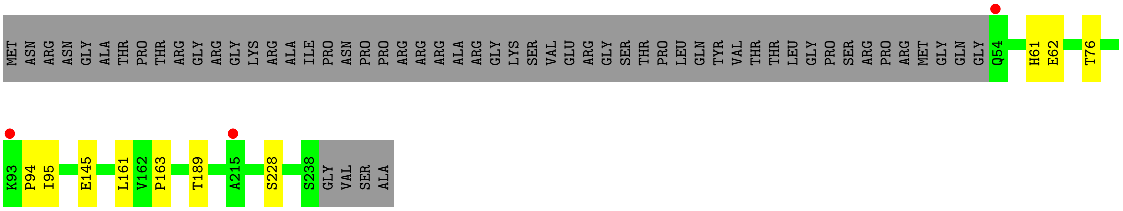
- Molecule 1: Capsid protein





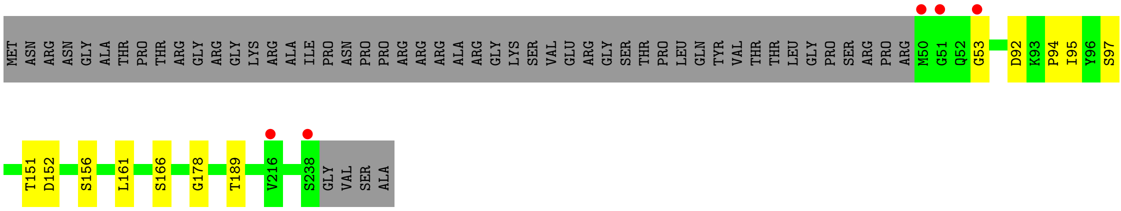
- Molecule 1: Capsid protein

Chain FZ:



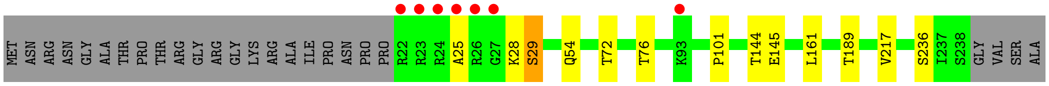
- Molecule 1: Capsid protein

Chain Fa:



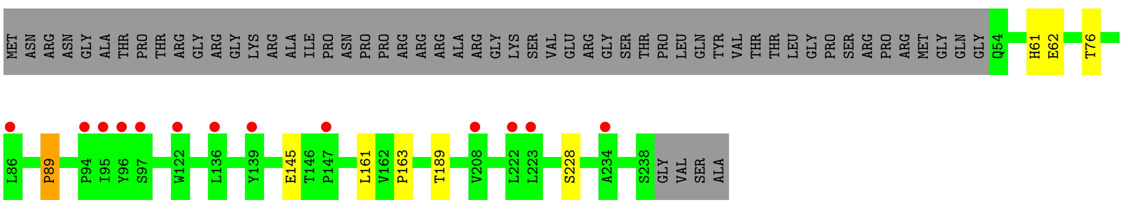
- Molecule 1: Capsid protein

Chain Fb:



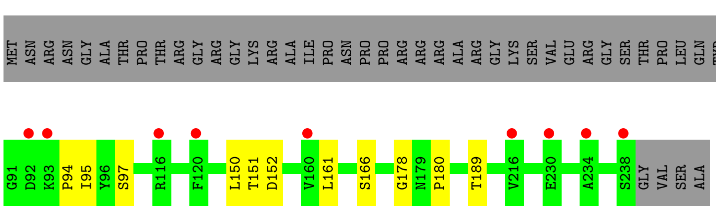
- Molecule 1: Capsid protein

Chain Fe:



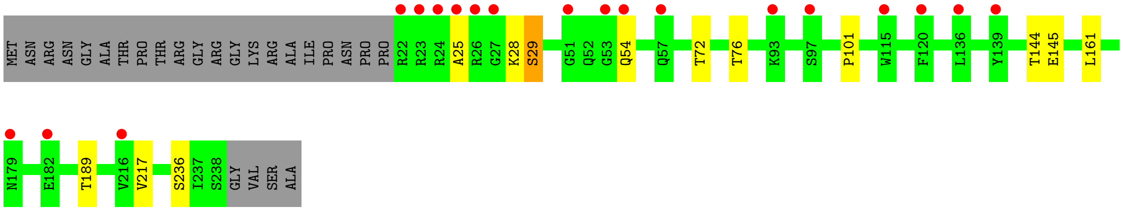
- Molecule 1: Capsid protein

Chain Ff:



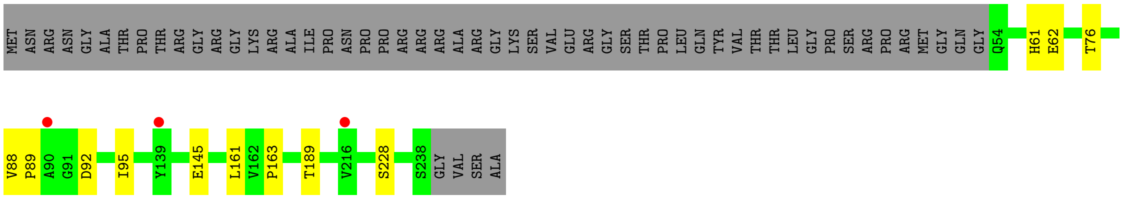
- Molecule 1: Capsid protein

Chain Fg:



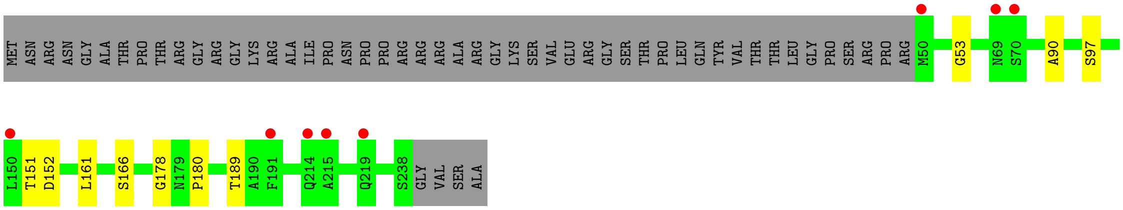
- Molecule 1: Capsid protein

Chain Fj:



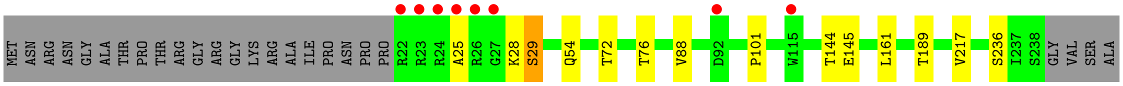
- Molecule 1: Capsid protein

Chain Fk:



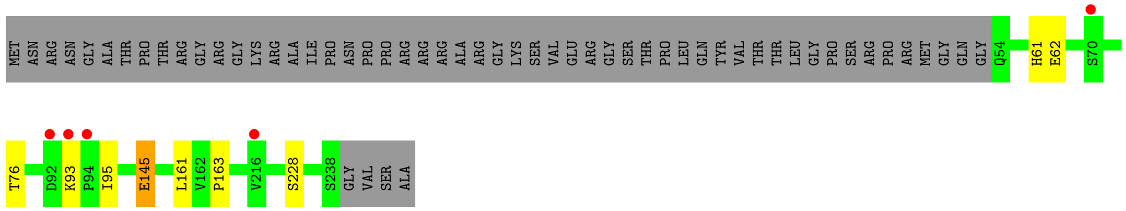
- Molecule 1: Capsid protein

Chain Fl:



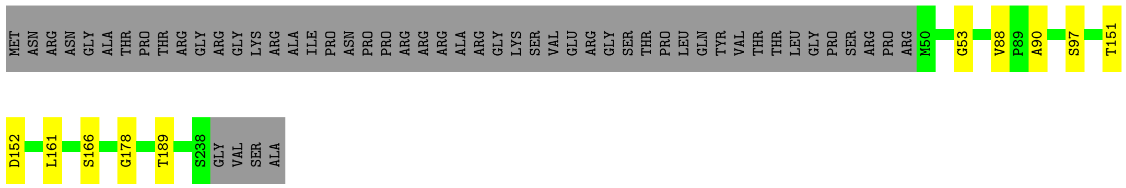
- Molecule 1: Capsid protein

Chain Fo:



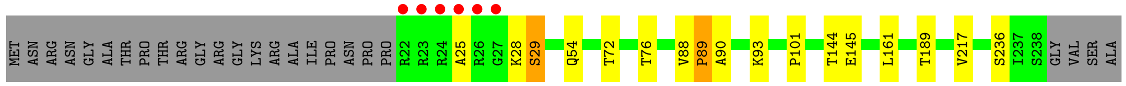
• Molecule 1: Capsid protein

Chain Fp:



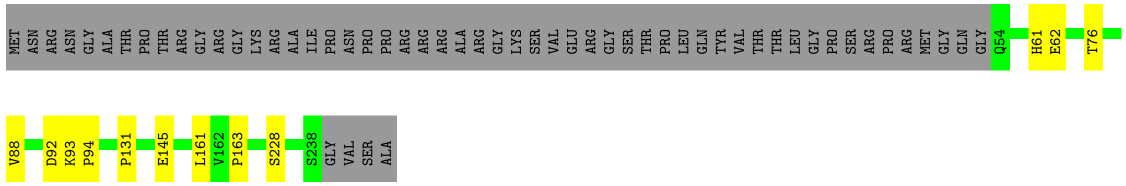
• Molecule 1: Capsid protein

Chain Fq:



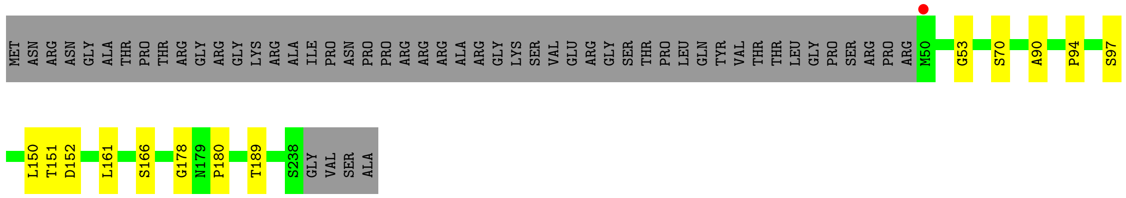
• Molecule 1: Capsid protein

Chain Ft:



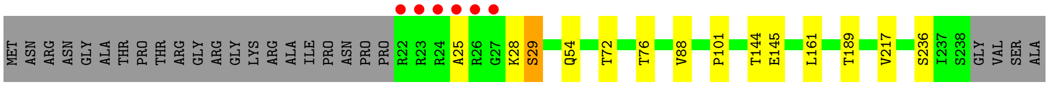
• Molecule 1: Capsid protein

Chain Fu:



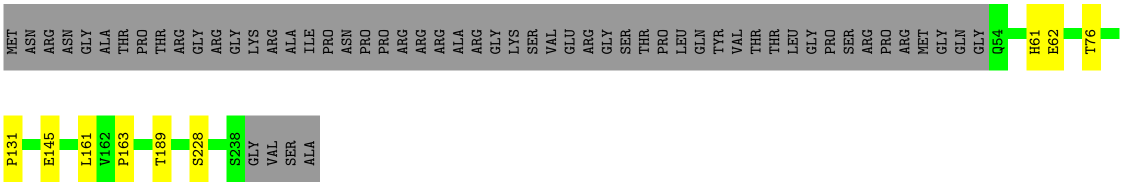
• Molecule 1: Capsid protein

Chain Fv:



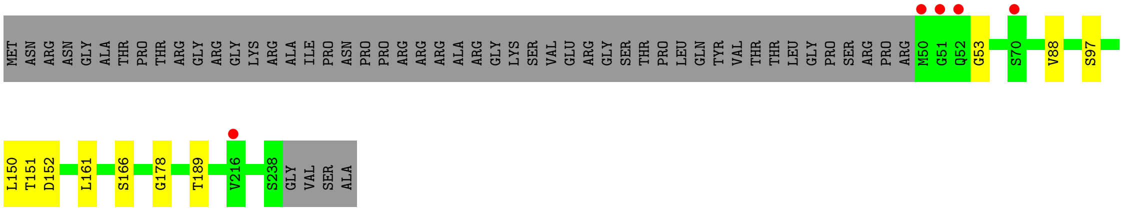
- Molecule 1: Capsid protein

Chain Fy:



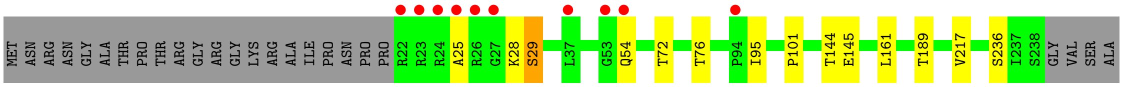
- Molecule 1: Capsid protein

Chain Fz:



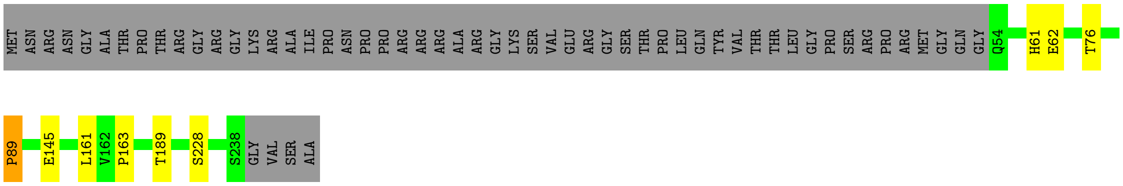
- Molecule 1: Capsid protein

Chain F1:



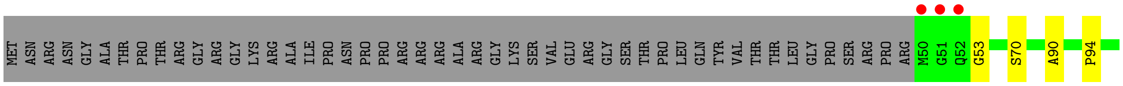
- Molecule 1: Capsid protein

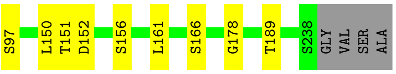
Chain F4:



- Molecule 1: Capsid protein

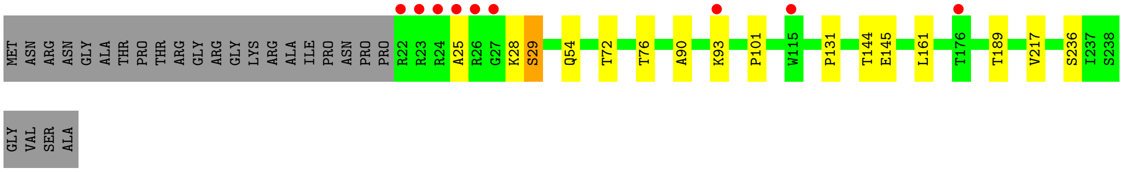
Chain F5:





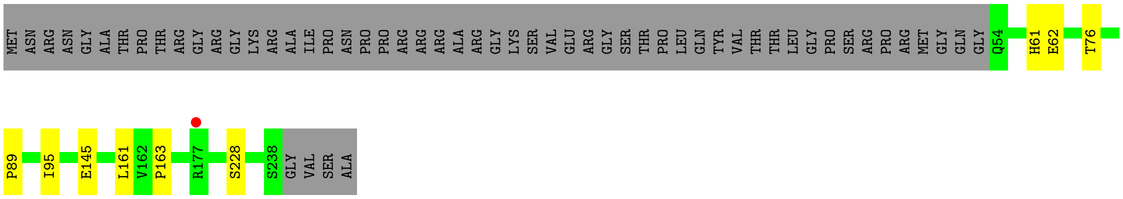
- Molecule 1: Capsid protein

Chain F6:



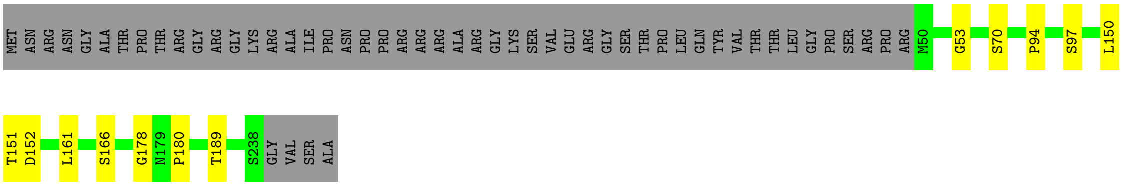
- Molecule 1: Capsid protein

Chain GA:



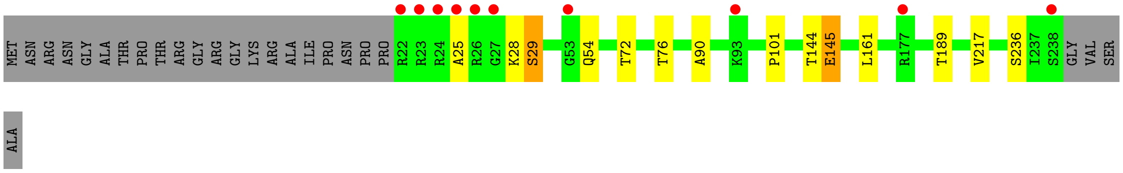
- Molecule 1: Capsid protein

Chain GB:



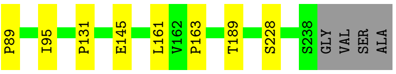
- Molecule 1: Capsid protein

Chain GC:

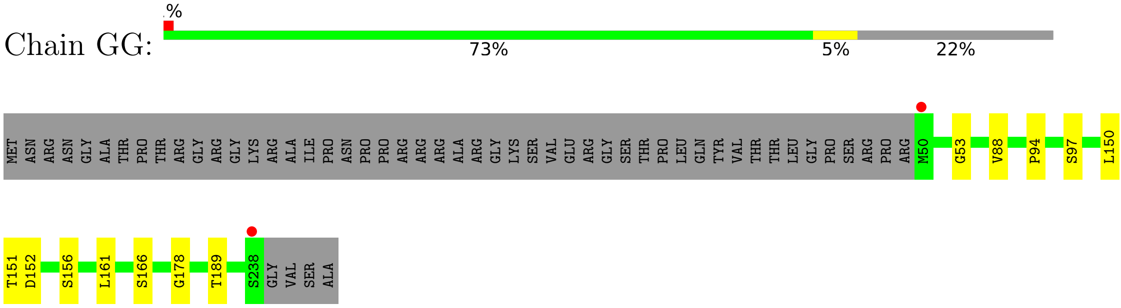


- Molecule 1: Capsid protein

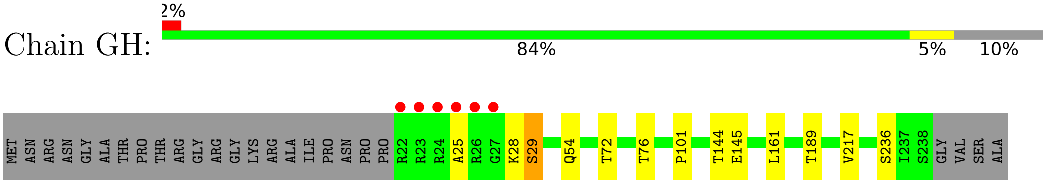
Chain GF:



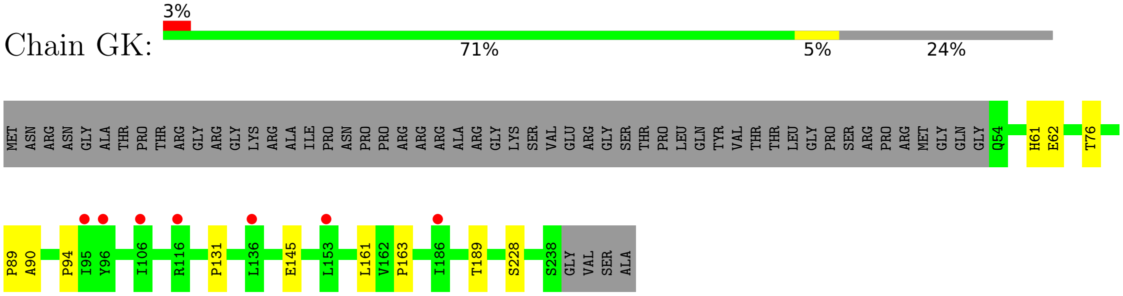
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



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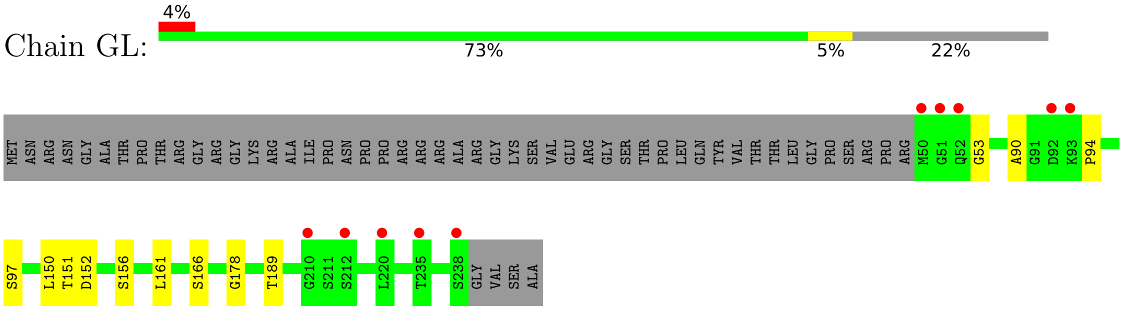

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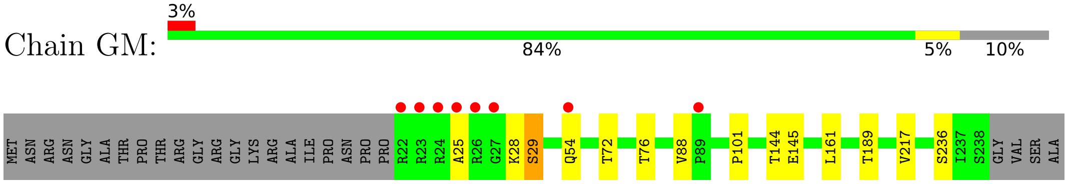

- Molecule 1: Capsid protein

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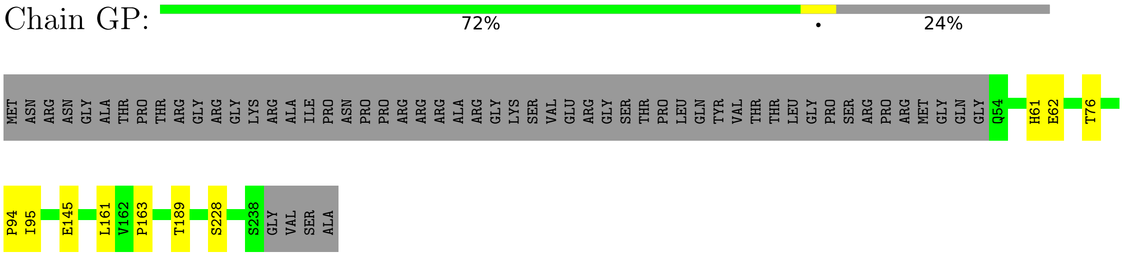
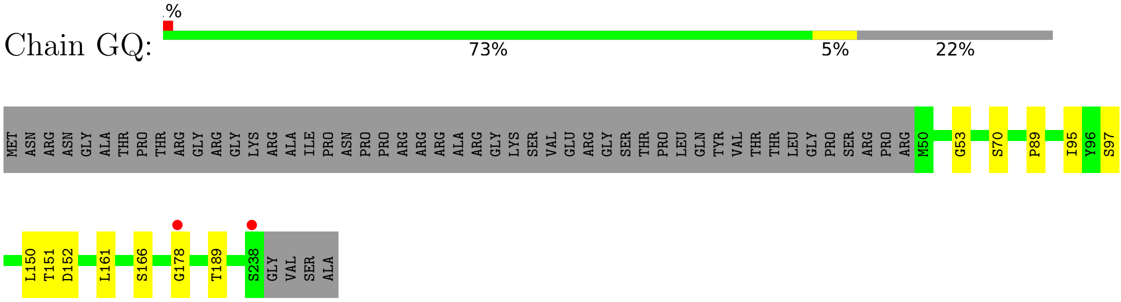


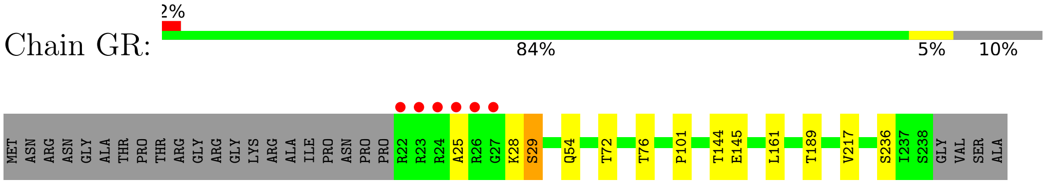
- Molecule 1: Capsid protein

Chain GQ:



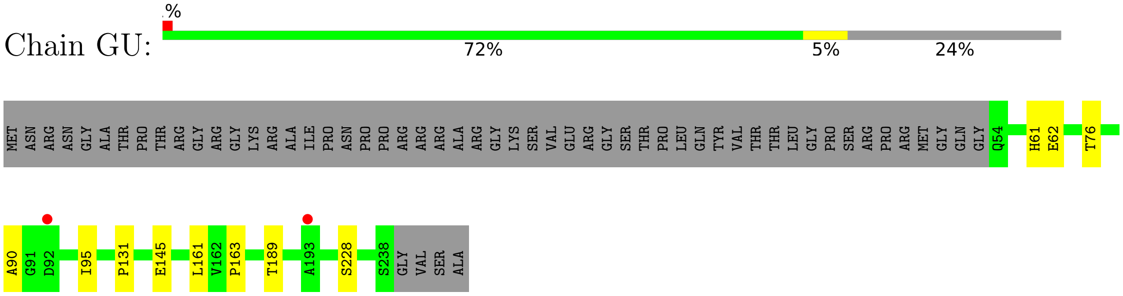
- Molecule 1: Capsid protein

Chain GR:



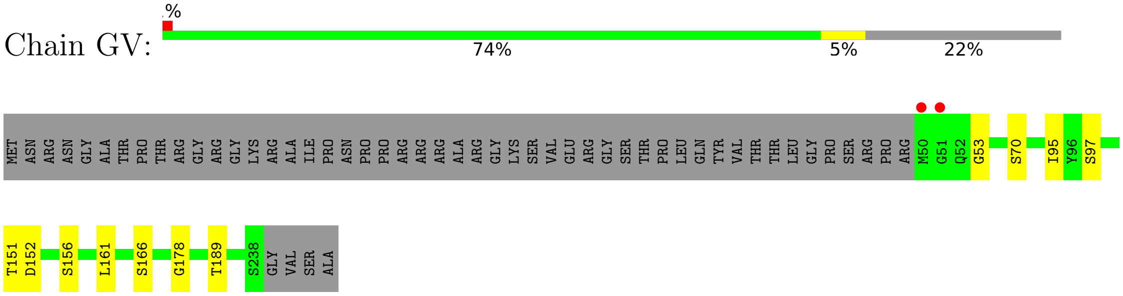
- Molecule 1: Capsid protein

Chain GU:

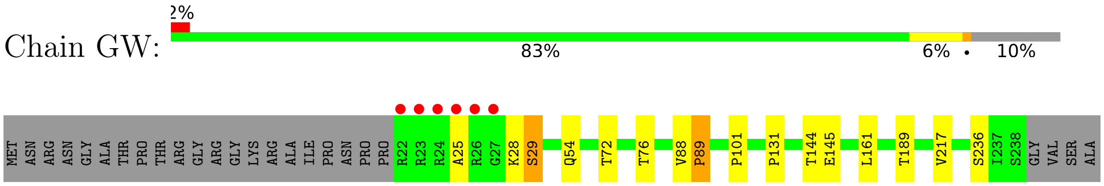


- Molecule 1: Capsid protein

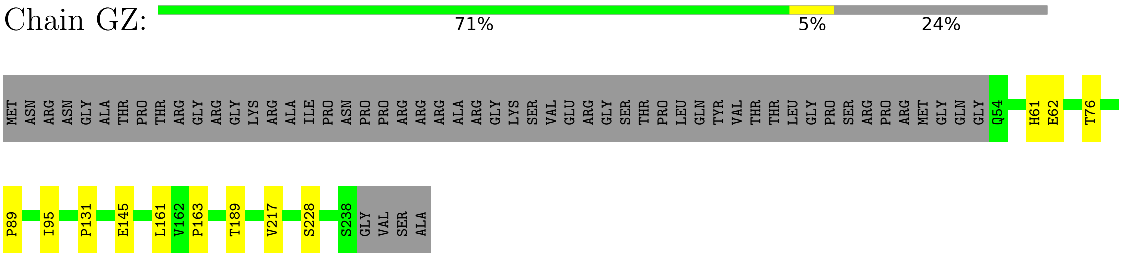
Chain GV:



- Molecule 1: Capsid protein



• Molecule 1: Capsid protein



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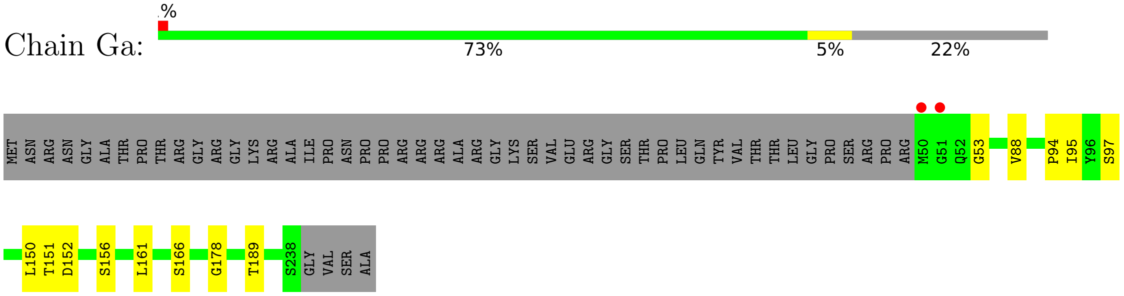

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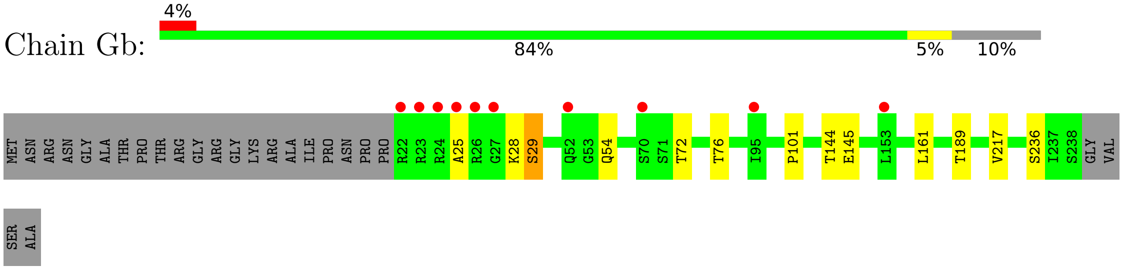

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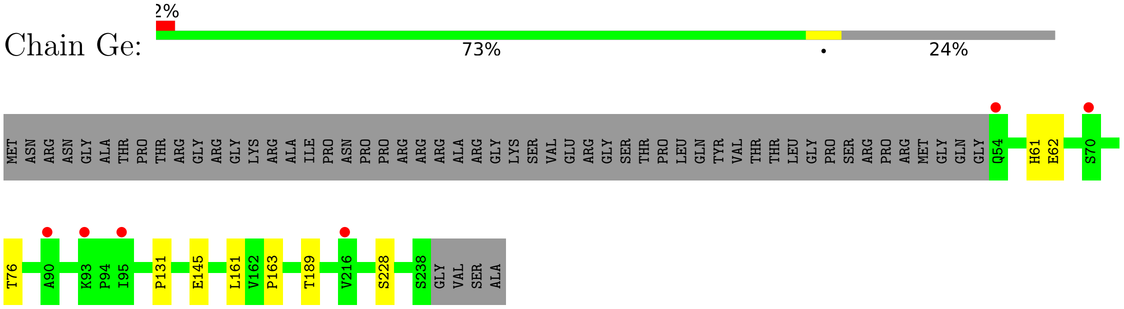

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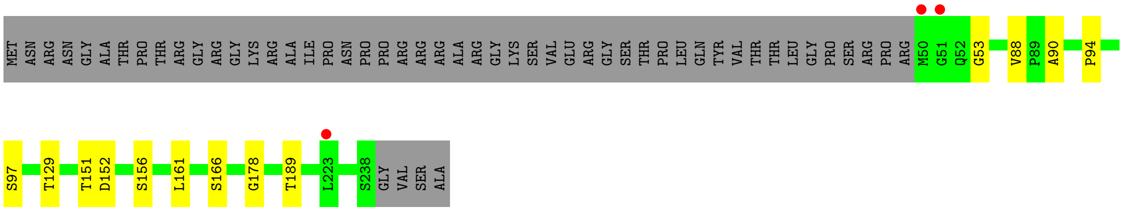
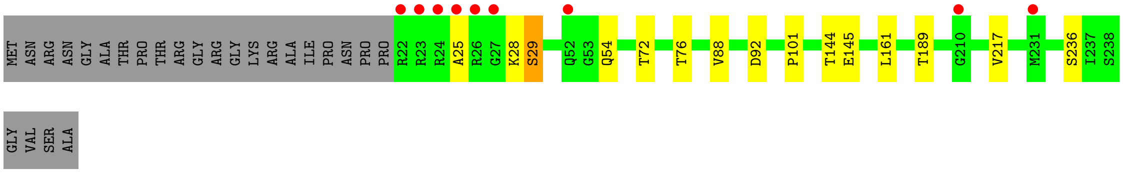


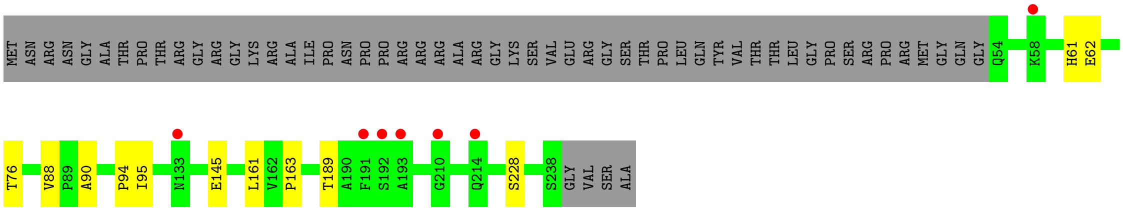
- Molecule 1: Capsid protein

Chain Gg:

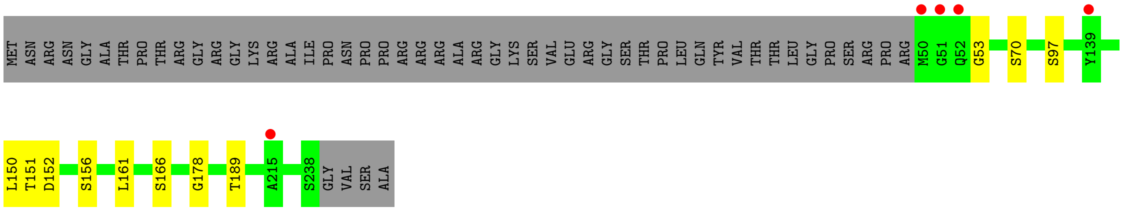
- Molecule 1: Capsid protein

Chain Gj:

- Molecule 1: Capsid protein

Chain Gk:

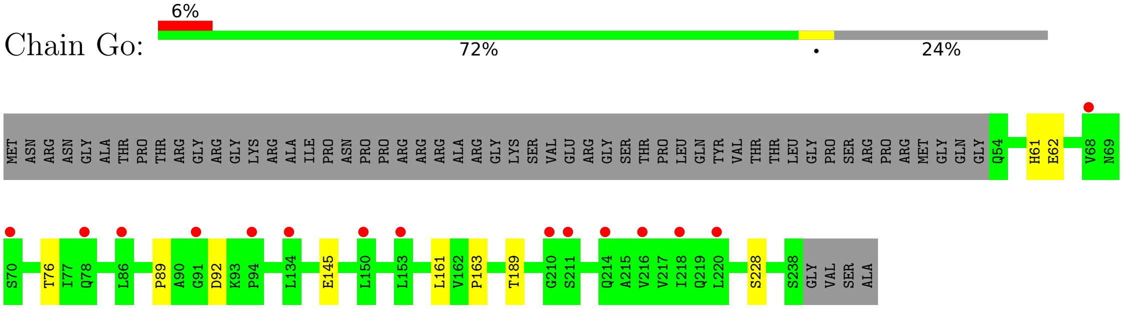



- Molecule 1: Capsid protein

Chain Gl:


- Molecule 1: Capsid protein

Chain Go:



- Molecule 1: Capsid protein

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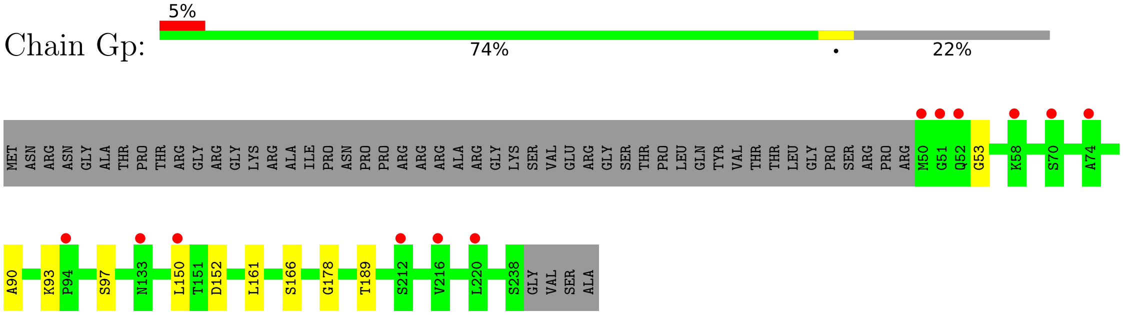
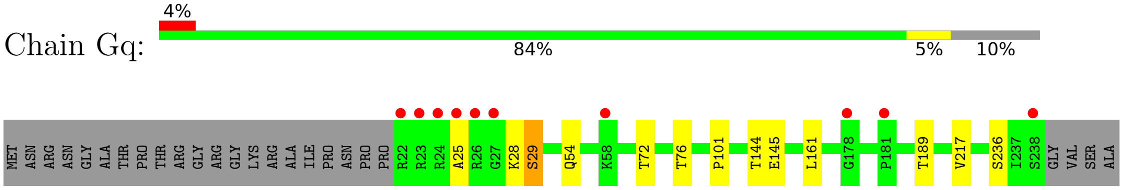


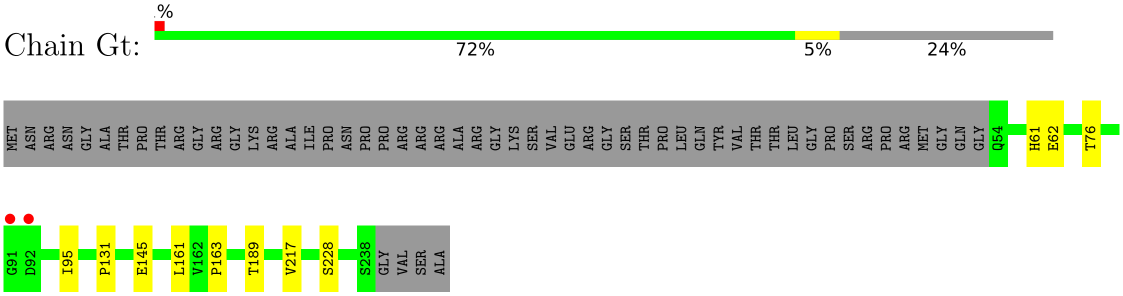
- Molecule 1: Capsid protein

Chain Gq:



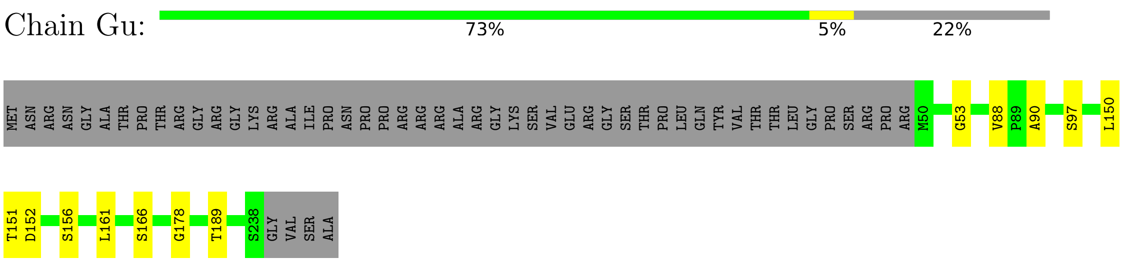
- Molecule 1: Capsid protein

Chain Gt:

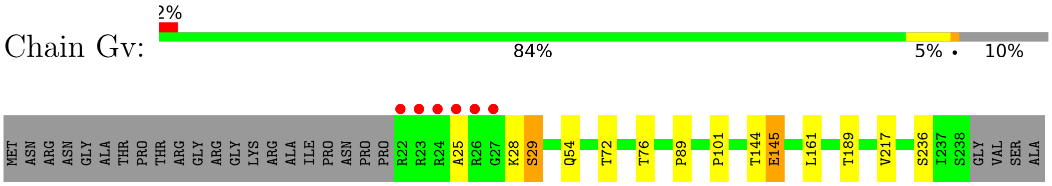


- Molecule 1: Capsid protein

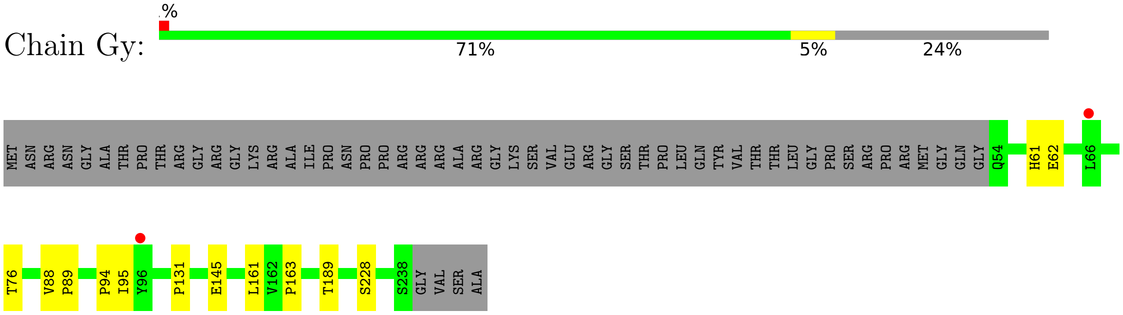
Chain Gu:



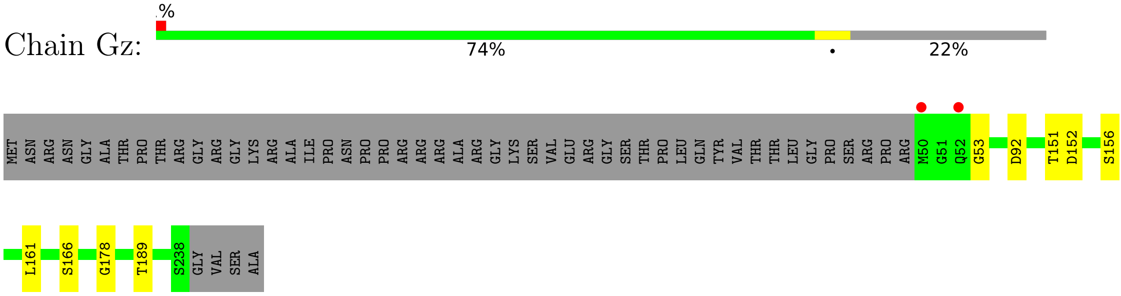
- Molecule 1: Capsid protein



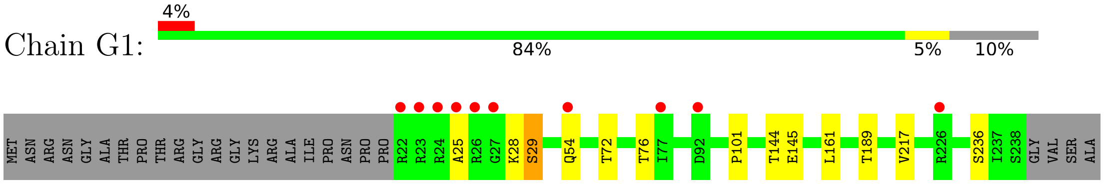
- Molecule 1: Capsid protein



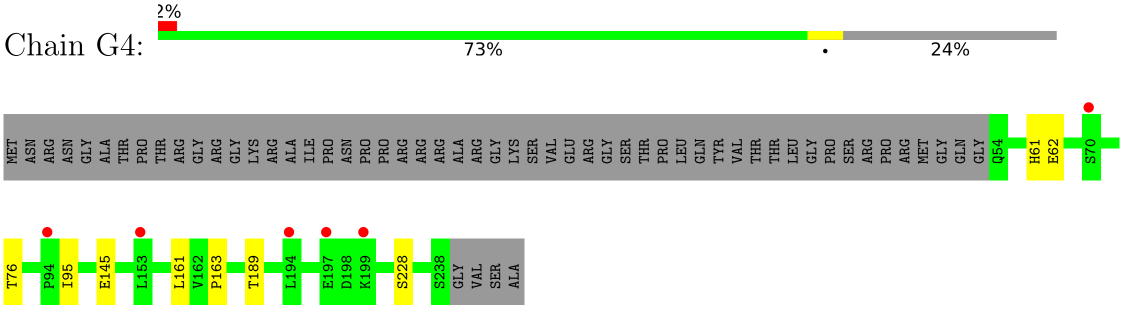
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



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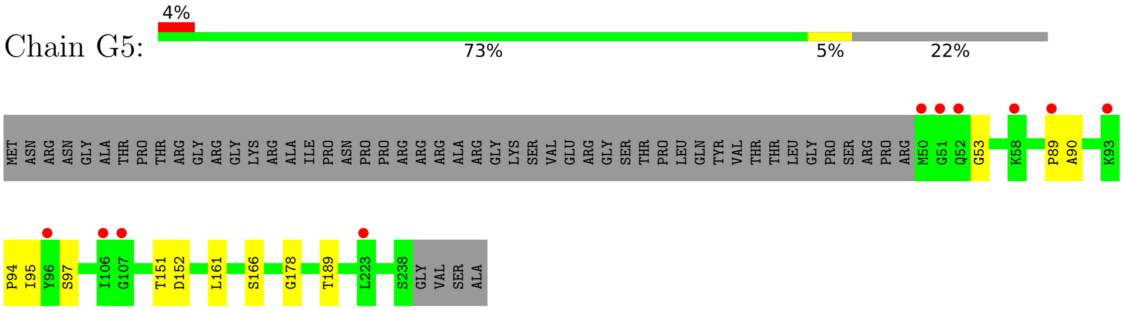

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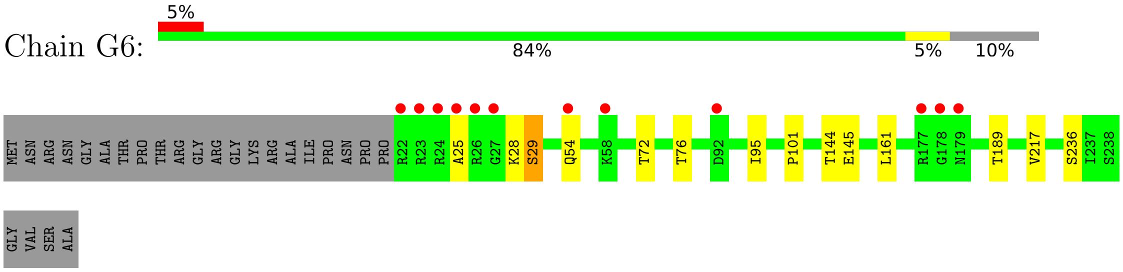
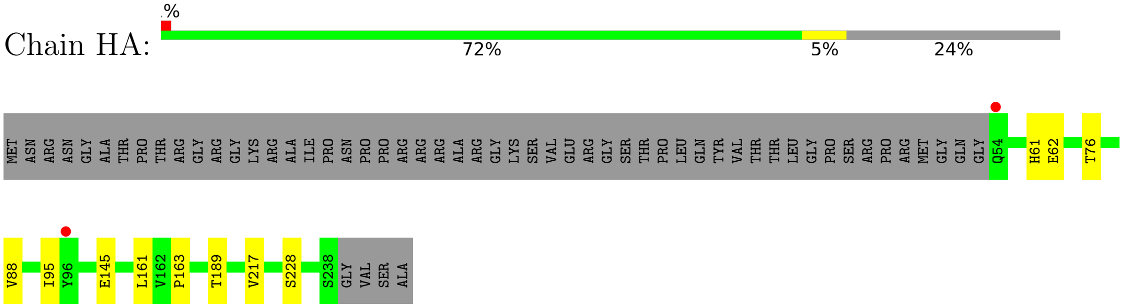
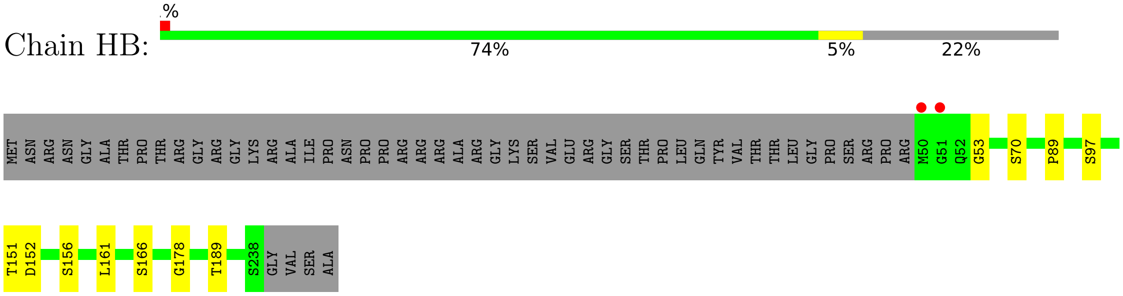


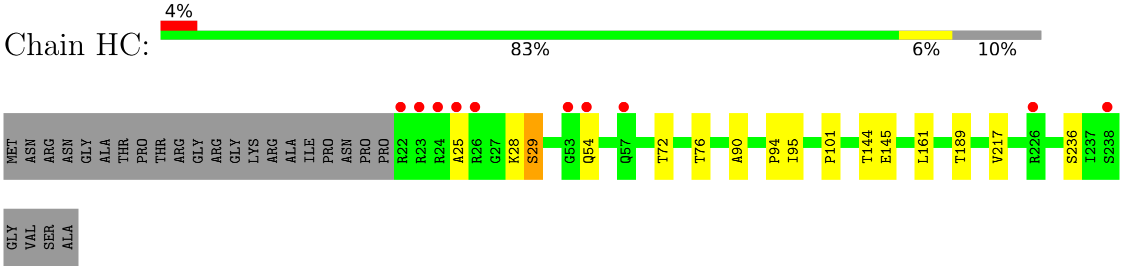
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

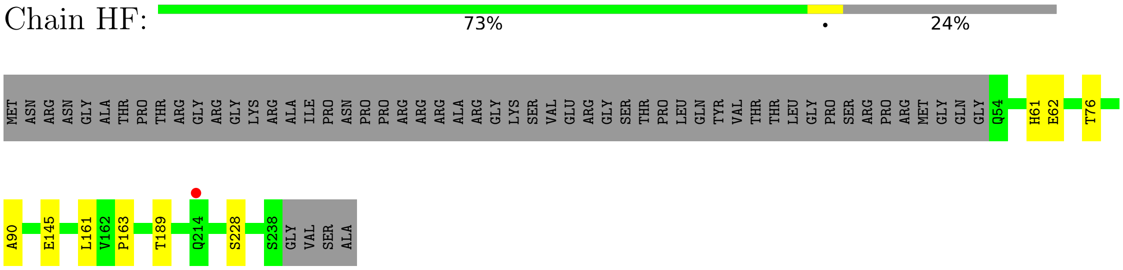


- Molecule 1: Capsid protein



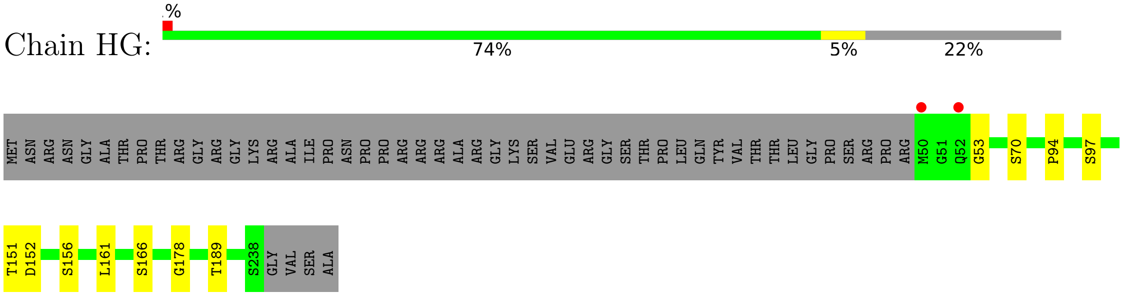
- Molecule 1: Capsid protein

Chain HF:



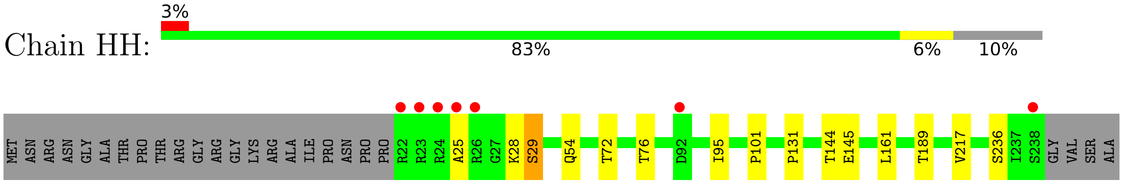
- Molecule 1: Capsid protein

Chain HG:



- Molecule 1: Capsid protein

Chain HH:



- Molecule 1: Capsid protein

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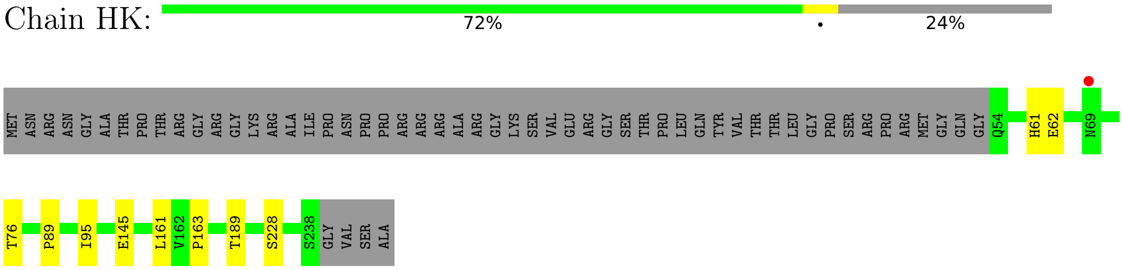
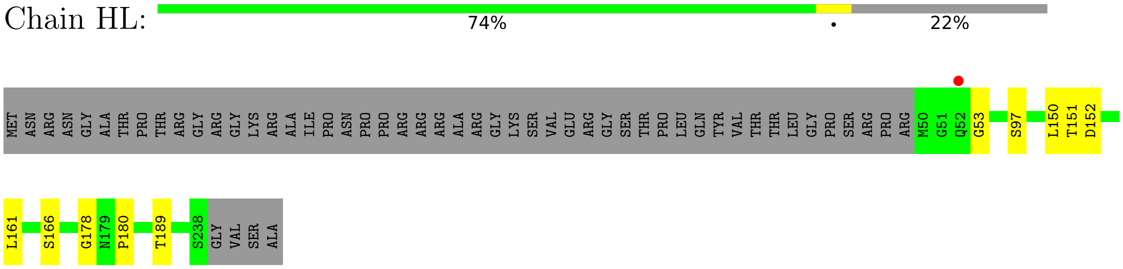
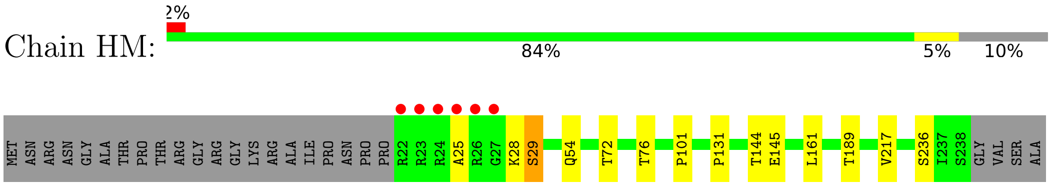


- Molecule 1: Capsid protein

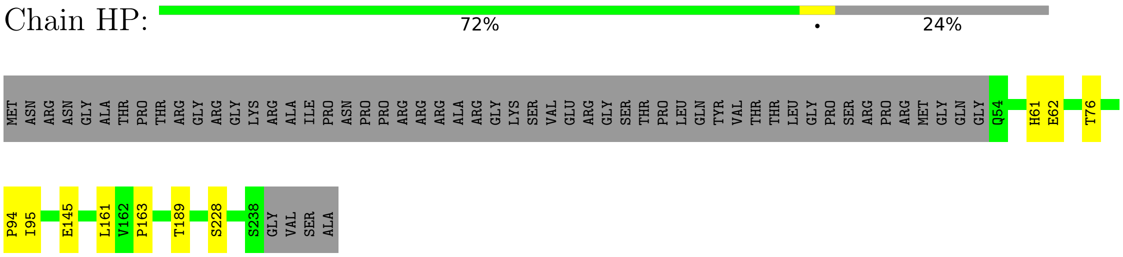
Chain HL:



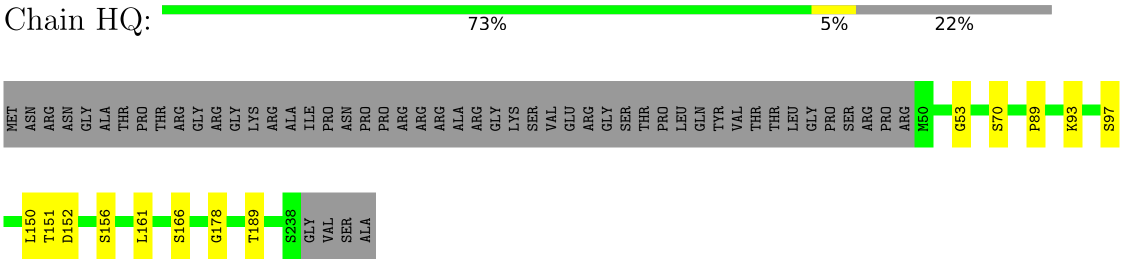
- Molecule 1: Capsid protein



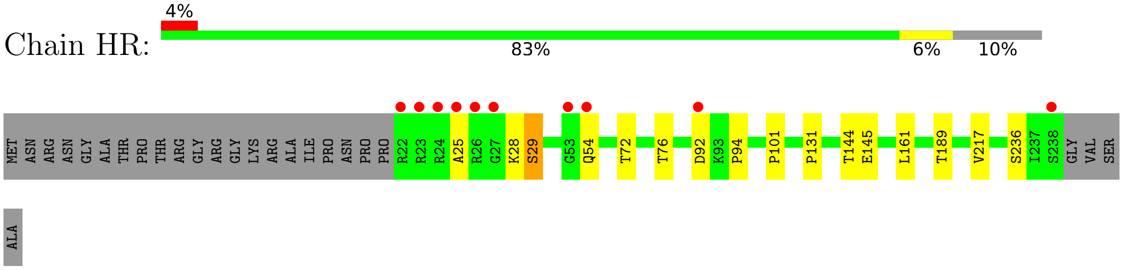
- Molecule 1: Capsid protein



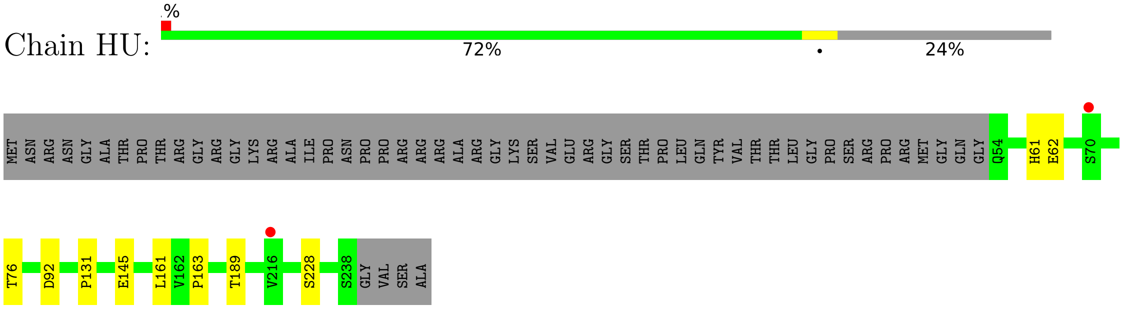
- Molecule 1: Capsid protein



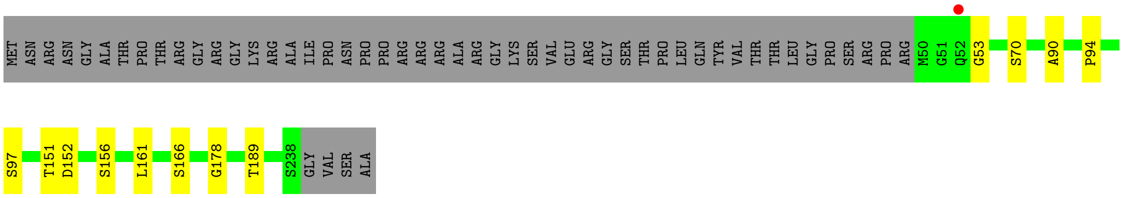
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

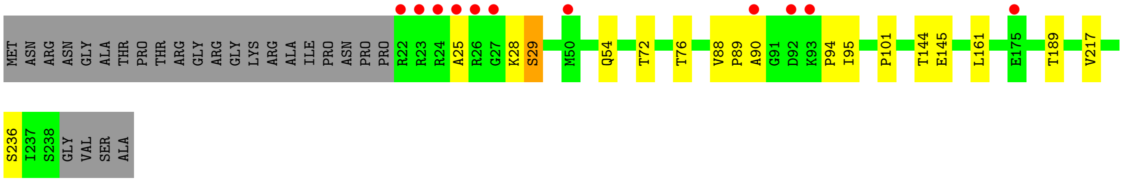


- Molecule 1: Capsid protein



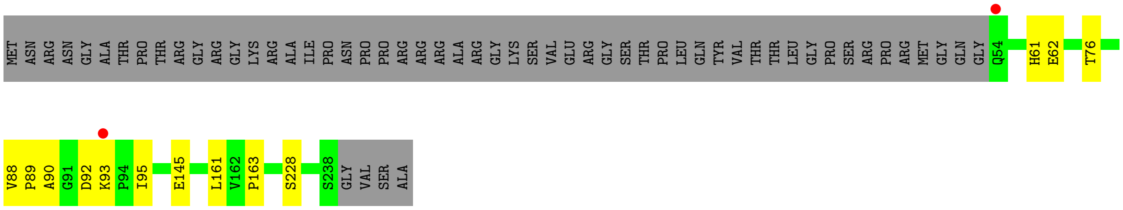
• Molecule 1: Capsid protein

Chain HW:



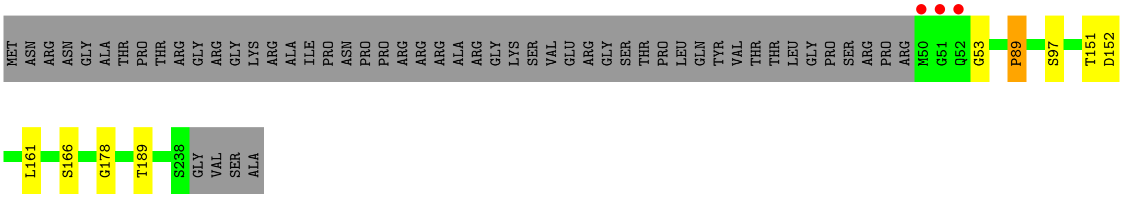
• Molecule 1: Capsid protein

Chain HZ:



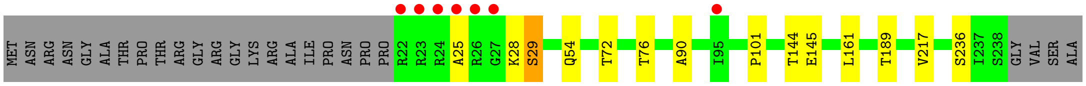
• Molecule 1: Capsid protein

Chain Ha:



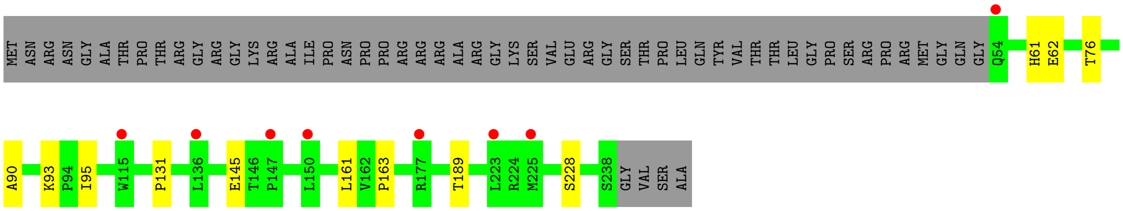
• Molecule 1: Capsid protein

Chain Hb:



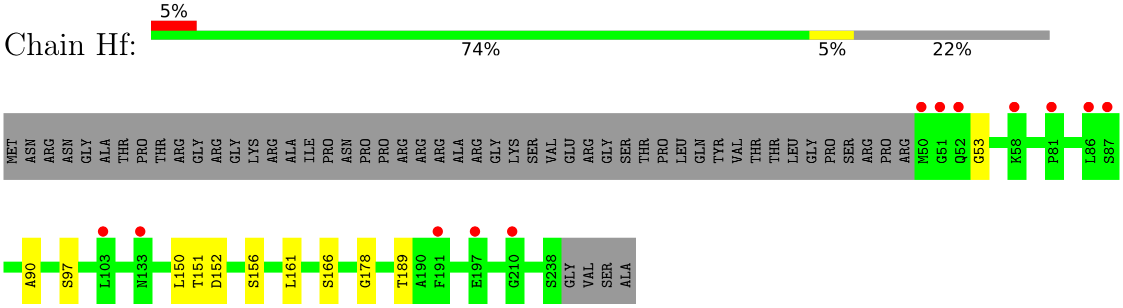
• Molecule 1: Capsid protein

Chain He:



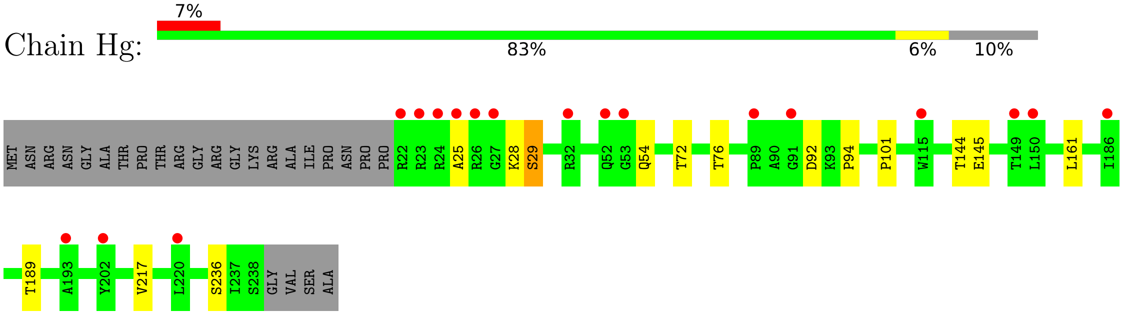
- Molecule 1: Capsid protein

Chain Hf:



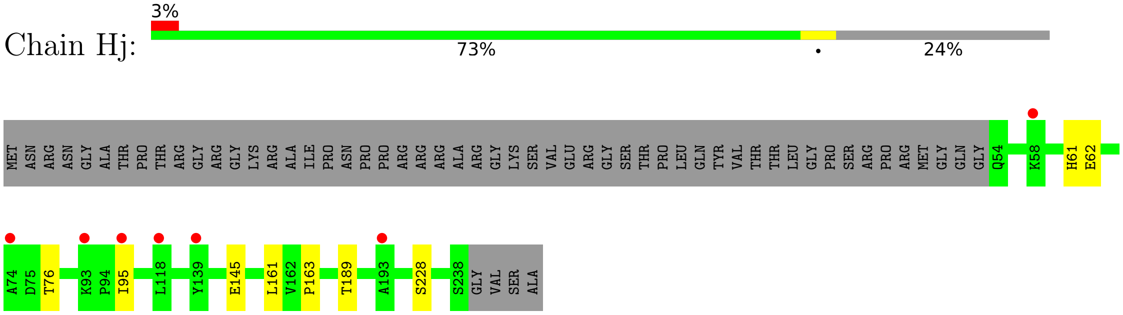
- Molecule 1: Capsid protein

Chain Hg:



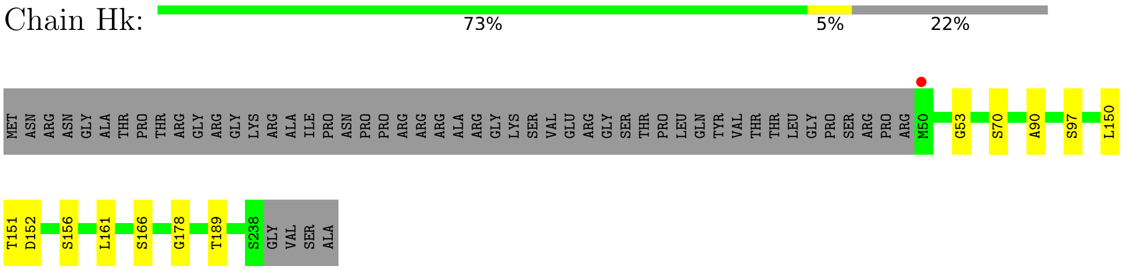
- Molecule 1: Capsid protein

Chain Hj:



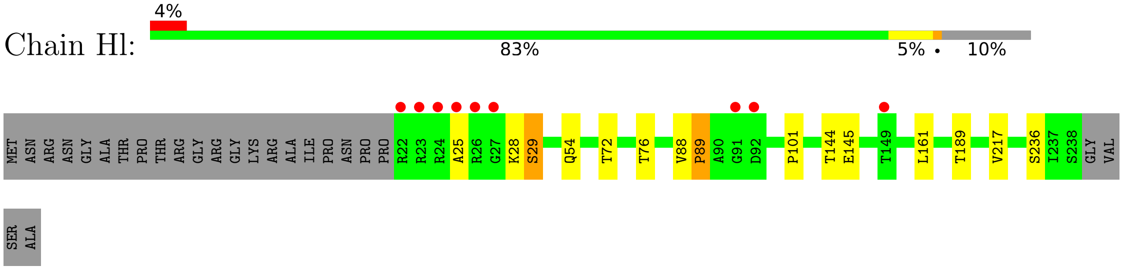
- Molecule 1: Capsid protein

Chain Hk:



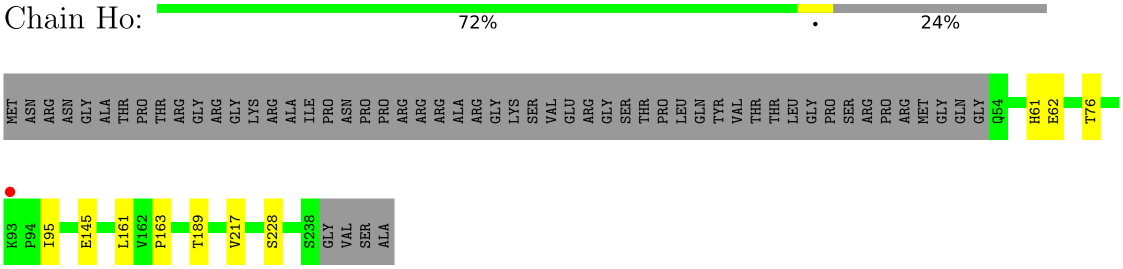
- Molecule 1: Capsid protein

Chain Hl:



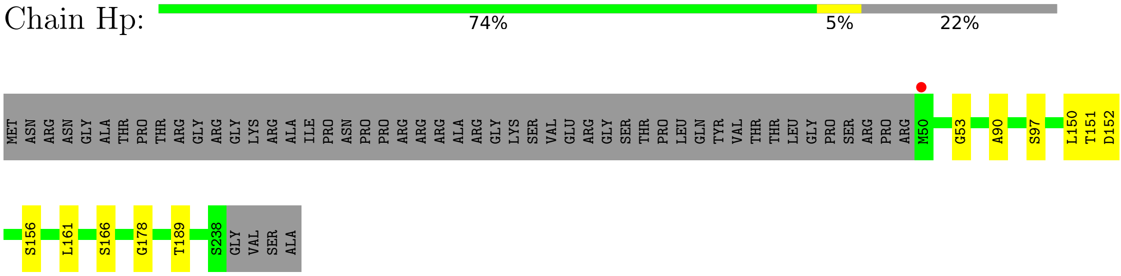
- Molecule 1: Capsid protein

Chain Ho:



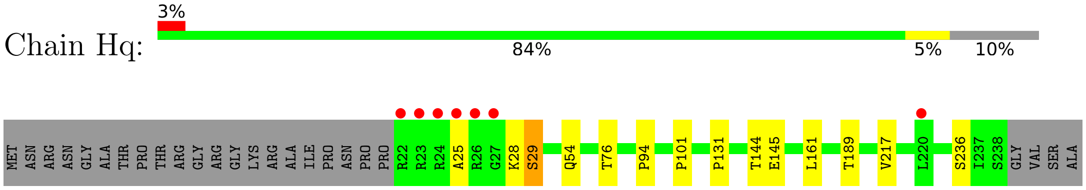
- Molecule 1: Capsid protein

Chain Hp:



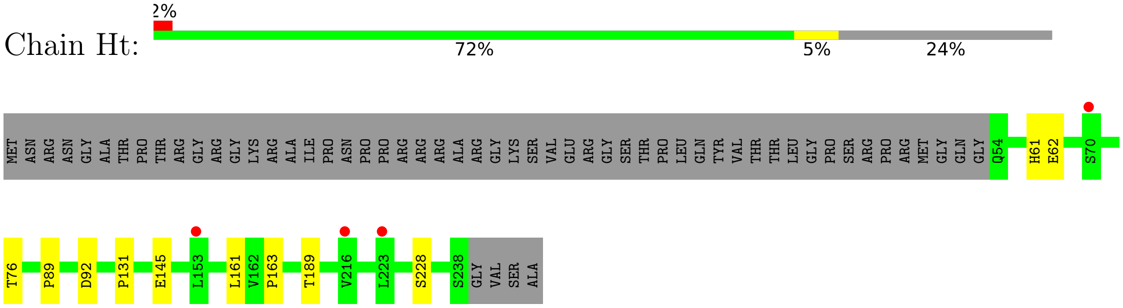
- Molecule 1: Capsid protein

Chain Hq:

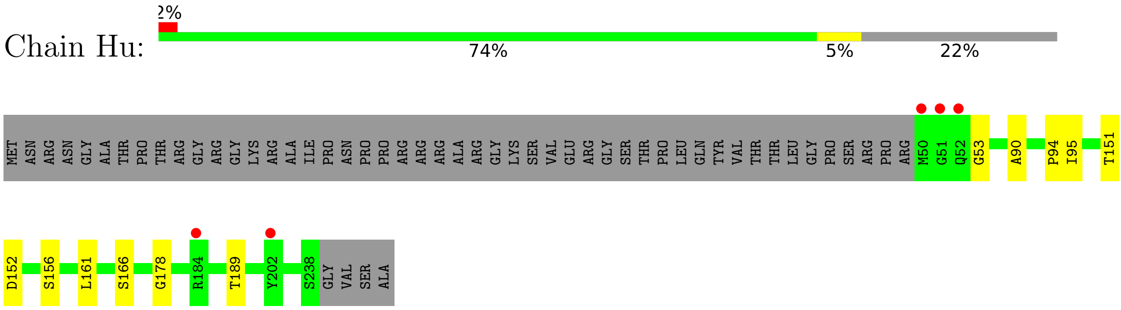


- Molecule 1: Capsid protein

Chain Ht:



- Molecule 1: Capsid protein



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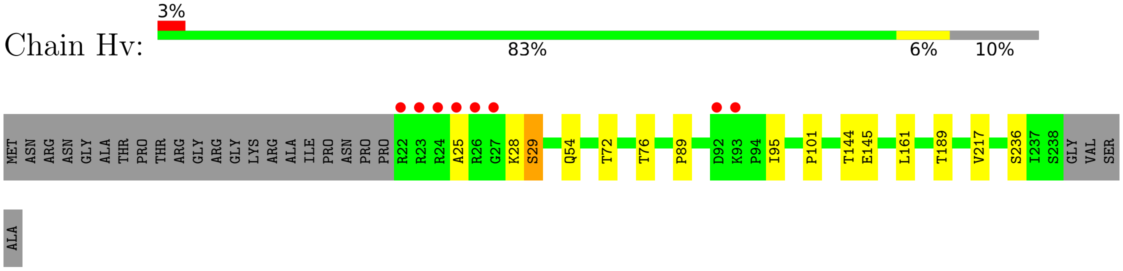

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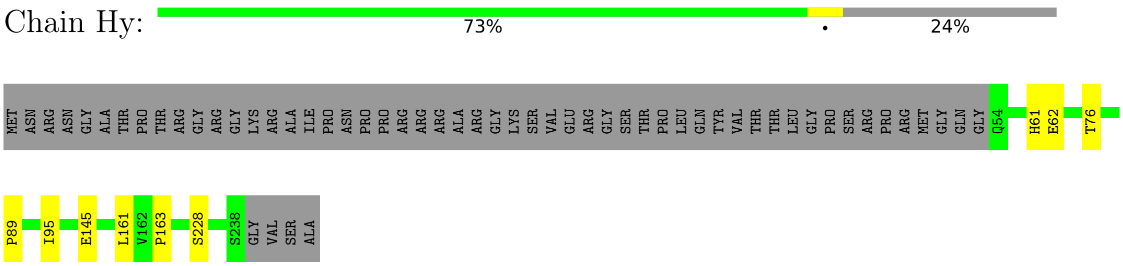
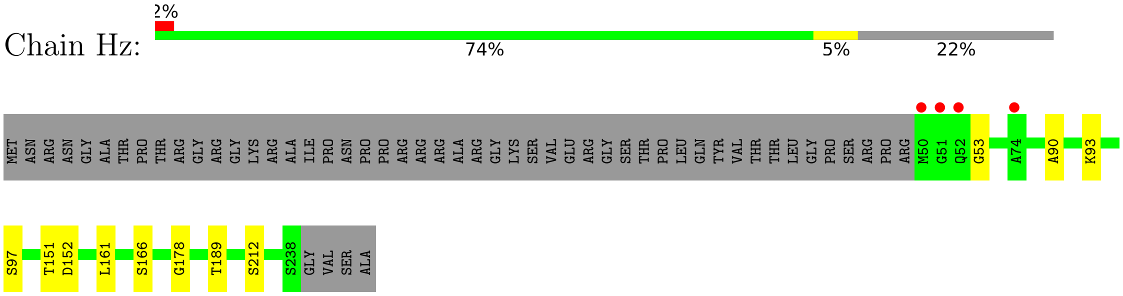
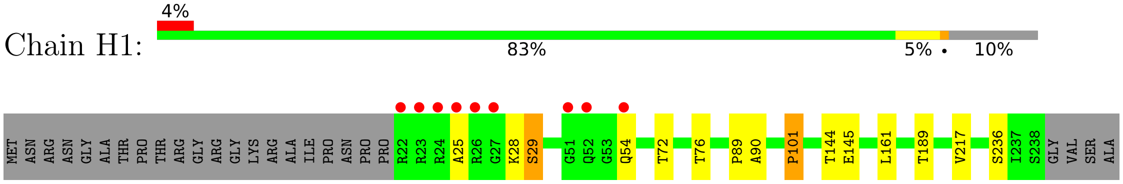


- Molecule 1: Capsid protein

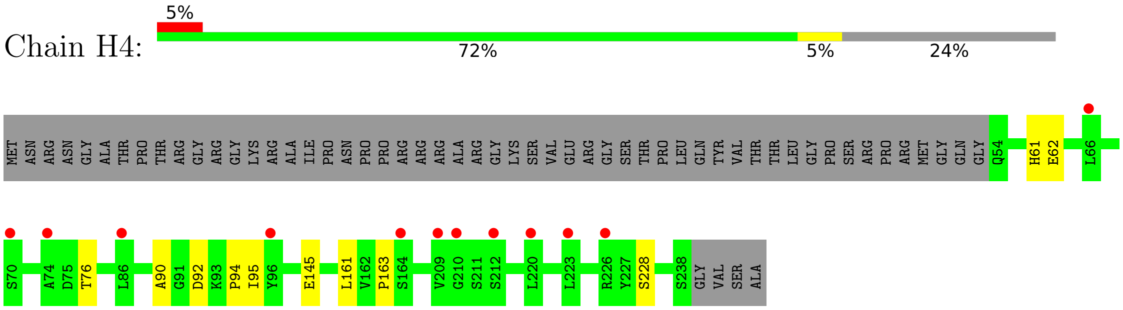


- Molecule 1: Capsid protein



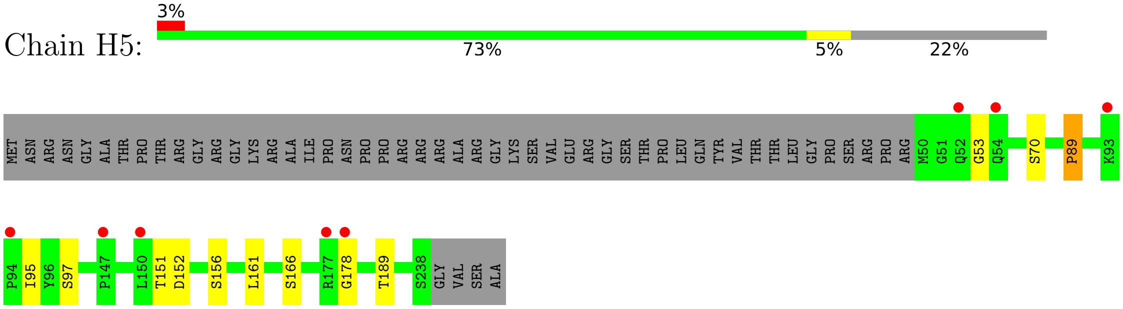
- Molecule 1: Capsid protein

Chain H4:



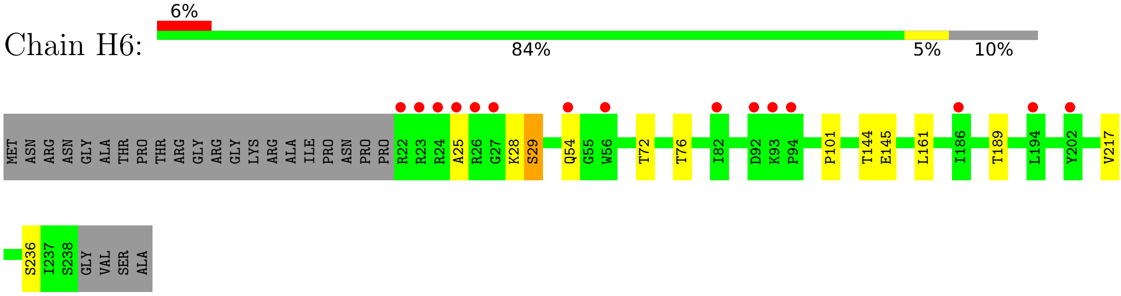
- Molecule 1: Capsid protein

Chain H5:



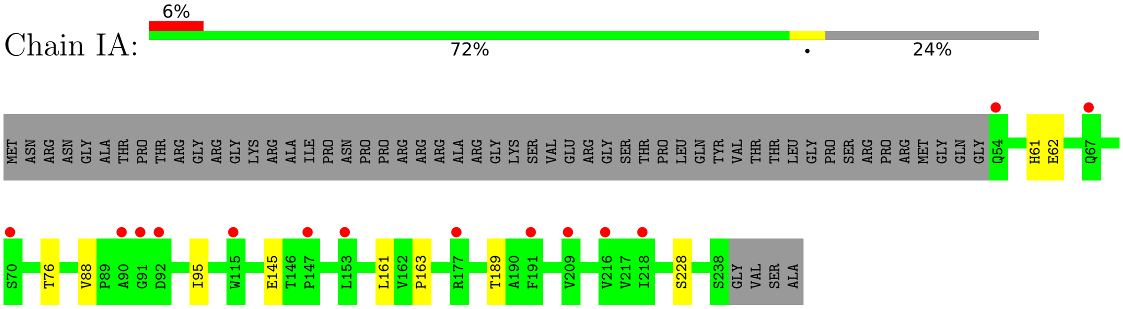
- Molecule 1: Capsid protein

Chain H6:



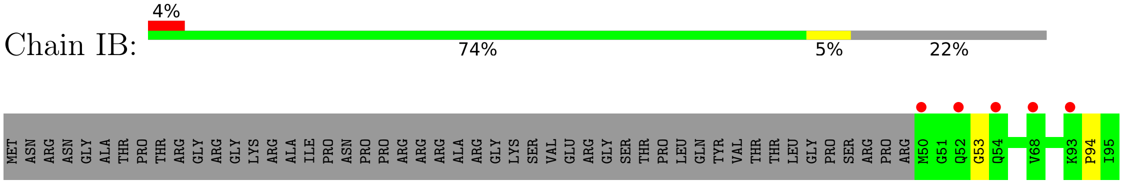
- Molecule 1: Capsid protein

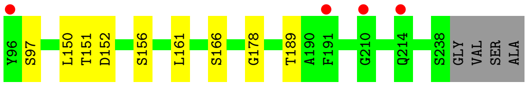
Chain IA:



- Molecule 1: Capsid protein

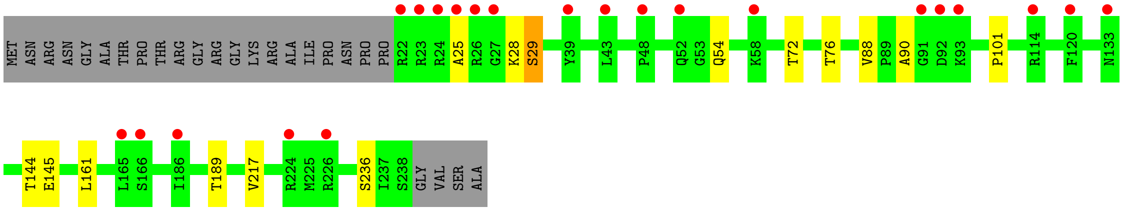
Chain IB:





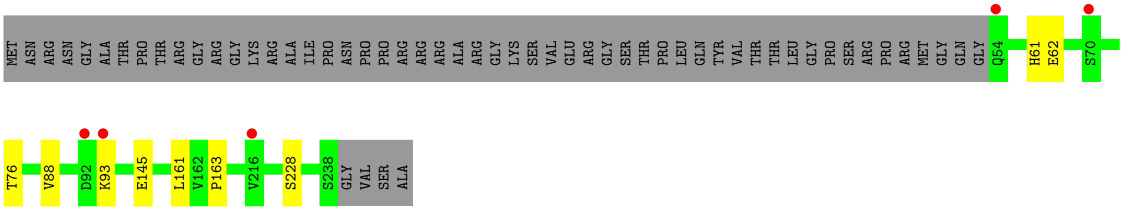
- Molecule 1: Capsid protein

Chain IC:



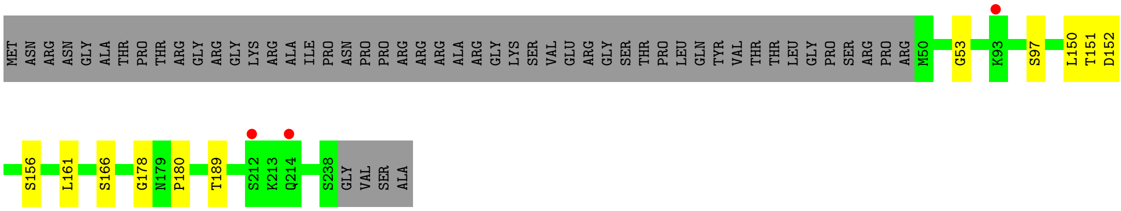
- Molecule 1: Capsid protein

Chain IF:



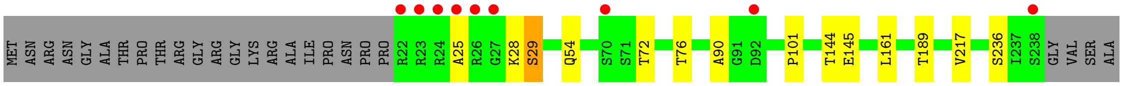
- Molecule 1: Capsid protein

Chain IG:



- Molecule 1: Capsid protein

Chain IH:



- Molecule 1: Capsid protein

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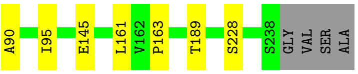
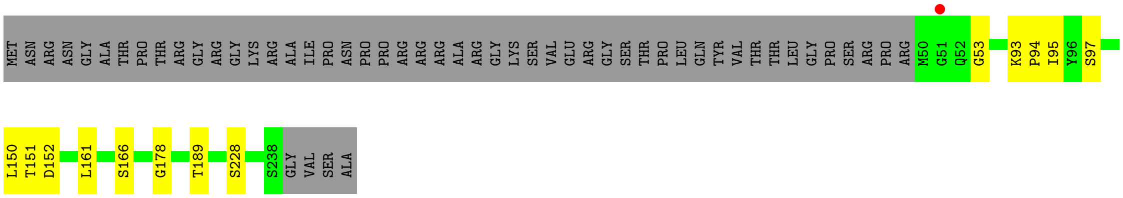


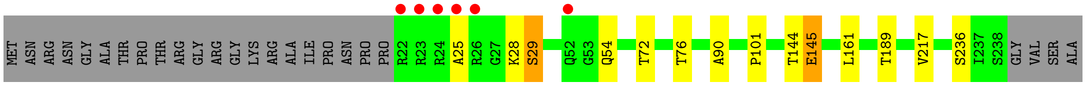
• Molecule 1: Capsid protein

Chain IL:



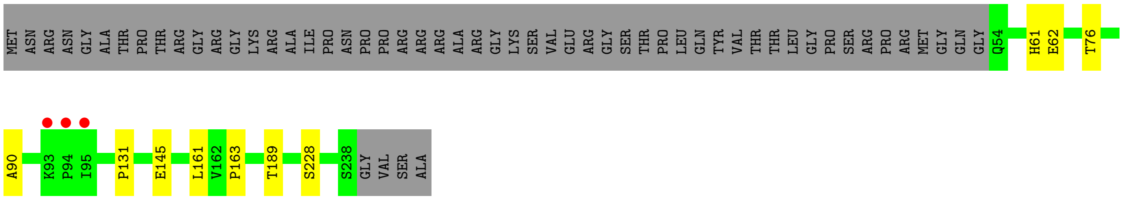
• Molecule 1: Capsid protein

Chain IM:



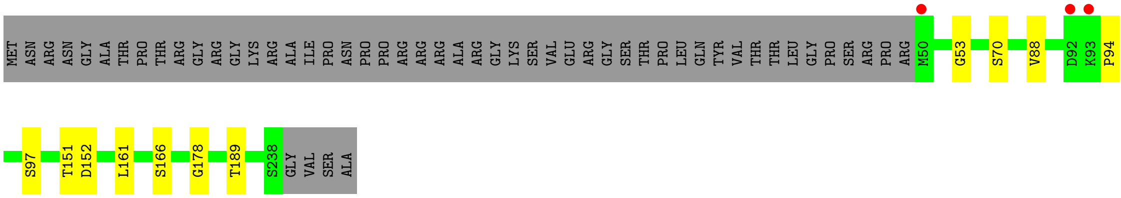
• Molecule 1: Capsid protein

Chain IP:



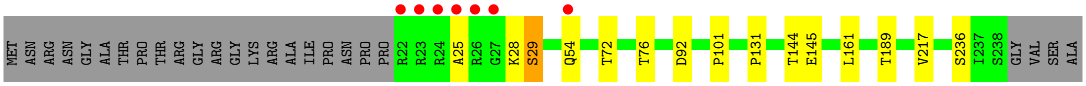
• Molecule 1: Capsid protein

Chain IQ:



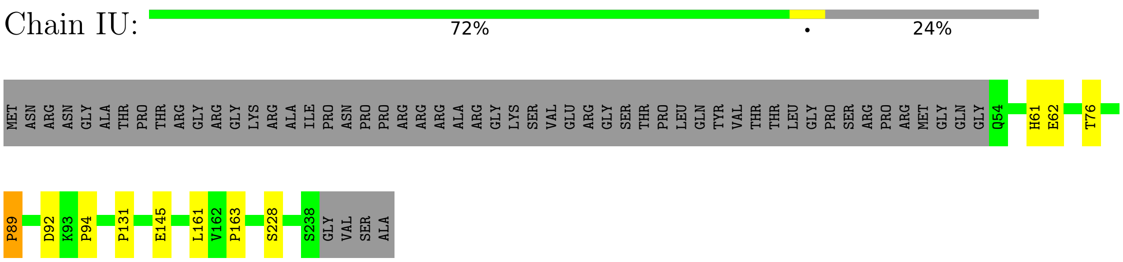
• Molecule 1: Capsid protein

Chain IR:



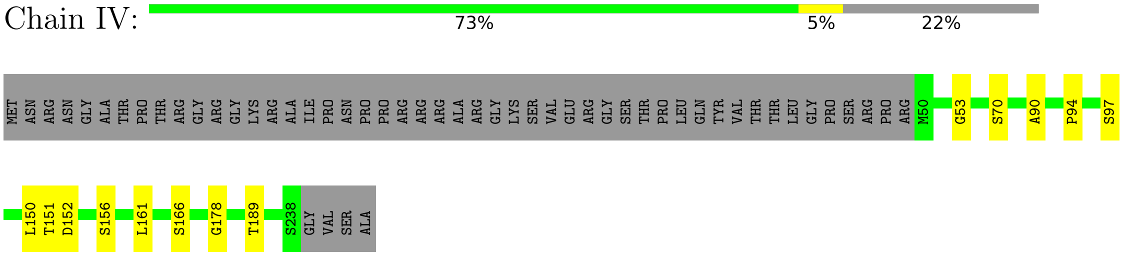
- Molecule 1: Capsid protein

Chain IU:



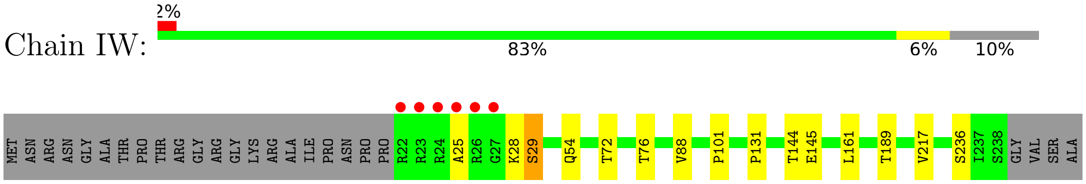
- Molecule 1: Capsid protein

Chain IV:



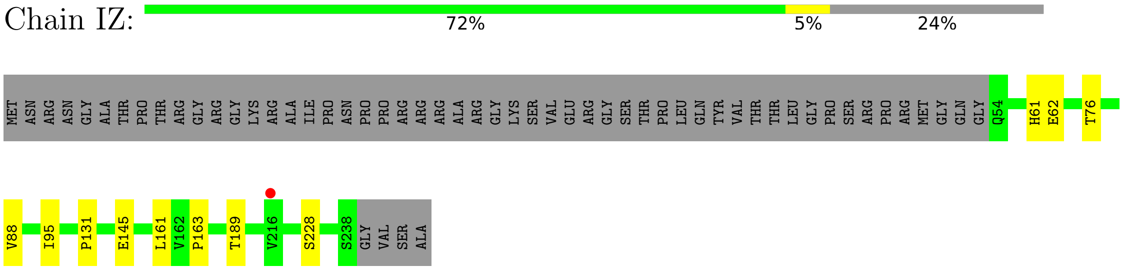
- Molecule 1: Capsid protein

Chain IW:



- Molecule 1: Capsid protein

Chain IZ:



- Molecule 1: Capsid protein

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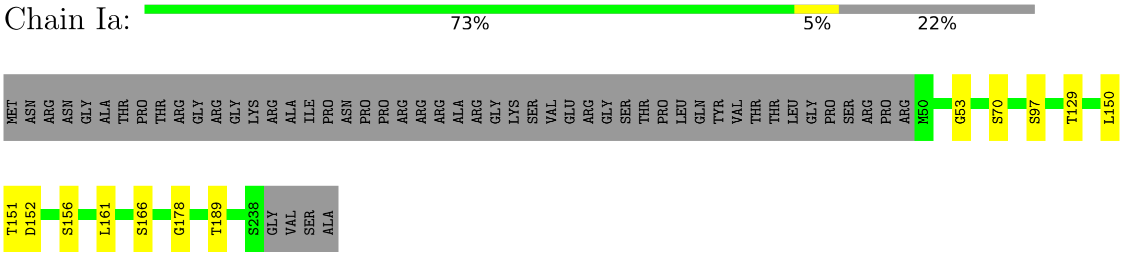
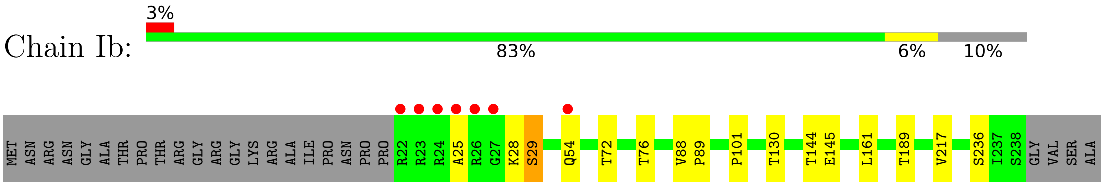


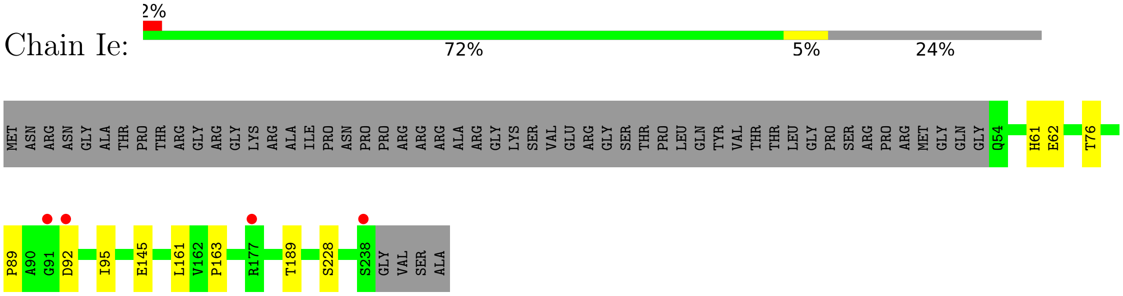
- Molecule 1: Capsid protein

Chain Ib:



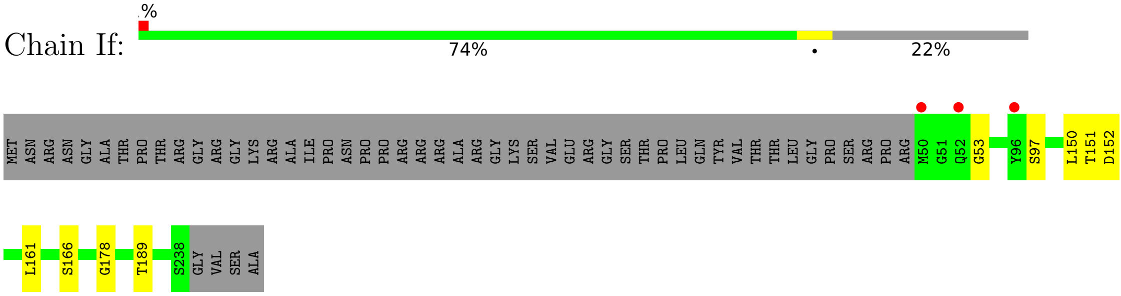
- Molecule 1: Capsid protein

Chain Ie:



- Molecule 1: Capsid protein

Chain If:



- Molecule 1: Capsid protein

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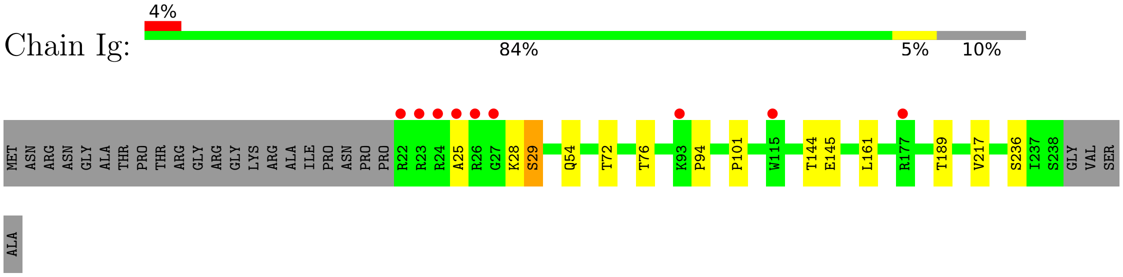

- Molecule 1: Capsid protein

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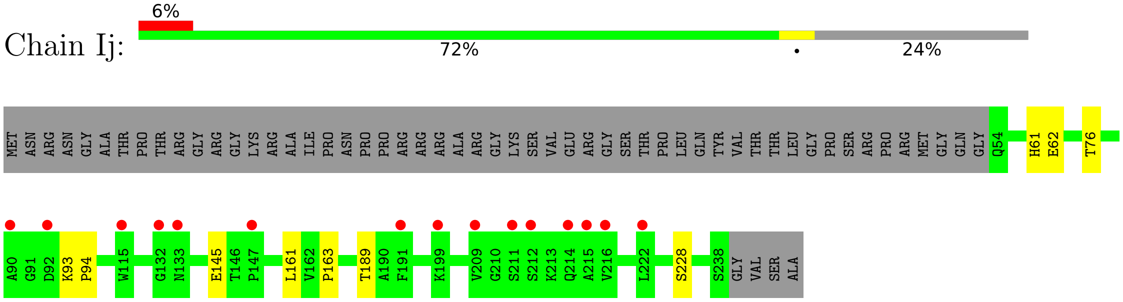

- Molecule 1: Capsid protein

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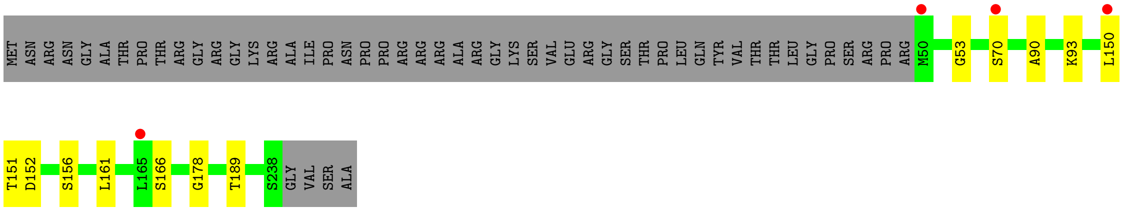

- Molecule 1: Capsid protein

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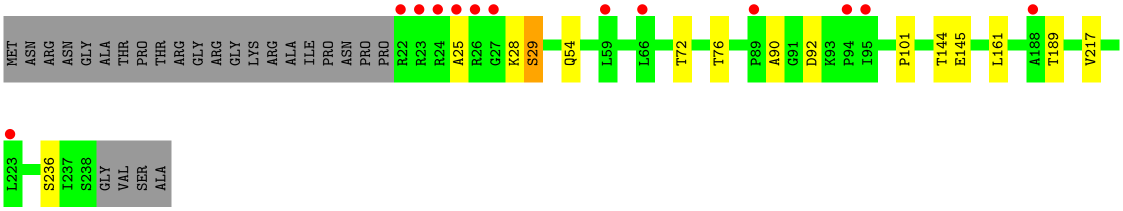
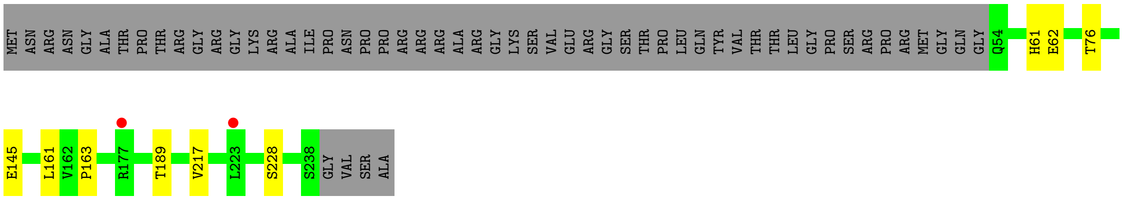


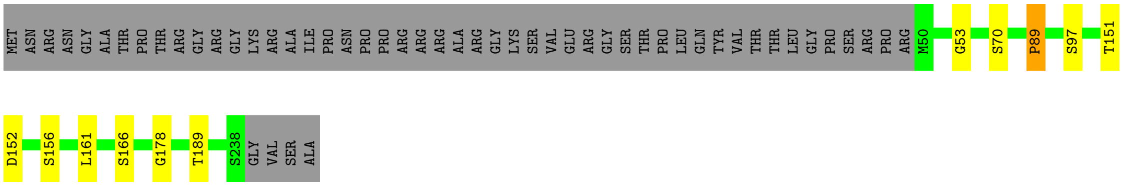
- Molecule 1: Capsid protein

Chain Io:



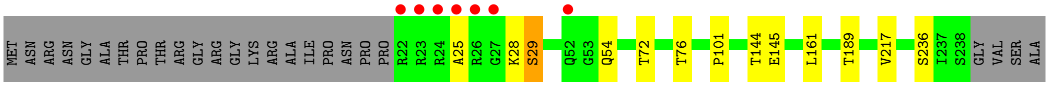
- Molecule 1: Capsid protein

Chain Ip:

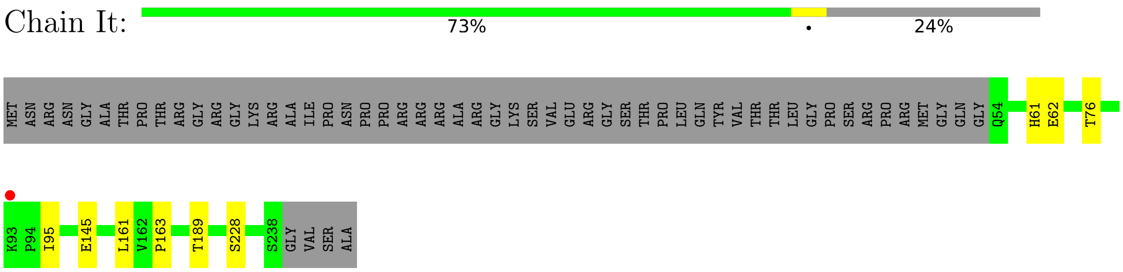


- Molecule 1: Capsid protein

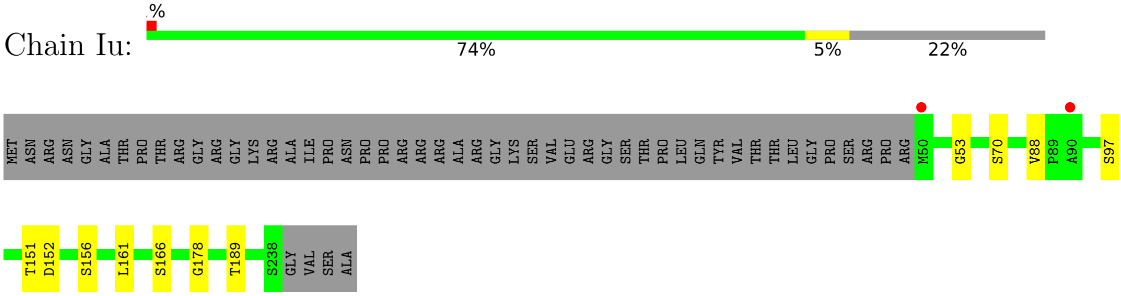
Chain Iq:



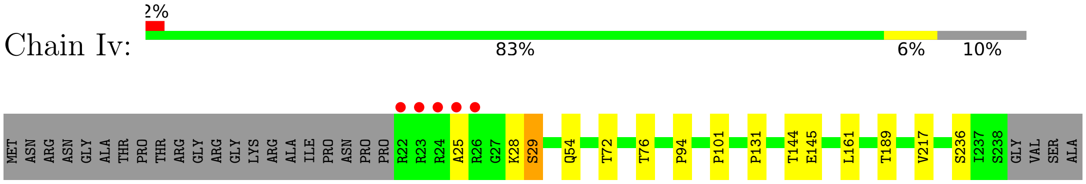
- Molecule 1: Capsid protein



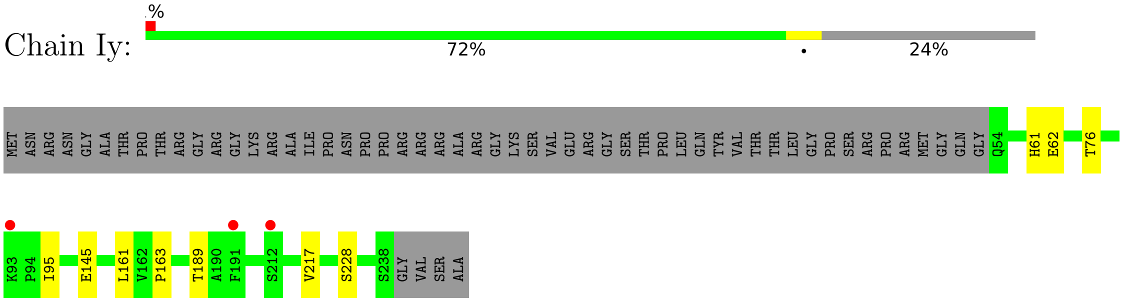
• Molecule 1: Capsid protein



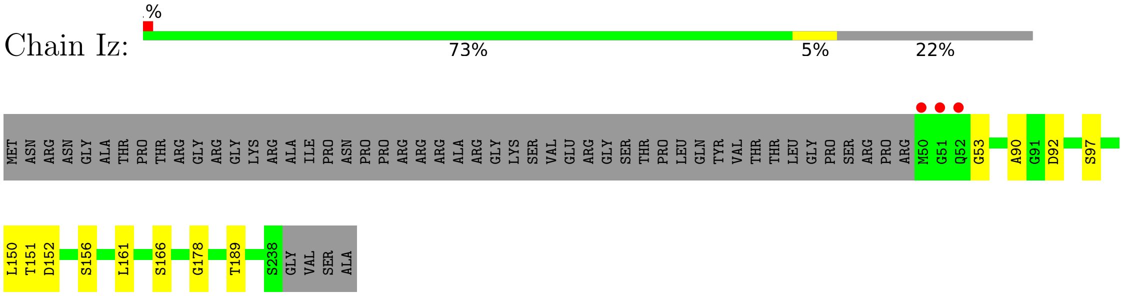
• Molecule 1: Capsid protein



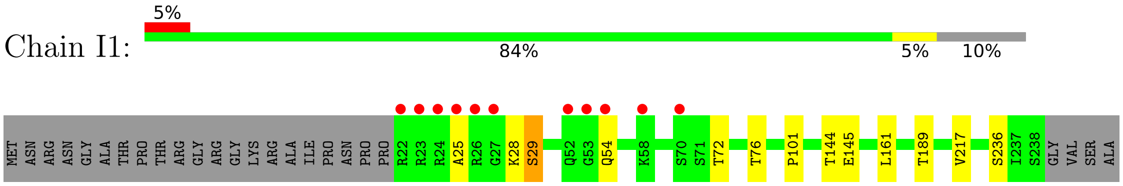
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



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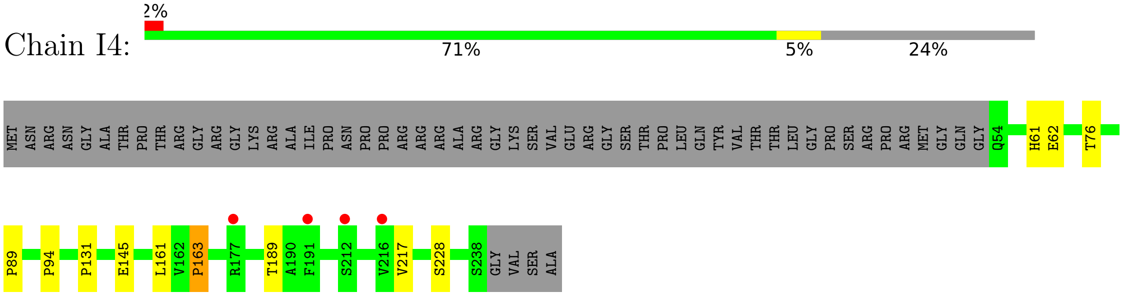

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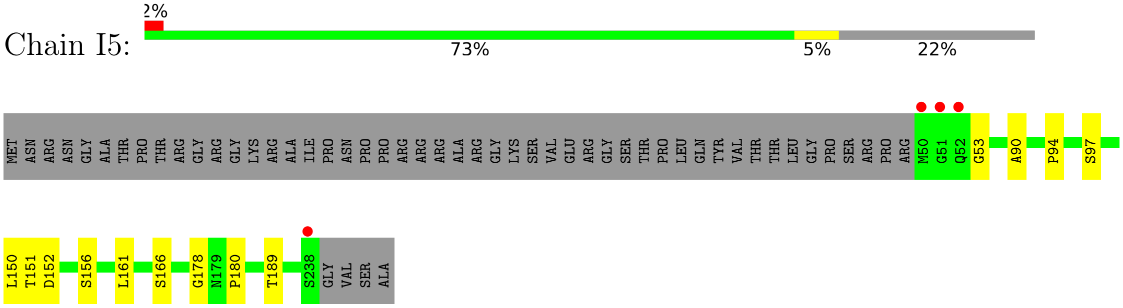

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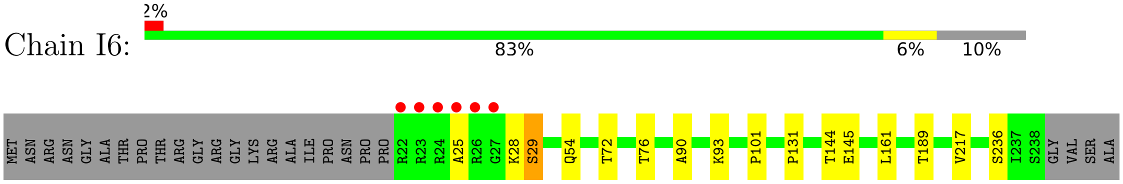

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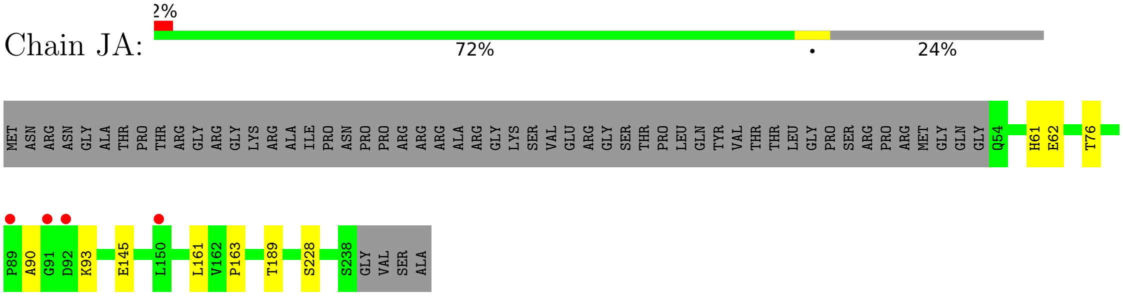
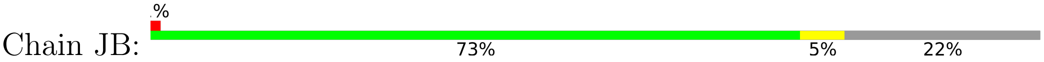
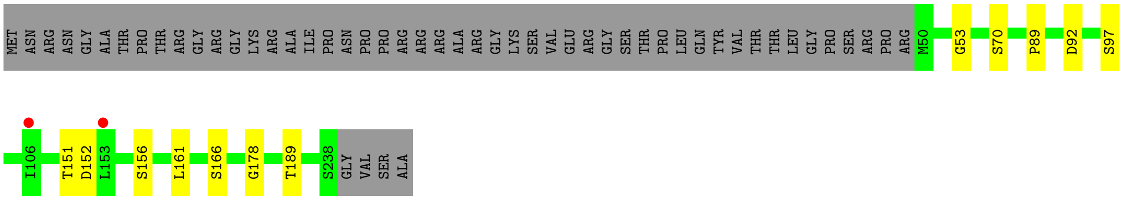


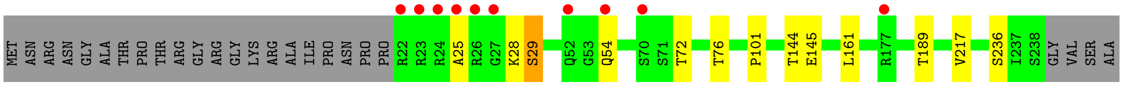
• Molecule 1: Capsid protein





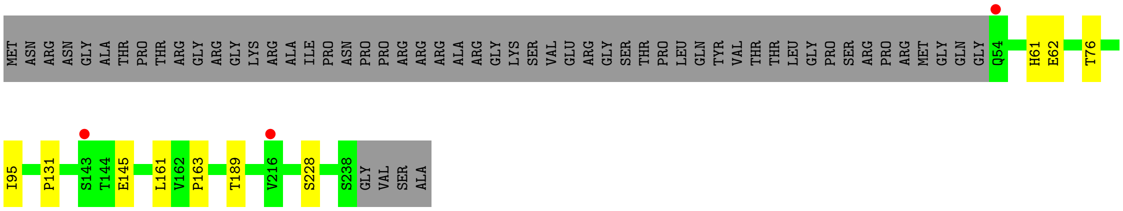
- Molecule 1: Capsid protein

Chain JC:



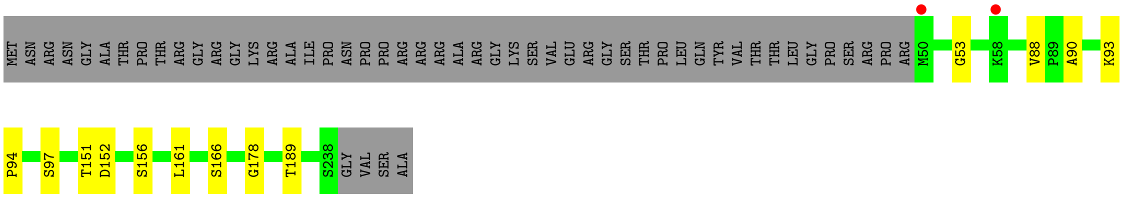
- Molecule 1: Capsid protein

Chain JF:



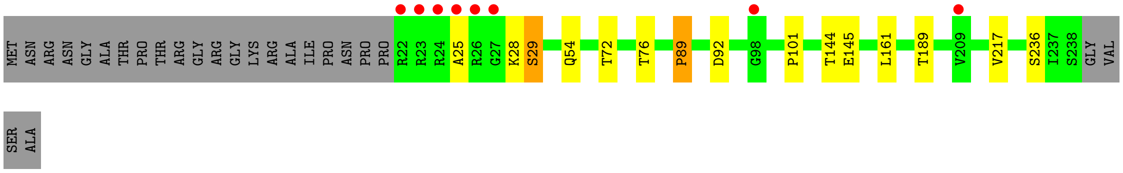
- Molecule 1: Capsid protein

Chain JG:



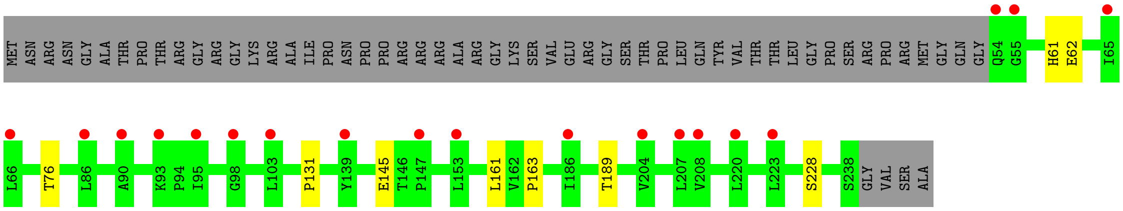
- Molecule 1: Capsid protein

Chain JH:

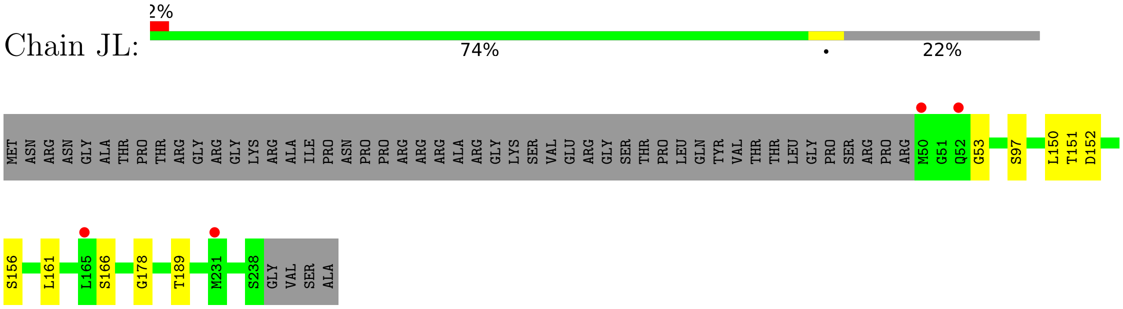


- Molecule 1: Capsid protein

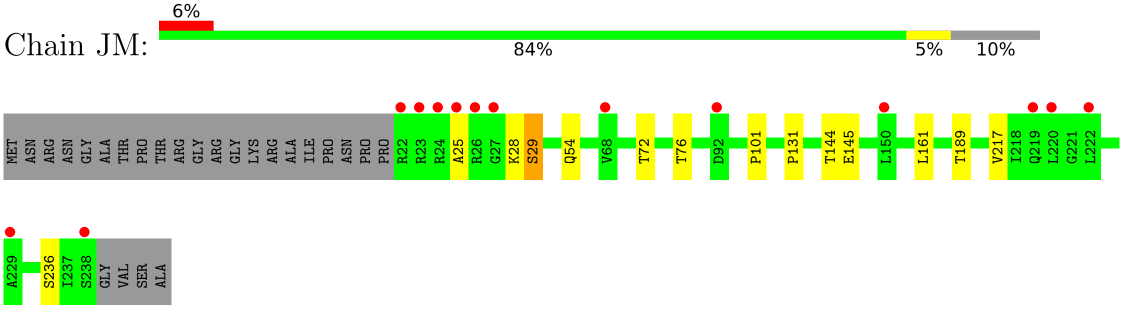
Chain JK:



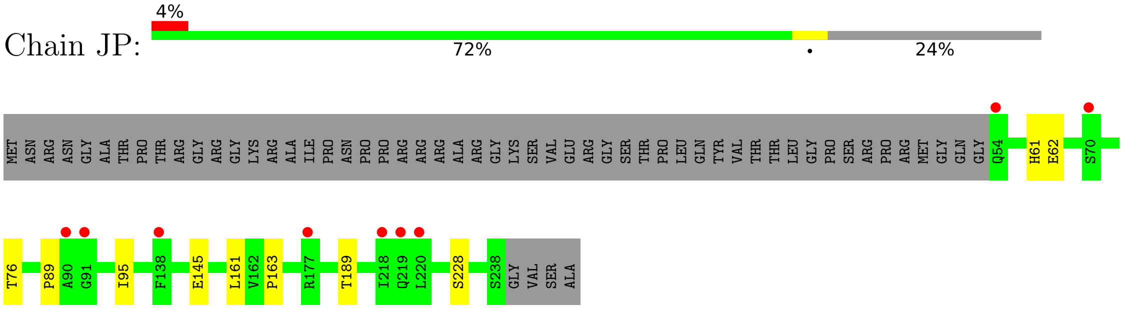
- Molecule 1: Capsid protein



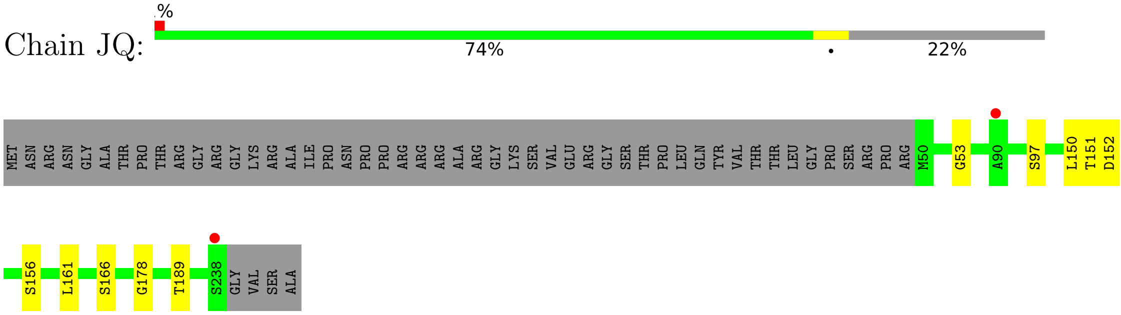
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

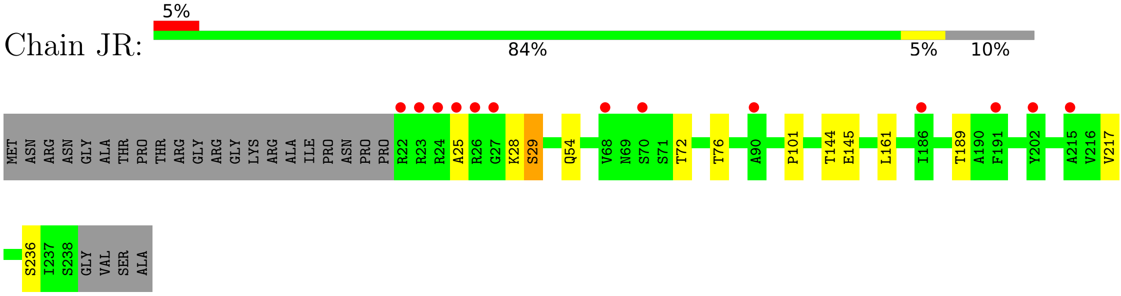


- Molecule 1: Capsid protein



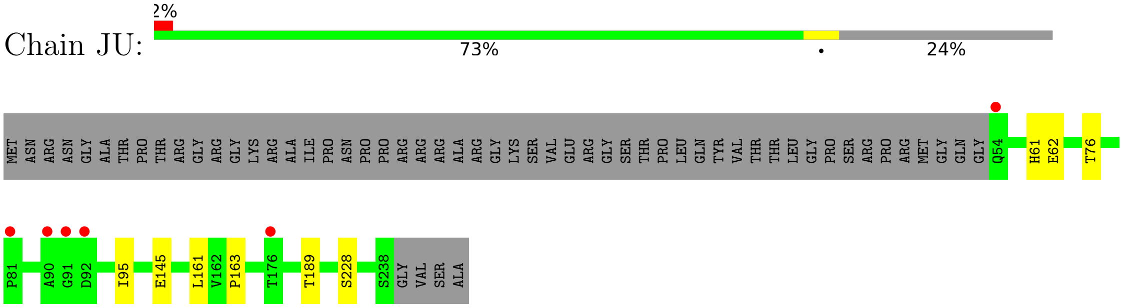
- Molecule 1: Capsid protein

Chain JR:



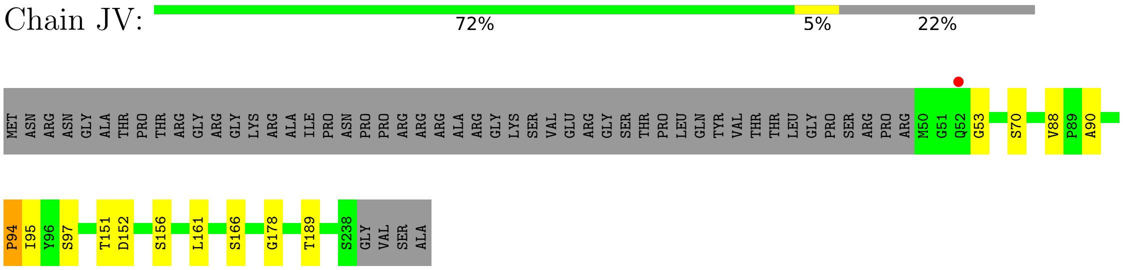
- Molecule 1: Capsid protein

Chain JU:



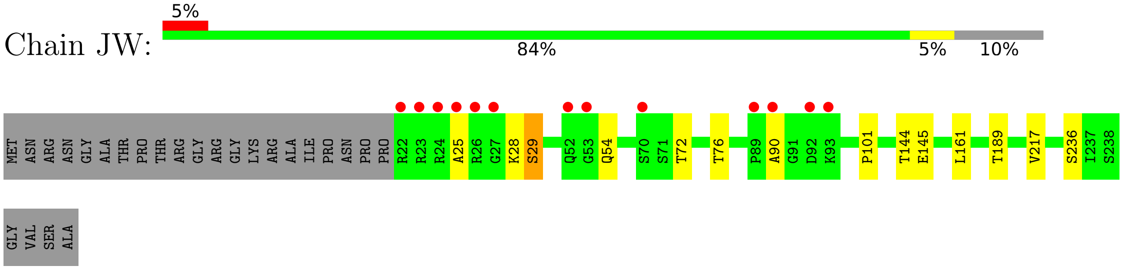
- Molecule 1: Capsid protein

Chain JV:



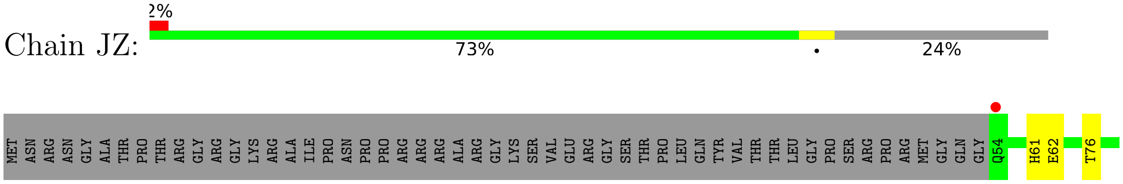
- Molecule 1: Capsid protein

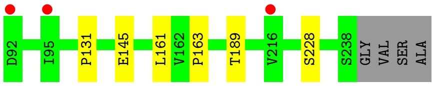
Chain JW:



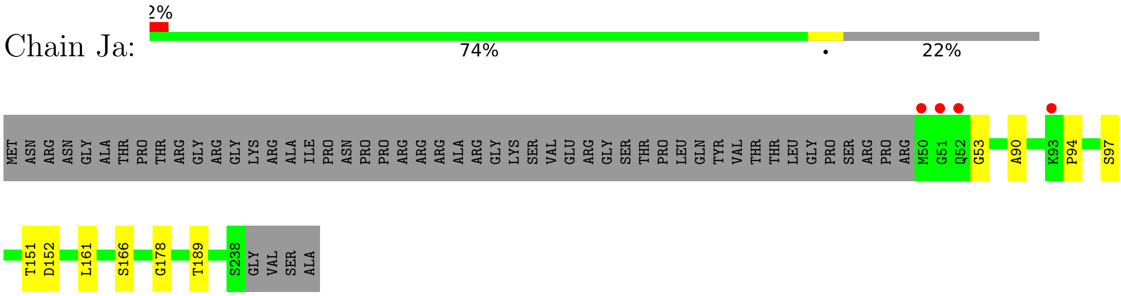
- Molecule 1: Capsid protein

Chain JZ:

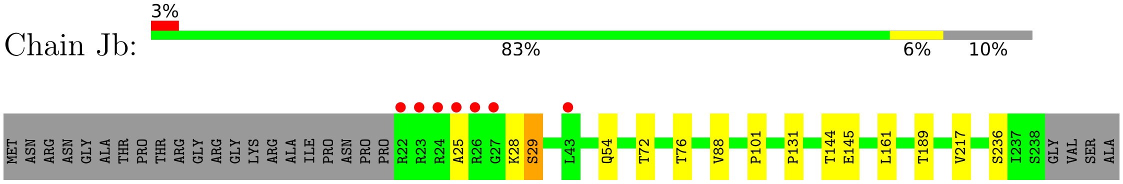




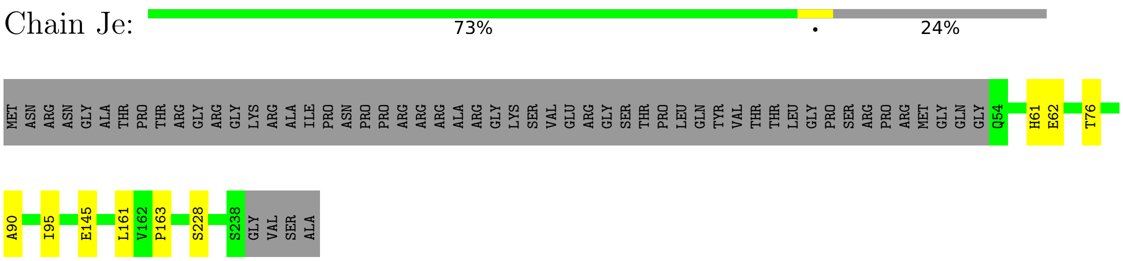
- Molecule 1: Capsid protein



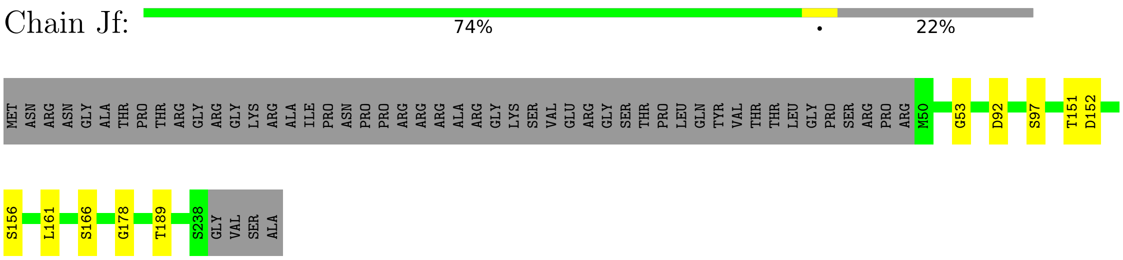
- Molecule 1: Capsid protein



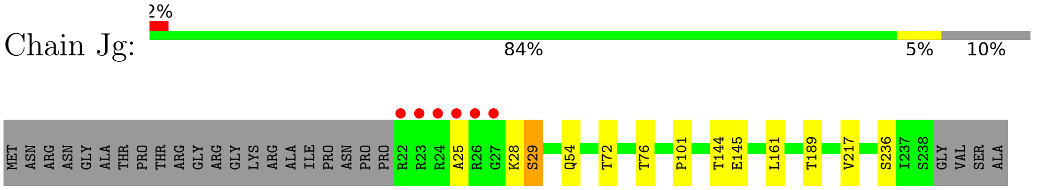
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

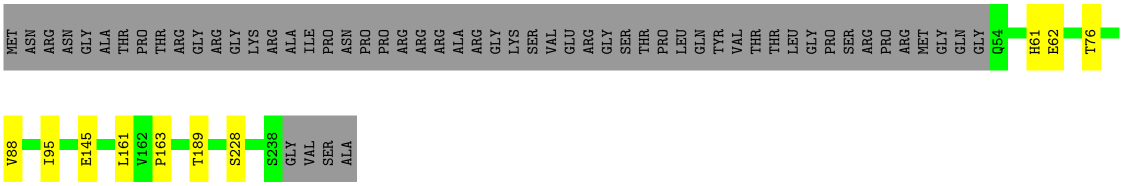


- Molecule 1: Capsid protein



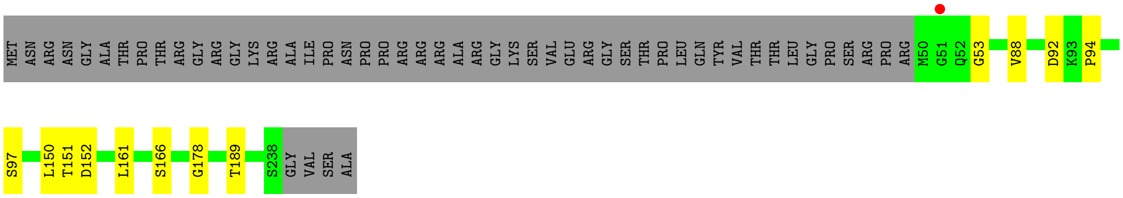
- Molecule 1: Capsid protein

Chain Jj:



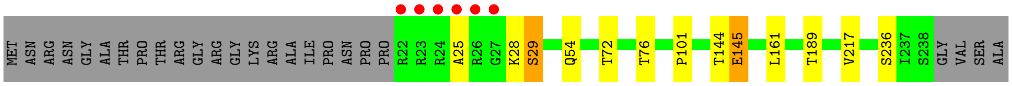
- Molecule 1: Capsid protein

Chain Jk:



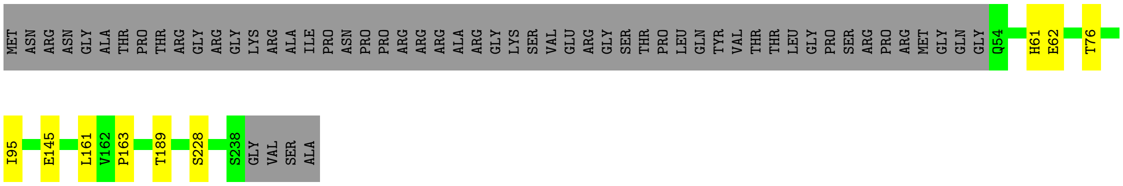
- Molecule 1: Capsid protein

Chain Jl:



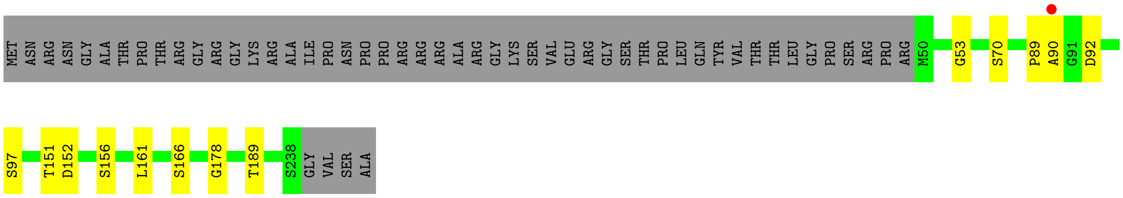
- Molecule 1: Capsid protein

Chain Jo:



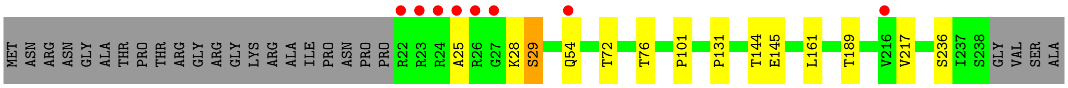
- Molecule 1: Capsid protein

Chain Jp:



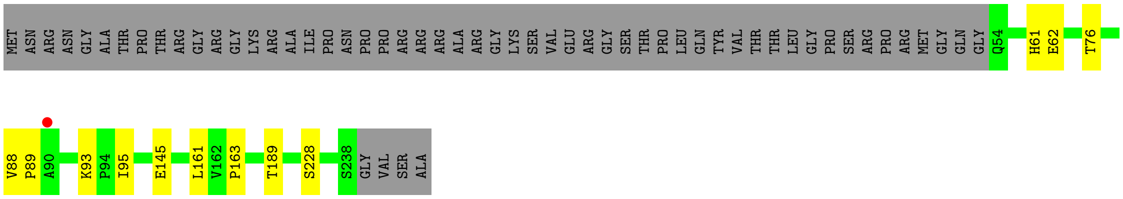
- Molecule 1: Capsid protein

Chain Jq:



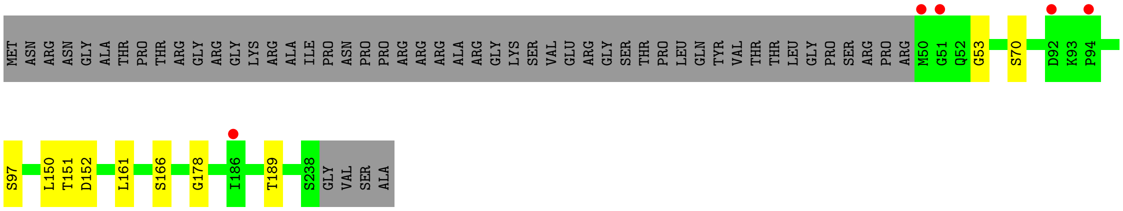
- Molecule 1: Capsid protein

Chain Jt:



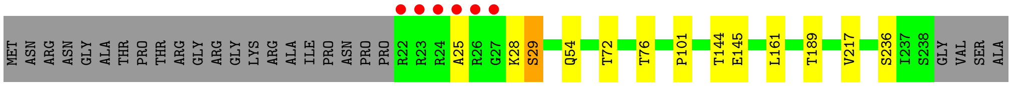
- Molecule 1: Capsid protein

Chain Ju:



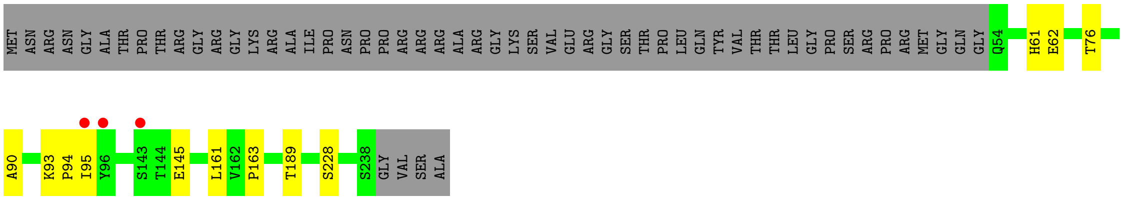
- Molecule 1: Capsid protein

Chain Jv:



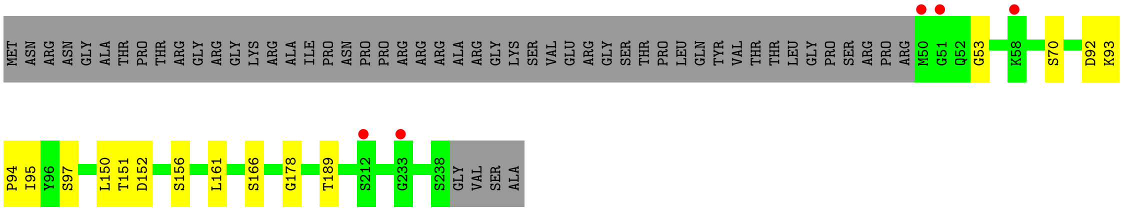
- Molecule 1: Capsid protein

Chain Jy:



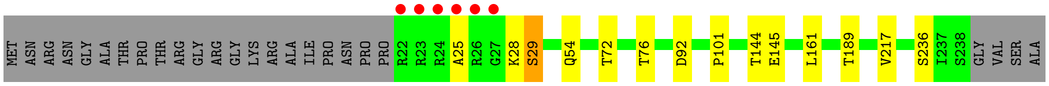
- Molecule 1: Capsid protein

Chain Jz:



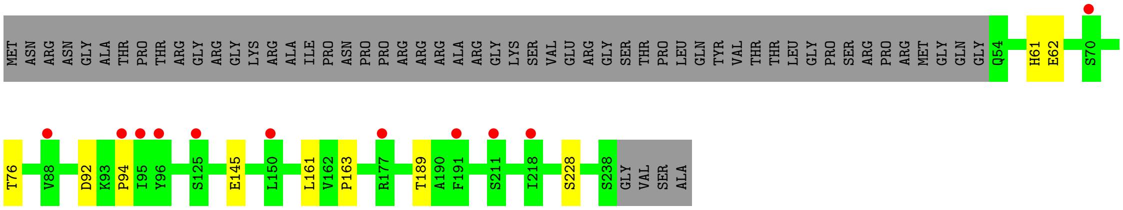
- Molecule 1: Capsid protein

Chain J1:



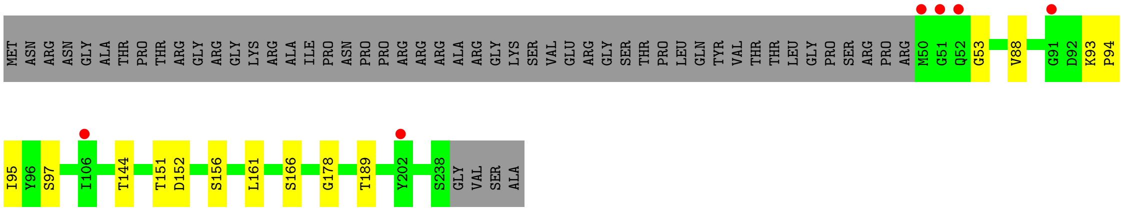
- Molecule 1: Capsid protein

Chain J4:



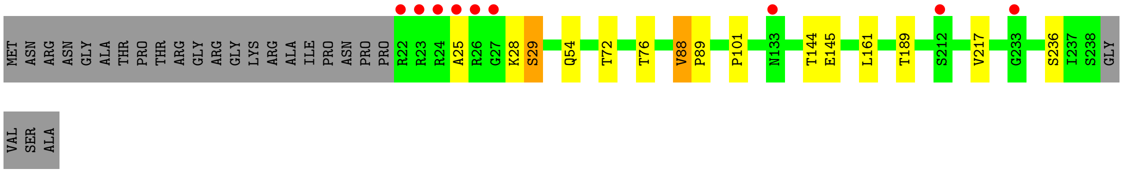
- Molecule 1: Capsid protein

Chain J5:



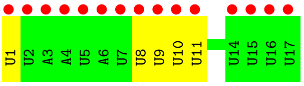
- Molecule 1: Capsid protein

Chain J6:



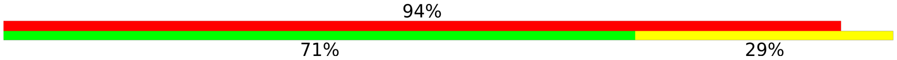
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

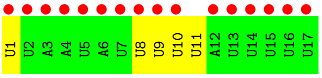
Chain AD:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

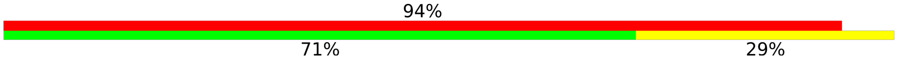
Chain AI:

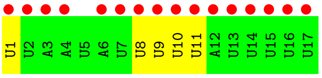




- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

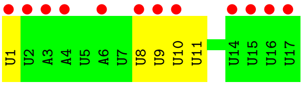
Chain AN:





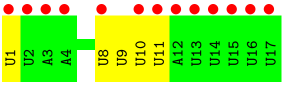
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain AS:



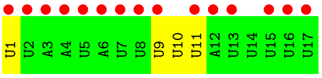
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain AX:



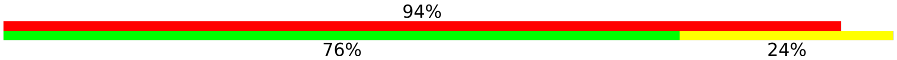
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

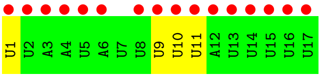
Chain Ac:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

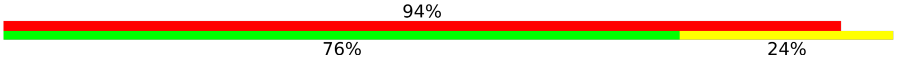
Chain Ah:

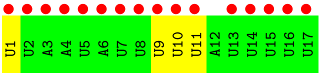




- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

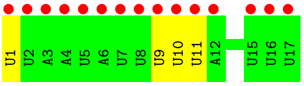
Chain Am:





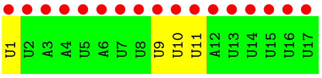
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain Ar:



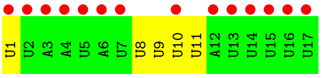
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain Aw:



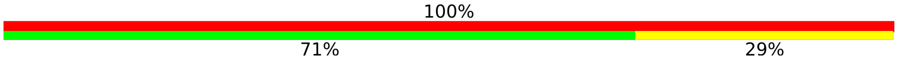
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

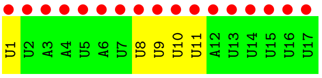
Chain A2:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

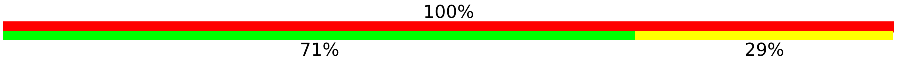
Chain A7:

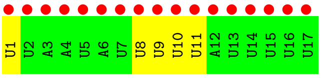




- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

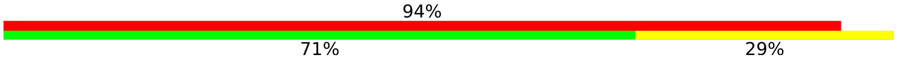
Chain BD:

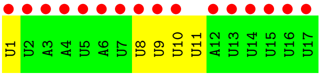




- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

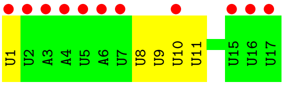
Chain BI:





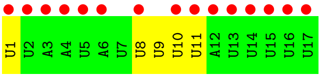
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain BN:



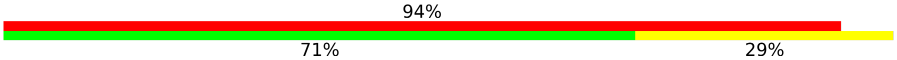
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

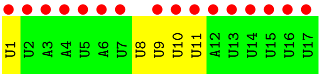
Chain BS:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

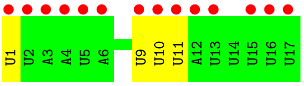
Chain BX:





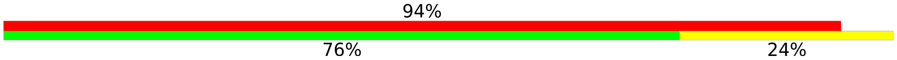
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

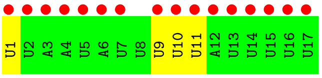
Chain Bc:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

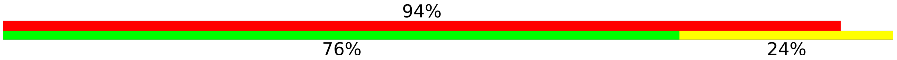
Chain Bh:

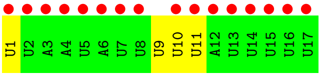




- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

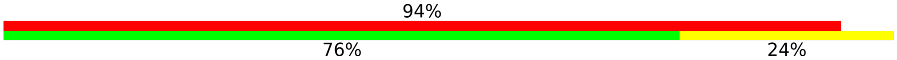
Chain Bm:

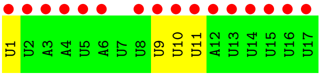




- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

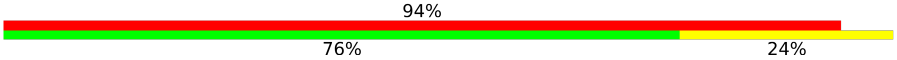
Chain Br:

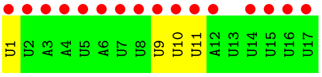




- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

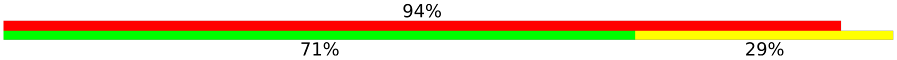
Chain Bw:

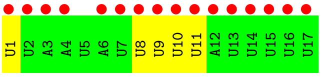




- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

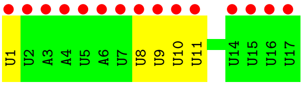
Chain B2:





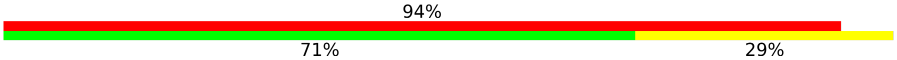
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

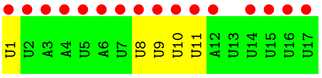
Chain B7:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

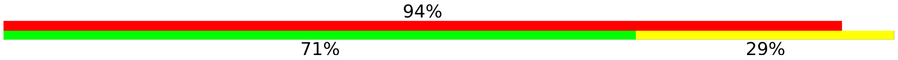
Chain CD:

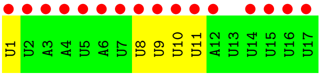




- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

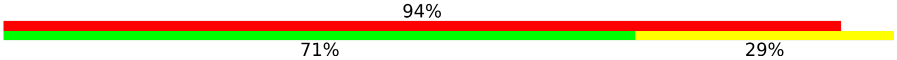
Chain CI:

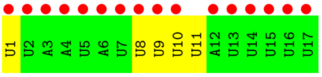




- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

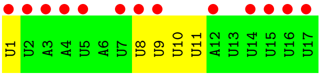
Chain CN:





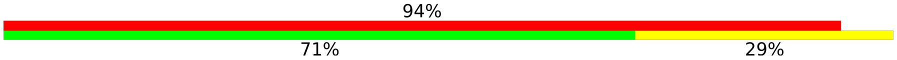
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

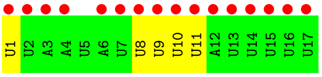
Chain CS:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

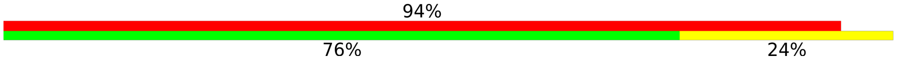
Chain CX:

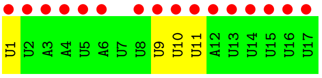




- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

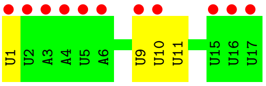
Chain Cc:





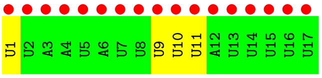
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain Ch:



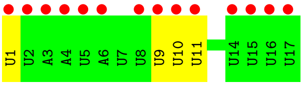
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain Cm:



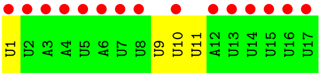
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain Cr:



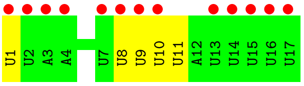
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain Cw:



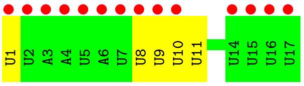
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain C2:



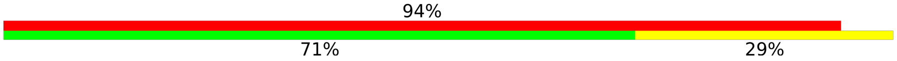
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

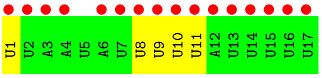
Chain C7:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

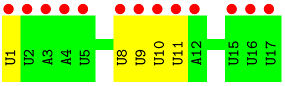
Chain DD:





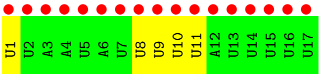
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain DI:



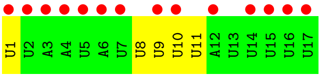
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain DN:



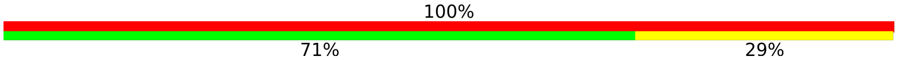
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

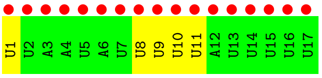
Chain DS:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

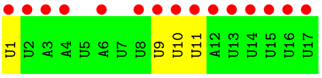
Chain DX:





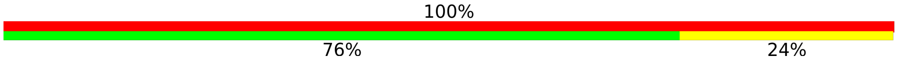
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

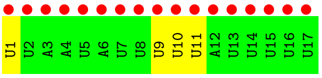
Chain Dc:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

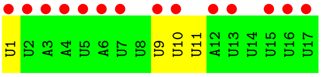
Chain Dh:





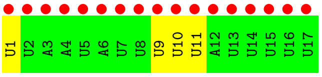
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3 ’

Chain Dm:



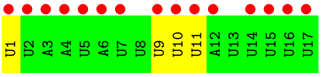
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3 ’

Chain Dr:



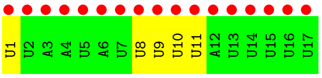
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3 ’

Chain Dw:



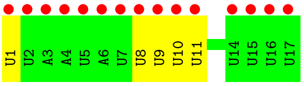
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3 ’

Chain D2:



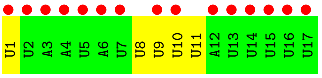
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3 ’

Chain D7:



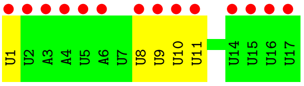
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3 ’

Chain ED:



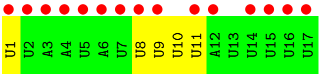
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain EI:



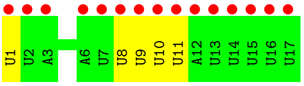
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain EN:



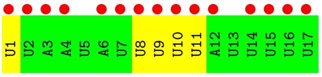
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain ES:



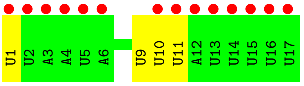
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain EX:



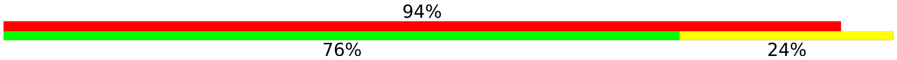
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

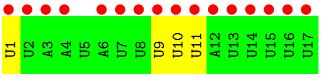
Chain Ec:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

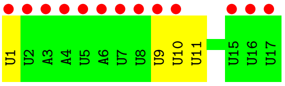
Chain Eh:





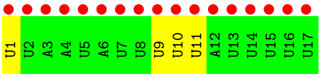
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain Em:



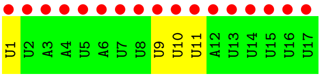
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain Er:



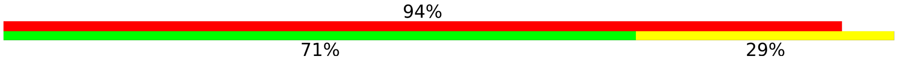
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

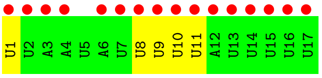
Chain Ew:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

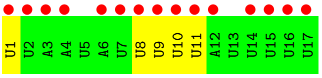
Chain E2:





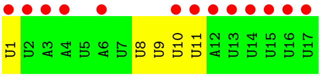
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain E7:



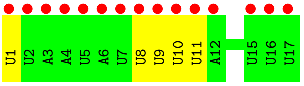
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain FD:



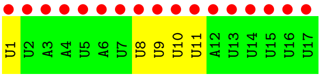
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain FI:



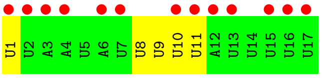
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain FN:



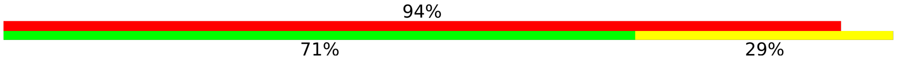
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

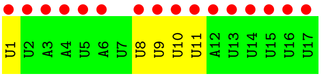
Chain FS:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

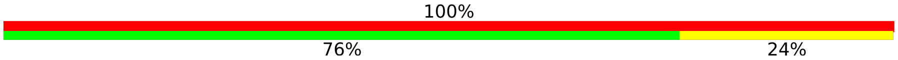
Chain FX:

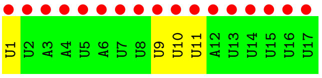




- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

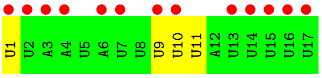
Chain Fc:





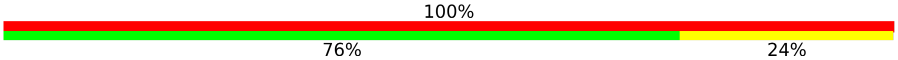
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

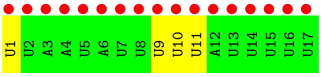
Chain Fh:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

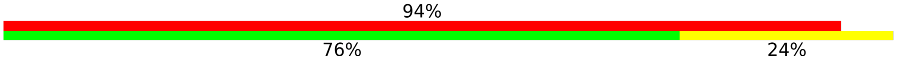
Chain Fm:

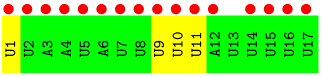




- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

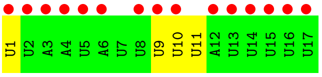
Chain Fr:





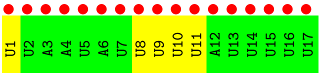
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain Fw:



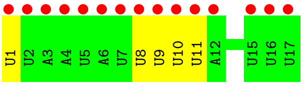
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain F2:



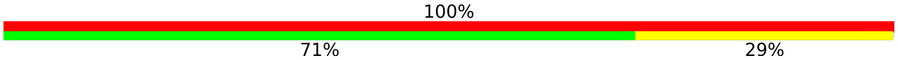
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

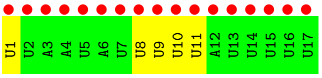
Chain F7:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

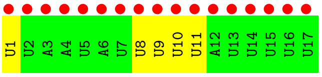
Chain GD:





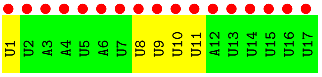
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain GI:



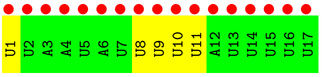
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain GN:



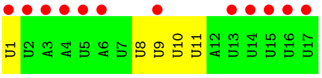
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain GS:



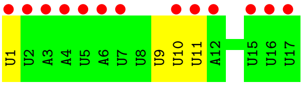
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain GX:



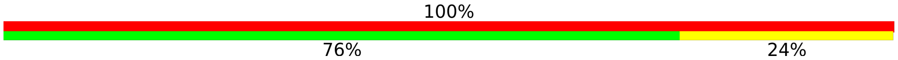
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

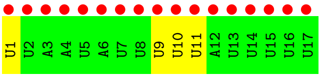
Chain Gc:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain Gh:





- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3
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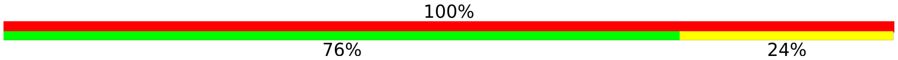
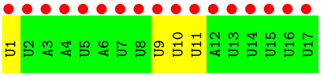
Chain Gm:





- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3
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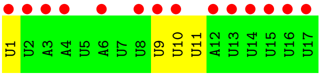
Chain Gr:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3
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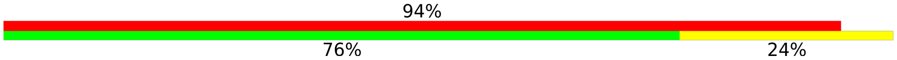
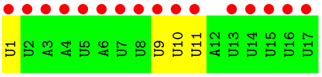
Chain Gw:





- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3
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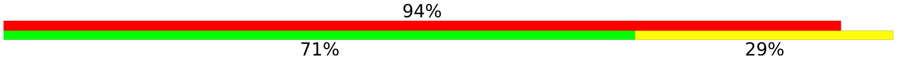
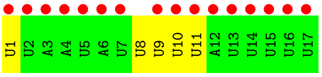
Chain G2:





- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3
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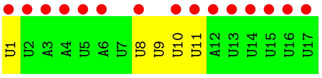
Chain G7:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3
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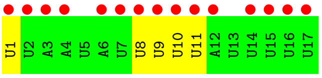
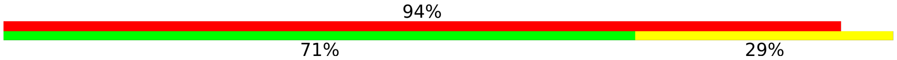
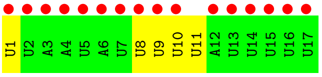
Chain HD:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3 ’

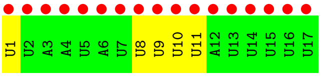
Chain HI:





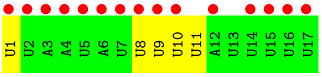
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3 ’

Chain HN:



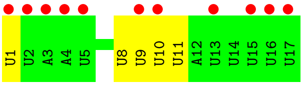
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3 ’

Chain HS:



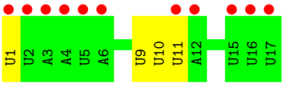
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3 ’

Chain HX:



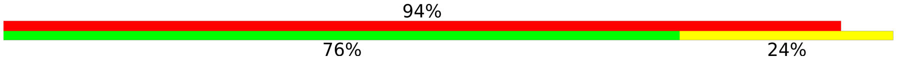
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3 ’

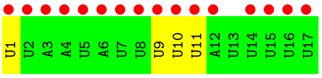
Chain Hc:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3 ’

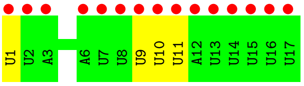
Chain Hh:





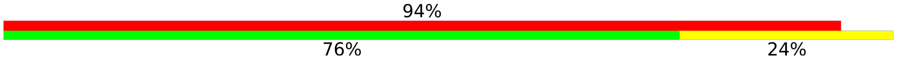
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

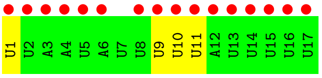
Chain Hm:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

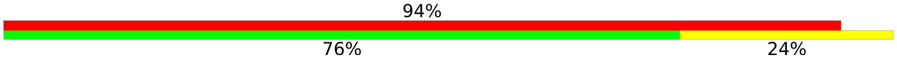
Chain Hr:

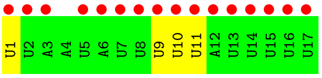




- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

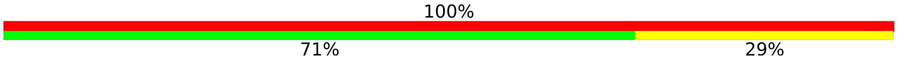
Chain Hw:

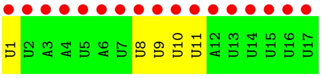




- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

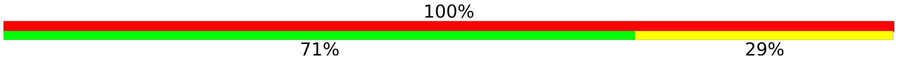
Chain H2:

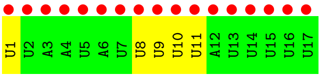




- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain H7:





- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

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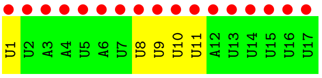
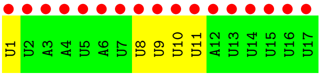


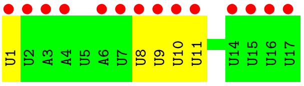
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain II:



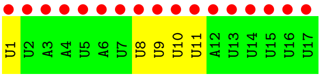
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain IN:



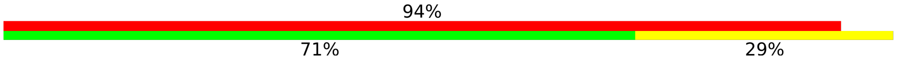
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

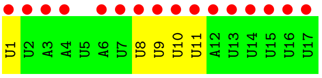
Chain IS:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

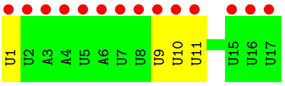
Chain IX:





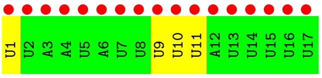
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain Ic:



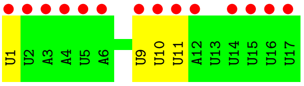
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain Ih:



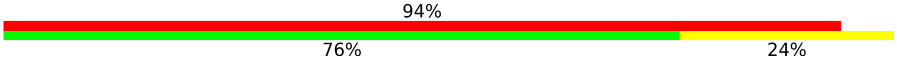
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

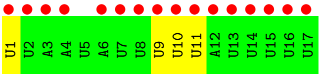
Chain Im:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

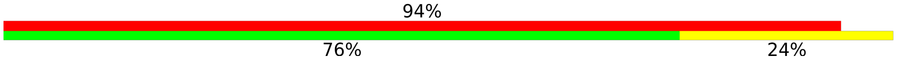
Chain Ir:

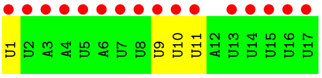




- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

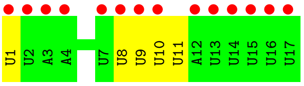
Chain Iw:





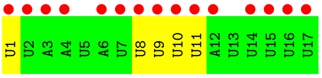
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain I2:



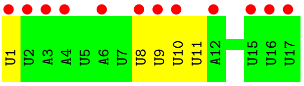
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain I7:



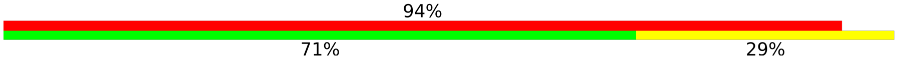
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

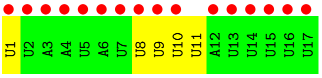
Chain JD:



- Molecule 2: 5'-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3'

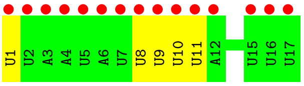
Chain JI:





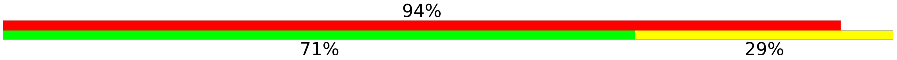
- Molecule 2: 5'-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3'

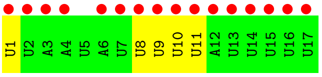
Chain JN:



- Molecule 2: 5'-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3'

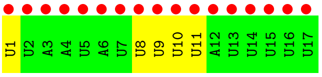
Chain JS:





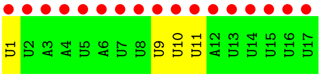
- Molecule 2: 5'-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3'

Chain JX:



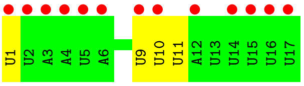
- Molecule 2: 5'-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3'

Chain Jc:



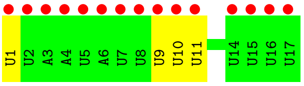
- Molecule 2: 5'-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3'

Chain Jh:



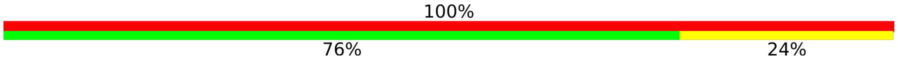
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

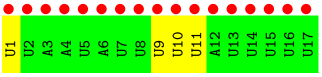
Chain Jm:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

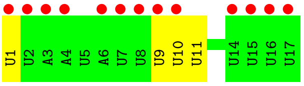
Chain Jr:





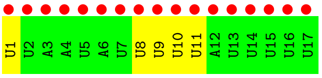
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain Jw:



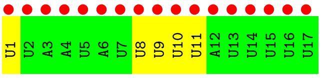
- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain J2:



- Molecule 2: 5’-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3’

Chain J7:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	411.74Å 403.90Å 412.46Å 90.00° 89.65° 90.00°	Depositor
Resolution (Å)	50.01 – 2.90 50.01 – 2.90	Depositor EDS
% Data completeness (in resolution range)	74.9 (50.01-2.90) 74.9 (50.01-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.91Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.251 , 0.285 0.235 , 0.267	Depositor DCC
R_{free} test set	221945 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 51.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.025 for -l,k,h 0.034 for -h,-l,-k 0.024 for -h,l,k 0.044 for -k,-h,-l 0.024 for k,h,-l 0.017 for -l,-h,k 0.030 for -k,l,-h 0.038 for l,h,k 0.027 for k,-l,-h 0.035 for h,-k,-l 0.030 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	588120	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A1	0.46	1/1710 (0.1%)	0.72	0/2323
1	A4	0.45	0/1458	0.72	0/1986
1	A5	0.41	0/1483	0.67	0/2018
1	A6	0.46	2/1710 (0.1%)	0.71	0/2323
1	AA	0.48	1/1458 (0.1%)	0.74	1/1986 (0.1%)
1	AB	0.43	0/1483	0.71	0/2018
1	AC	0.48	1/1710 (0.1%)	0.72	0/2323
1	AF	0.51	1/1458 (0.1%)	0.75	0/1986
1	AG	0.47	0/1483	0.71	0/2018
1	AH	0.47	0/1710	0.72	0/2323
1	AK	0.49	1/1458 (0.1%)	0.74	0/1986
1	AL	0.46	0/1483	0.69	0/2018
1	AM	0.48	1/1710 (0.1%)	0.73	0/2323
1	AP	0.49	1/1458 (0.1%)	0.75	0/1986
1	AQ	0.43	0/1483	0.69	0/2018
1	AR	0.48	2/1710 (0.1%)	0.72	0/2323
1	AU	0.45	1/1458 (0.1%)	0.71	0/1986
1	AV	0.39	0/1483	0.67	0/2018
1	AW	0.45	0/1710	0.70	0/2323
1	AZ	0.52	2/1458 (0.1%)	0.76	0/1986
1	Aa	0.45	0/1483	0.70	0/2018
1	Ab	0.49	2/1710 (0.1%)	0.73	0/2323
1	Ae	0.50	1/1458 (0.1%)	0.76	0/1986
1	Af	0.46	0/1483	0.70	0/2018
1	Ag	0.51	2/1710 (0.1%)	0.74	0/2323
1	Aj	0.47	1/1458 (0.1%)	0.73	0/1986
1	Ak	0.44	0/1483	0.70	0/2018
1	Al	0.51	2/1710 (0.1%)	0.73	0/2323
1	Ao	0.51	1/1458 (0.1%)	0.76	0/1986
1	Ap	0.49	0/1483	0.70	0/2018
1	Aq	0.51	1/1710 (0.1%)	0.74	0/2323
1	At	0.51	2/1458 (0.1%)	0.76	0/1986

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	Au	0.45	0/1483	0.69	0/2018
1	Av	0.51	1/1710 (0.1%)	0.73	0/2323
1	Ay	0.46	1/1458 (0.1%)	0.72	0/1986
1	Az	0.40	0/1483	0.67	0/2018
1	B1	0.49	1/1710 (0.1%)	0.72	0/2323
1	B4	0.44	1/1458 (0.1%)	0.72	0/1986
1	B5	0.42	0/1483	0.67	0/2018
1	B6	0.45	0/1710	0.71	0/2323
1	BA	0.49	1/1458 (0.1%)	0.74	0/1986
1	BB	0.46	0/1483	0.69	0/2018
1	BC	0.49	0/1710	0.72	0/2323
1	BF	0.48	1/1458 (0.1%)	0.75	0/1986
1	BG	0.45	0/1483	0.71	0/2018
1	BH	0.50	1/1710 (0.1%)	0.74	0/2323
1	BK	0.53	1/1458 (0.1%)	0.76	0/1986
1	BL	0.45	0/1483	0.69	0/2018
1	BM	0.49	1/1710 (0.1%)	0.72	0/2323
1	BP	0.47	2/1458 (0.1%)	0.73	0/1986
1	BQ	0.42	0/1483	0.68	0/2018
1	BR	0.48	1/1710 (0.1%)	0.72	0/2323
1	BU	0.44	1/1458 (0.1%)	0.71	0/1986
1	BV	0.42	0/1483	0.67	0/2018
1	BW	0.44	1/1710 (0.1%)	0.71	0/2323
1	BZ	0.50	1/1458 (0.1%)	0.75	0/1986
1	Ba	0.43	0/1483	0.68	0/2018
1	Bb	0.49	2/1710 (0.1%)	0.73	0/2323
1	Be	0.50	1/1458 (0.1%)	0.74	0/1986
1	Bf	0.45	0/1483	0.71	0/2018
1	Bg	0.51	2/1710 (0.1%)	0.73	0/2323
1	Bj	0.50	1/1458 (0.1%)	0.74	0/1986
1	Bk	0.45	0/1483	0.70	0/2018
1	Bl	0.49	2/1710 (0.1%)	0.72	0/2323
1	Bo	0.49	1/1458 (0.1%)	0.74	0/1986
1	Bp	0.44	0/1483	0.70	0/2018
1	Bq	0.48	2/1710 (0.1%)	0.72	0/2323
1	Bt	0.47	1/1458 (0.1%)	0.73	0/1986
1	Bu	0.43	0/1483	0.69	0/2018
1	Bv	0.46	1/1710 (0.1%)	0.72	0/2323
1	By	0.51	2/1458 (0.1%)	0.74	0/1986
1	Bz	0.46	0/1483	0.71	0/2018
1	C1	0.50	2/1710 (0.1%)	0.73	0/2323
1	C4	0.48	2/1458 (0.1%)	0.73	0/1986
1	C5	0.43	0/1483	0.68	0/2018

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	C6	0.47	0/1710	0.71	0/2323
1	CA	0.49	1/1458 (0.1%)	0.75	0/1986
1	CB	0.45	0/1483	0.69	0/2018
1	CC	0.47	1/1710 (0.1%)	0.73	0/2323
1	CF	0.56	2/1458 (0.1%)	0.77	0/1986
1	CG	0.47	0/1483	0.70	0/2018
1	CH	0.52	0/1710	0.75	0/2323
1	CK	0.50	1/1458 (0.1%)	0.74	0/1986
1	CL	0.46	0/1483	0.71	0/2018
1	CM	0.48	0/1710	0.73	0/2323
1	CP	0.47	2/1458 (0.1%)	0.73	0/1986
1	CQ	0.42	0/1483	0.68	0/2018
1	CR	0.46	0/1710	0.71	0/2323
1	CU	0.49	1/1458 (0.1%)	0.73	0/1986
1	CV	0.44	0/1483	0.69	0/2018
1	CW	0.47	0/1710	0.73	0/2323
1	CZ	0.45	1/1458 (0.1%)	0.73	0/1986
1	Ca	0.42	0/1483	0.68	0/2018
1	Cb	0.47	0/1710	0.71	0/2323
1	Ce	0.51	1/1458 (0.1%)	0.74	0/1986
1	Cf	0.43	0/1483	0.69	0/2018
1	Cg	0.47	2/1710 (0.1%)	0.71	0/2323
1	Cj	0.48	1/1458 (0.1%)	0.75	0/1986
1	Ck	0.45	0/1483	0.70	0/2018
1	Cl	0.50	2/1710 (0.1%)	0.74	0/2323
1	Co	0.49	1/1458 (0.1%)	0.75	0/1986
1	Cp	0.43	0/1483	0.68	0/2018
1	Cq	0.49	2/1710 (0.1%)	0.72	0/2323
1	Ct	0.49	1/1458 (0.1%)	0.74	0/1986
1	Cu	0.45	0/1483	0.69	0/2018
1	Cv	0.49	2/1710 (0.1%)	0.73	0/2323
1	Cy	0.52	2/1458 (0.1%)	0.75	0/1986
1	Cz	0.47	0/1483	0.70	0/2018
1	D1	0.51	2/1710 (0.1%)	0.75	0/2323
1	D4	0.51	1/1458 (0.1%)	0.75	0/1986
1	D5	0.48	0/1483	0.71	0/2018
1	D6	0.51	1/1710 (0.1%)	0.74	0/2323
1	DA	0.49	1/1458 (0.1%)	0.75	0/1986
1	DB	0.46	0/1483	0.70	0/2018
1	DC	0.48	1/1710 (0.1%)	0.73	0/2323
1	DF	0.49	2/1458 (0.1%)	0.75	0/1986
1	DG	0.42	0/1483	0.68	0/2018
1	DH	0.48	1/1710 (0.1%)	0.71	0/2323

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	DK	0.50	2/1458 (0.1%)	0.75	0/1986
1	DL	0.47	0/1483	0.70	0/2018
1	DM	0.50	0/1710	0.73	0/2323
1	DP	0.44	0/1458	0.72	0/1986
1	DQ	0.42	0/1483	0.69	0/2018
1	DR	0.48	0/1710	0.72	0/2323
1	DU	0.46	2/1458 (0.1%)	0.73	0/1986
1	DV	0.41	0/1483	0.68	0/2018
1	DW	0.45	1/1710 (0.1%)	0.71	0/2323
1	DZ	0.50	1/1458 (0.1%)	0.75	0/1986
1	Da	0.47	0/1483	0.71	0/2018
1	Db	0.50	1/1710 (0.1%)	0.74	0/2323
1	De	0.46	1/1458 (0.1%)	0.72	0/1986
1	Df	0.40	0/1483	0.68	0/2018
1	Dg	0.44	0/1710	0.70	0/2323
1	Dj	0.51	2/1458 (0.1%)	0.75	0/1986
1	Dk	0.46	0/1483	0.70	0/2018
1	Dl	0.49	1/1710 (0.1%)	0.73	0/2323
1	Do	0.47	1/1458 (0.1%)	0.71	0/1986
1	Dp	0.41	0/1483	0.67	0/2018
1	Dq	0.45	0/1710	0.70	0/2323
1	Dt	0.51	1/1458 (0.1%)	0.74	0/1986
1	Du	0.44	0/1483	0.70	0/2018
1	Dv	0.48	1/1710 (0.1%)	0.73	0/2323
1	Dy	0.52	2/1458 (0.1%)	0.77	0/1986
1	Dz	0.46	0/1483	0.72	0/2018
1	E1	0.50	0/1710	0.73	0/2323
1	E4	0.52	2/1458 (0.1%)	0.77	0/1986
1	E5	0.47	0/1483	0.70	0/2018
1	E6	0.49	0/1710	0.72	0/2323
1	EA	0.50	2/1458 (0.1%)	0.74	0/1986
1	EB	0.47	0/1483	0.70	0/2018
1	EC	0.49	0/1710	0.74	0/2323
1	EF	0.47	1/1458 (0.1%)	0.73	0/1986
1	EG	0.40	0/1483	0.68	0/2018
1	EH	0.46	0/1710	0.70	0/2323
1	EK	0.46	1/1458 (0.1%)	0.73	0/1986
1	EL	0.42	0/1483	0.69	0/2018
1	EM	0.48	2/1710 (0.1%)	0.72	0/2323
1	EP	0.51	2/1458 (0.1%)	0.75	0/1986
1	EQ	0.49	0/1483	0.71	0/2018
1	ER	0.48	0/1710	0.72	0/2323
1	EU	0.47	1/1458 (0.1%)	0.74	0/1986

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	EV	0.46	0/1483	0.69	0/2018
1	EW	0.49	0/1710	0.72	0/2323
1	EZ	0.46	1/1458 (0.1%)	0.73	0/1986
1	Ea	0.43	0/1483	0.70	0/2018
1	Eb	0.49	1/1710 (0.1%)	0.73	0/2323
1	Ee	0.48	2/1458 (0.1%)	0.72	0/1986
1	Ef	0.42	0/1483	0.68	0/2018
1	Eg	0.45	0/1710	0.70	0/2323
1	Ej	0.46	1/1458 (0.1%)	0.72	0/1986
1	Ek	0.39	0/1483	0.66	0/2018
1	El	0.44	1/1710 (0.1%)	0.70	0/2323
1	Eo	0.46	1/1458 (0.1%)	0.71	0/1986
1	Ep	0.42	0/1483	0.68	0/2018
1	Eq	0.45	0/1710	0.71	0/2323
1	Et	0.51	2/1458 (0.1%)	0.75	0/1986
1	Eu	0.47	0/1483	0.71	0/2018
1	Ev	0.51	2/1710 (0.1%)	0.73	0/2323
1	Ey	0.49	1/1458 (0.1%)	0.74	0/1986
1	Ez	0.44	0/1483	0.69	0/2018
1	F1	0.39	0/1710	0.64	0/2323
1	F4	0.48	0/1458	0.71	0/1986
1	F5	0.43	0/1483	0.67	0/2018
1	F6	0.47	0/1710	0.67	0/2323
1	FA	0.46	1/1458 (0.1%)	0.69	0/1986
1	FB	0.43	0/1483	0.67	0/2018
1	FC	0.45	0/1710	0.67	0/2323
1	FF	0.46	0/1458	0.71	0/1986
1	FG	0.44	0/1483	0.68	0/2018
1	FH	0.46	2/1710 (0.1%)	0.68	0/2323
1	FK	0.45	0/1458	0.69	0/1986
1	FL	0.41	0/1483	0.66	0/2018
1	FM	0.48	1/1710 (0.1%)	0.69	0/2323
1	FP	0.48	0/1458	0.70	0/1986
1	FQ	0.44	0/1483	0.67	0/2018
1	FR	0.47	0/1710	0.70	0/2323
1	FU	0.45	0/1458	0.69	0/1986
1	FV	0.43	0/1483	0.66	0/2018
1	FW	0.48	0/1710	0.70	0/2323
1	FZ	0.40	0/1458	0.67	0/1986
1	Fa	0.37	0/1483	0.63	0/2018
1	Fb	0.40	0/1710	0.66	0/2323
1	Fe	0.40	0/1458	0.66	0/1986
1	Ff	0.36	0/1483	0.63	0/2018

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	Fg	0.39	0/1710	0.66	0/2323
1	Fj	0.46	0/1458	0.69	0/1986
1	Fk	0.42	0/1483	0.66	0/2018
1	Fl	0.44	0/1710	0.67	0/2323
1	Fo	0.46	1/1458 (0.1%)	0.70	0/1986
1	Fp	0.44	0/1483	0.68	0/2018
1	Fq	0.51	0/1710	0.71	0/2323
1	Ft	0.45	0/1458	0.70	0/1986
1	Fu	0.43	0/1483	0.66	0/2018
1	Fv	0.47	0/1710	0.69	0/2323
1	Fy	0.38	0/1458	0.65	0/1986
1	Fz	0.36	0/1483	0.63	0/2018
1	G1	0.43	0/1710	0.66	0/2323
1	G4	0.39	0/1458	0.66	0/1986
1	G5	0.38	0/1483	0.63	0/2018
1	G6	0.43	0/1710	0.67	0/2323
1	GA	0.47	0/1458	0.71	0/1986
1	GB	0.42	0/1483	0.66	0/2018
1	GC	0.47	1/1710 (0.1%)	0.68	0/2323
1	GF	0.47	0/1458	0.71	0/1986
1	GG	0.43	0/1483	0.67	0/2018
1	GH	0.46	0/1710	0.68	0/2323
1	GK	0.38	0/1458	0.66	0/1986
1	GL	0.36	0/1483	0.63	0/2018
1	GM	0.41	0/1710	0.65	0/2323
1	GP	0.47	0/1458	0.70	0/1986
1	GQ	0.46	0/1483	0.67	0/2018
1	GR	0.47	0/1710	0.70	0/2323
1	GU	0.44	0/1458	0.69	0/1986
1	GV	0.43	0/1483	0.67	0/2018
1	GW	0.47	0/1710	0.69	0/2323
1	GZ	0.44	0/1458	0.70	0/1986
1	Ga	0.42	0/1483	0.66	0/2018
1	Gb	0.45	0/1710	0.67	0/2323
1	Ge	0.47	0/1458	0.71	0/1986
1	Gf	0.46	0/1483	0.68	0/2018
1	Gg	0.46	0/1710	0.69	0/2323
1	Gj	0.42	0/1458	0.67	0/1986
1	Gk	0.39	0/1483	0.64	0/2018
1	Gl	0.42	0/1710	0.66	0/2323
1	Go	0.38	0/1458	0.66	0/1986
1	Gp	0.35	0/1483	0.62	0/2018
1	Gq	0.39	0/1710	0.65	0/2323

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	Gt	0.49	0/1458	0.72	0/1986
1	Gu	0.44	0/1483	0.67	0/2018
1	Gv	0.49	1/1710 (0.1%)	0.70	0/2323
1	Gy	0.43	0/1458	0.67	0/1986
1	Gz	0.38	0/1483	0.65	0/2018
1	H1	0.45	0/1710	0.68	0/2323
1	H4	0.38	0/1458	0.66	0/1986
1	H5	0.36	0/1483	0.64	0/2018
1	H6	0.39	0/1710	0.65	0/2323
1	HA	0.41	0/1458	0.68	0/1986
1	HB	0.38	0/1483	0.65	0/2018
1	HC	0.41	0/1710	0.66	0/2323
1	HF	0.43	0/1458	0.68	0/1986
1	HG	0.40	0/1483	0.66	0/2018
1	HH	0.43	0/1710	0.67	0/2323
1	HK	0.44	0/1458	0.69	0/1986
1	HL	0.44	0/1483	0.67	0/2018
1	HM	0.43	0/1710	0.67	0/2323
1	HP	0.45	0/1458	0.69	0/1986
1	HQ	0.46	0/1483	0.69	0/2018
1	HR	0.45	0/1710	0.68	0/2323
1	HU	0.45	0/1458	0.69	0/1986
1	HV	0.40	0/1483	0.65	0/2018
1	HW	0.43	0/1710	0.67	0/2323
1	HZ	0.44	0/1458	0.69	0/1986
1	Ha	0.40	0/1483	0.66	0/2018
1	Hb	0.43	0/1710	0.67	0/2323
1	He	0.40	0/1458	0.66	0/1986
1	Hf	0.37	0/1483	0.62	0/2018
1	Hg	0.40	0/1710	0.65	0/2323
1	Hj	0.39	0/1458	0.67	0/1986
1	Hk	0.37	0/1483	0.63	0/2018
1	Hl	0.41	0/1710	0.66	0/2323
1	Ho	0.43	0/1458	0.68	0/1986
1	Hp	0.40	0/1483	0.65	0/2018
1	Hq	0.43	0/1710	0.68	0/2323
1	Ht	0.47	0/1458	0.70	0/1986
1	Hu	0.42	0/1483	0.67	0/2018
1	Hv	0.49	0/1710	0.69	0/2323
1	Hy	0.44	0/1458	0.68	0/1986
1	Hz	0.43	0/1483	0.67	0/2018
1	I1	0.41	0/1710	0.66	0/2323
1	I4	0.47	0/1458	0.70	0/1986

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	I5	0.44	0/1483	0.67	0/2018
1	I6	0.45	0/1710	0.69	0/2323
1	IA	0.38	0/1458	0.65	0/1986
1	IB	0.35	0/1483	0.63	0/2018
1	IC	0.38	0/1710	0.65	0/2323
1	IF	0.41	0/1458	0.66	0/1986
1	IG	0.37	0/1483	0.64	0/2018
1	IH	0.41	0/1710	0.67	0/2323
1	IK	0.42	0/1458	0.68	0/1986
1	IL	0.42	0/1483	0.67	0/2018
1	IM	0.46	2/1710 (0.1%)	0.68	0/2323
1	IP	0.41	0/1458	0.67	0/1986
1	IQ	0.38	0/1483	0.64	0/2018
1	IR	0.41	0/1710	0.66	0/2323
1	IU	0.48	0/1458	0.72	0/1986
1	IV	0.44	0/1483	0.69	0/2018
1	IW	0.48	0/1710	0.69	0/2323
1	IZ	0.45	0/1458	0.70	0/1986
1	Ia	0.45	0/1483	0.67	0/2018
1	Ib	0.48	0/1710	0.69	0/2323
1	Ie	0.40	0/1458	0.65	0/1986
1	If	0.38	0/1483	0.65	0/2018
1	Ig	0.42	0/1710	0.66	0/2323
1	Ij	0.42	0/1458	0.67	0/1986
1	Ik	0.43	0/1483	0.68	0/2018
1	Il	0.43	0/1710	0.67	0/2323
1	Io	0.48	0/1458	0.71	0/1986
1	Ip	0.44	0/1483	0.67	0/2018
1	Iq	0.45	0/1710	0.68	0/2323
1	It	0.45	0/1458	0.70	0/1986
1	Iu	0.43	0/1483	0.68	0/2018
1	Iv	0.46	0/1710	0.70	0/2323
1	Iy	0.41	0/1458	0.67	0/1986
1	Iz	0.37	0/1483	0.64	0/2018
1	J1	0.47	0/1710	0.68	0/2323
1	J4	0.44	0/1458	0.68	0/1986
1	J5	0.43	0/1483	0.70	0/2018
1	J6	0.46	0/1710	0.68	0/2323
1	JA	0.47	0/1458	0.69	0/1986
1	JB	0.45	0/1483	0.67	0/2018
1	JC	0.46	0/1710	0.68	0/2323
1	JF	0.45	0/1458	0.69	0/1986
1	JG	0.41	0/1483	0.66	0/2018

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	JH	0.44	0/1710	0.67	0/2323
1	JK	0.38	0/1458	0.65	0/1986
1	JL	0.37	0/1483	0.63	0/2018
1	JM	0.39	0/1710	0.64	0/2323
1	JP	0.40	0/1458	0.65	0/1986
1	JQ	0.37	0/1483	0.64	0/2018
1	JR	0.39	0/1710	0.65	0/2323
1	JU	0.42	0/1458	0.68	0/1986
1	JV	0.39	0/1483	0.65	0/2018
1	JW	0.41	0/1710	0.66	0/2323
1	JZ	0.42	0/1458	0.68	0/1986
1	Ja	0.36	0/1483	0.63	0/2018
1	Jb	0.42	0/1710	0.67	0/2323
1	Je	0.46	0/1458	0.69	0/1986
1	Jf	0.41	0/1483	0.67	0/2018
1	Jg	0.48	0/1710	0.70	0/2323
1	Jj	0.46	0/1458	0.70	0/1986
1	Jk	0.45	0/1483	0.68	0/2018
1	Jl	0.48	2/1710 (0.1%)	0.71	0/2323
1	Jo	0.43	0/1458	0.67	0/1986
1	Jp	0.39	0/1483	0.65	0/2018
1	Jq	0.45	0/1710	0.68	0/2323
1	Jt	0.42	0/1458	0.68	0/1986
1	Ju	0.40	0/1483	0.66	0/2018
1	Jv	0.44	0/1710	0.67	0/2323
1	Jy	0.46	0/1458	0.70	0/1986
1	Jz	0.43	0/1483	0.67	0/2018
2	A2	0.56	1/386 (0.3%)	0.70	0/594
2	A7	0.56	1/386 (0.3%)	0.70	0/594
2	AD	0.55	1/386 (0.3%)	0.69	0/594
2	AI	0.56	1/386 (0.3%)	0.69	0/594
2	AN	0.55	1/386 (0.3%)	0.68	0/594
2	AS	0.56	1/386 (0.3%)	0.69	0/594
2	AX	0.54	1/386 (0.3%)	0.70	0/594
2	Ac	0.56	1/386 (0.3%)	0.70	0/594
2	Ah	0.55	1/386 (0.3%)	0.69	0/594
2	Am	0.55	1/386 (0.3%)	0.69	0/594
2	Ar	0.55	1/386 (0.3%)	0.70	0/594
2	Aw	0.55	1/386 (0.3%)	0.69	0/594
2	B2	0.56	1/386 (0.3%)	0.69	0/594
2	B7	0.55	1/386 (0.3%)	0.69	0/594
2	BD	0.55	1/386 (0.3%)	0.69	0/594
2	BI	0.55	1/386 (0.3%)	0.70	0/594

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	BN	0.56	1/386 (0.3%)	0.70	0/594
2	BS	0.55	1/386 (0.3%)	0.69	0/594
2	BX	0.54	1/386 (0.3%)	0.69	0/594
2	Bc	0.55	1/386 (0.3%)	0.69	0/594
2	Bh	0.56	1/386 (0.3%)	0.69	0/594
2	Bm	0.56	1/386 (0.3%)	0.70	0/594
2	Br	0.55	1/386 (0.3%)	0.70	0/594
2	Bw	0.55	1/386 (0.3%)	0.69	0/594
2	C2	0.57	1/386 (0.3%)	0.69	0/594
2	C7	0.56	1/386 (0.3%)	0.69	0/594
2	CD	0.55	1/386 (0.3%)	0.70	0/594
2	CI	0.57	1/386 (0.3%)	0.71	0/594
2	CN	0.56	1/386 (0.3%)	0.69	0/594
2	CS	0.55	1/386 (0.3%)	0.69	0/594
2	CX	0.55	1/386 (0.3%)	0.69	0/594
2	Cc	0.55	1/386 (0.3%)	0.70	0/594
2	Ch	0.56	1/386 (0.3%)	0.70	0/594
2	Cm	0.56	1/386 (0.3%)	0.70	0/594
2	Cr	0.55	1/386 (0.3%)	0.70	0/594
2	Cw	0.56	1/386 (0.3%)	0.70	0/594
2	D2	0.55	1/386 (0.3%)	0.70	0/594
2	D7	0.54	1/386 (0.3%)	0.70	0/594
2	DD	0.55	1/386 (0.3%)	0.68	0/594
2	DI	0.56	1/386 (0.3%)	0.70	0/594
2	DN	0.56	1/386 (0.3%)	0.69	0/594
2	DS	0.54	1/386 (0.3%)	0.70	0/594
2	DX	0.54	1/386 (0.3%)	0.69	0/594
2	Dc	0.55	1/386 (0.3%)	0.69	0/594
2	Dh	0.55	1/386 (0.3%)	0.69	0/594
2	Dm	0.56	1/386 (0.3%)	0.70	0/594
2	Dr	0.55	1/386 (0.3%)	0.68	0/594
2	Dw	0.56	1/386 (0.3%)	0.68	0/594
2	E2	0.56	1/386 (0.3%)	0.71	0/594
2	E7	0.54	1/386 (0.3%)	0.70	0/594
2	ED	0.56	1/386 (0.3%)	0.70	0/594
2	EI	0.55	1/386 (0.3%)	0.70	0/594
2	EN	0.54	1/386 (0.3%)	0.69	0/594
2	ES	0.55	1/386 (0.3%)	0.69	0/594
2	EX	0.56	1/386 (0.3%)	0.71	0/594
2	Ec	0.55	1/386 (0.3%)	0.70	0/594
2	Eh	0.56	1/386 (0.3%)	0.69	0/594
2	Em	0.55	1/386 (0.3%)	0.69	0/594
2	Er	0.55	1/386 (0.3%)	0.70	0/594

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	Ew	0.55	1/386 (0.3%)	0.70	0/594
2	F2	0.54	1/386 (0.3%)	0.70	0/594
2	F7	0.55	1/386 (0.3%)	0.70	0/594
2	FD	0.56	1/386 (0.3%)	0.71	0/594
2	FI	0.54	1/386 (0.3%)	0.71	0/594
2	FN	0.57	1/386 (0.3%)	0.69	0/594
2	FS	0.55	1/386 (0.3%)	0.70	0/594
2	FX	0.55	1/386 (0.3%)	0.69	0/594
2	Fc	0.54	1/386 (0.3%)	0.71	0/594
2	Fh	0.54	1/386 (0.3%)	0.70	0/594
2	Fm	0.54	1/386 (0.3%)	0.70	0/594
2	Fr	0.55	1/386 (0.3%)	0.70	0/594
2	Fw	0.55	1/386 (0.3%)	0.70	0/594
2	G2	0.54	1/386 (0.3%)	0.70	0/594
2	G7	0.54	1/386 (0.3%)	0.70	0/594
2	GD	0.55	1/386 (0.3%)	0.70	0/594
2	GI	0.56	1/386 (0.3%)	0.70	0/594
2	GN	0.54	1/386 (0.3%)	0.70	0/594
2	GS	0.55	1/386 (0.3%)	0.69	0/594
2	GX	0.55	1/386 (0.3%)	0.71	0/594
2	Gc	0.56	1/386 (0.3%)	0.71	0/594
2	Gh	0.55	1/386 (0.3%)	0.71	0/594
2	Gm	0.54	1/386 (0.3%)	0.70	0/594
2	Gr	0.54	1/386 (0.3%)	0.69	0/594
2	Gw	0.56	1/386 (0.3%)	0.70	0/594
2	H2	0.54	1/386 (0.3%)	0.70	0/594
2	H7	0.53	1/386 (0.3%)	0.70	0/594
2	HD	0.54	1/386 (0.3%)	0.69	0/594
2	HI	0.54	1/386 (0.3%)	0.71	0/594
2	HN	0.55	1/386 (0.3%)	0.70	0/594
2	HS	0.54	1/386 (0.3%)	0.70	0/594
2	HX	0.55	1/386 (0.3%)	0.71	0/594
2	Hc	0.54	1/386 (0.3%)	0.69	0/594
2	Hh	0.54	1/386 (0.3%)	0.70	0/594
2	Hm	0.54	1/386 (0.3%)	0.71	0/594
2	Hr	0.54	1/386 (0.3%)	0.70	0/594
2	Hw	0.55	1/386 (0.3%)	0.70	0/594
2	I2	0.55	1/386 (0.3%)	0.71	0/594
2	I7	0.54	1/386 (0.3%)	0.70	0/594
2	ID	0.53	1/386 (0.3%)	0.70	0/594
2	II	0.55	1/386 (0.3%)	0.70	0/594
2	IN	0.55	1/386 (0.3%)	0.70	0/594
2	IS	0.54	1/386 (0.3%)	0.70	0/594

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	IX	0.55	1/386 (0.3%)	0.70	0/594
2	Ic	0.54	1/386 (0.3%)	0.71	0/594
2	Ih	0.53	1/386 (0.3%)	0.69	0/594
2	Im	0.54	1/386 (0.3%)	0.70	0/594
2	Ir	0.55	1/386 (0.3%)	0.71	0/594
2	Iw	0.54	1/386 (0.3%)	0.71	0/594
2	J2	0.54	1/386 (0.3%)	0.70	0/594
2	J7	0.54	1/386 (0.3%)	0.70	0/594
2	JD	0.53	1/386 (0.3%)	0.70	0/594
2	JI	0.54	1/386 (0.3%)	0.70	0/594
2	JN	0.54	1/386 (0.3%)	0.71	0/594
2	JS	0.54	1/386 (0.3%)	0.71	0/594
2	JX	0.54	1/386 (0.3%)	0.71	0/594
2	Jc	0.53	1/386 (0.3%)	0.71	0/594
2	Jh	0.55	1/386 (0.3%)	0.71	0/594
2	Jm	0.54	1/386 (0.3%)	0.70	0/594
2	Jr	0.54	1/386 (0.3%)	0.70	0/594
2	Jw	0.55	1/386 (0.3%)	0.70	0/594
All	All	0.46	262/604440 (0.0%)	0.70	1/830520 (0.0%)

The worst 5 of 262 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BN	1	U	OP3-P	-7.52	1.52	1.61
2	FN	1	U	OP3-P	-7.50	1.52	1.61
2	Dw	1	U	OP3-P	-7.50	1.52	1.61
2	C2	1	U	OP3-P	-7.44	1.52	1.61
2	Dc	1	U	OP3-P	-7.43	1.52	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	91	GLY	N-CA-C	-5.08	100.40	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	A1	215/242 (89%)	187 (87%)	19 (9%)	9 (4%)	3	10
1	A4	183/242 (76%)	165 (90%)	14 (8%)	4 (2%)	6	24
1	A5	187/242 (77%)	160 (86%)	19 (10%)	8 (4%)	2	10
1	A6	215/242 (89%)	187 (87%)	18 (8%)	10 (5%)	2	8
1	AA	183/242 (76%)	165 (90%)	13 (7%)	5 (3%)	5	19
1	AB	187/242 (77%)	158 (84%)	21 (11%)	8 (4%)	2	10
1	AC	215/242 (89%)	187 (87%)	18 (8%)	10 (5%)	2	8
1	AF	183/242 (76%)	167 (91%)	12 (7%)	4 (2%)	6	24
1	AG	187/242 (77%)	161 (86%)	20 (11%)	6 (3%)	4	16
1	AH	215/242 (89%)	189 (88%)	17 (8%)	9 (4%)	3	10
1	AK	183/242 (76%)	163 (89%)	14 (8%)	6 (3%)	4	15
1	AL	187/242 (77%)	160 (86%)	19 (10%)	8 (4%)	2	10
1	AM	215/242 (89%)	188 (87%)	19 (9%)	8 (4%)	3	13
1	AP	183/242 (76%)	164 (90%)	13 (7%)	6 (3%)	4	15
1	AQ	187/242 (77%)	163 (87%)	18 (10%)	6 (3%)	4	16
1	AR	215/242 (89%)	188 (87%)	19 (9%)	8 (4%)	3	13
1	AU	183/242 (76%)	165 (90%)	11 (6%)	7 (4%)	3	13
1	AV	187/242 (77%)	159 (85%)	22 (12%)	6 (3%)	4	16
1	AW	215/242 (89%)	190 (88%)	16 (7%)	9 (4%)	3	10
1	AZ	183/242 (76%)	167 (91%)	12 (7%)	4 (2%)	6	24
1	Aa	187/242 (77%)	161 (86%)	20 (11%)	6 (3%)	4	16
1	Ab	215/242 (89%)	189 (88%)	17 (8%)	9 (4%)	3	10
1	Ae	183/242 (76%)	164 (90%)	14 (8%)	5 (3%)	5	19
1	Af	187/242 (77%)	160 (86%)	19 (10%)	8 (4%)	2	10
1	Ag	215/242 (89%)	188 (87%)	18 (8%)	9 (4%)	3	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aj	183/242 (76%)	165 (90%)	14 (8%)	4 (2%)	6	24
1	Ak	187/242 (77%)	159 (85%)	21 (11%)	7 (4%)	3	13
1	Al	215/242 (89%)	185 (86%)	21 (10%)	9 (4%)	3	10
1	Ao	183/242 (76%)	166 (91%)	13 (7%)	4 (2%)	6	24
1	Ap	187/242 (77%)	160 (86%)	20 (11%)	7 (4%)	3	13
1	Aq	215/242 (89%)	185 (86%)	21 (10%)	9 (4%)	3	10
1	At	183/242 (76%)	163 (89%)	16 (9%)	4 (2%)	6	24
1	Au	187/242 (77%)	159 (85%)	21 (11%)	7 (4%)	3	13
1	Av	215/242 (89%)	186 (86%)	20 (9%)	9 (4%)	3	10
1	Ay	183/242 (76%)	163 (89%)	16 (9%)	4 (2%)	6	24
1	Az	187/242 (77%)	161 (86%)	19 (10%)	7 (4%)	3	13
1	B1	215/242 (89%)	187 (87%)	19 (9%)	9 (4%)	3	10
1	B4	183/242 (76%)	164 (90%)	13 (7%)	6 (3%)	4	15
1	B5	187/242 (77%)	159 (85%)	22 (12%)	6 (3%)	4	16
1	B6	215/242 (89%)	189 (88%)	18 (8%)	8 (4%)	3	13
1	BA	183/242 (76%)	163 (89%)	14 (8%)	6 (3%)	4	15
1	BB	187/242 (77%)	158 (84%)	22 (12%)	7 (4%)	3	13
1	BC	215/242 (89%)	186 (86%)	20 (9%)	9 (4%)	3	10
1	BF	183/242 (76%)	167 (91%)	12 (7%)	4 (2%)	6	24
1	BG	187/242 (77%)	161 (86%)	17 (9%)	9 (5%)	2	8
1	BH	215/242 (89%)	189 (88%)	18 (8%)	8 (4%)	3	13
1	BK	183/242 (76%)	166 (91%)	13 (7%)	4 (2%)	6	24
1	BL	187/242 (77%)	160 (86%)	20 (11%)	7 (4%)	3	13
1	BM	215/242 (89%)	187 (87%)	18 (8%)	10 (5%)	2	8
1	BP	183/242 (76%)	165 (90%)	14 (8%)	4 (2%)	6	24
1	BQ	187/242 (77%)	155 (83%)	22 (12%)	10 (5%)	2	6
1	BR	215/242 (89%)	188 (87%)	17 (8%)	10 (5%)	2	8
1	BU	183/242 (76%)	166 (91%)	13 (7%)	4 (2%)	6	24
1	BV	187/242 (77%)	160 (86%)	21 (11%)	6 (3%)	4	16
1	BW	215/242 (89%)	188 (87%)	18 (8%)	9 (4%)	3	10
1	BZ	183/242 (76%)	166 (91%)	13 (7%)	4 (2%)	6	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ba	187/242 (77%)	160 (86%)	21 (11%)	6 (3%)	4	16
1	Bb	215/242 (89%)	188 (87%)	17 (8%)	10 (5%)	2	8
1	Be	183/242 (76%)	166 (91%)	12 (7%)	5 (3%)	5	19
1	Bf	187/242 (77%)	159 (85%)	20 (11%)	8 (4%)	2	10
1	Bg	215/242 (89%)	189 (88%)	15 (7%)	11 (5%)	2	7
1	Bj	183/242 (76%)	162 (88%)	16 (9%)	5 (3%)	5	19
1	Bk	187/242 (77%)	157 (84%)	25 (13%)	5 (3%)	5	19
1	Bl	215/242 (89%)	188 (87%)	18 (8%)	9 (4%)	3	10
1	Bo	183/242 (76%)	163 (89%)	15 (8%)	5 (3%)	5	19
1	Bp	187/242 (77%)	158 (84%)	21 (11%)	8 (4%)	2	10
1	Bq	215/242 (89%)	190 (88%)	17 (8%)	8 (4%)	3	13
1	Bt	183/242 (76%)	165 (90%)	14 (8%)	4 (2%)	6	24
1	Bu	187/242 (77%)	160 (86%)	21 (11%)	6 (3%)	4	16
1	Bv	215/242 (89%)	188 (87%)	19 (9%)	8 (4%)	3	13
1	By	183/242 (76%)	162 (88%)	13 (7%)	8 (4%)	2	10
1	Bz	187/242 (77%)	163 (87%)	17 (9%)	7 (4%)	3	13
1	C1	215/242 (89%)	190 (88%)	15 (7%)	10 (5%)	2	8
1	C4	183/242 (76%)	166 (91%)	12 (7%)	5 (3%)	5	19
1	C5	187/242 (77%)	158 (84%)	23 (12%)	6 (3%)	4	16
1	C6	215/242 (89%)	188 (87%)	18 (8%)	9 (4%)	3	10
1	CA	183/242 (76%)	166 (91%)	13 (7%)	4 (2%)	6	24
1	CB	187/242 (77%)	161 (86%)	20 (11%)	6 (3%)	4	16
1	CC	215/242 (89%)	186 (86%)	19 (9%)	10 (5%)	2	8
1	CF	183/242 (76%)	166 (91%)	12 (7%)	5 (3%)	5	19
1	CG	187/242 (77%)	162 (87%)	19 (10%)	6 (3%)	4	16
1	CH	215/242 (89%)	188 (87%)	19 (9%)	8 (4%)	3	13
1	CK	183/242 (76%)	164 (90%)	15 (8%)	4 (2%)	6	24
1	CL	187/242 (77%)	161 (86%)	21 (11%)	5 (3%)	5	19
1	CM	215/242 (89%)	191 (89%)	15 (7%)	9 (4%)	3	10
1	CP	183/242 (76%)	164 (90%)	15 (8%)	4 (2%)	6	24
1	CQ	187/242 (77%)	159 (85%)	22 (12%)	6 (3%)	4	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CR	215/242 (89%)	191 (89%)	15 (7%)	9 (4%)	3	10
1	CU	183/242 (76%)	163 (89%)	15 (8%)	5 (3%)	5	19
1	CV	187/242 (77%)	159 (85%)	23 (12%)	5 (3%)	5	19
1	CW	215/242 (89%)	189 (88%)	18 (8%)	8 (4%)	3	13
1	CZ	183/242 (76%)	164 (90%)	14 (8%)	5 (3%)	5	19
1	Ca	187/242 (77%)	161 (86%)	19 (10%)	7 (4%)	3	13
1	Cb	215/242 (89%)	186 (86%)	18 (8%)	11 (5%)	2	7
1	Ce	183/242 (76%)	165 (90%)	13 (7%)	5 (3%)	5	19
1	Cf	187/242 (77%)	159 (85%)	21 (11%)	7 (4%)	3	13
1	Cg	215/242 (89%)	190 (88%)	15 (7%)	10 (5%)	2	8
1	Cj	183/242 (76%)	166 (91%)	13 (7%)	4 (2%)	6	24
1	Ck	187/242 (77%)	160 (86%)	19 (10%)	8 (4%)	2	10
1	Cl	215/242 (89%)	185 (86%)	20 (9%)	10 (5%)	2	8
1	Co	183/242 (76%)	167 (91%)	12 (7%)	4 (2%)	6	24
1	Cp	187/242 (77%)	159 (85%)	22 (12%)	6 (3%)	4	16
1	Cq	215/242 (89%)	188 (87%)	19 (9%)	8 (4%)	3	13
1	Ct	183/242 (76%)	164 (90%)	13 (7%)	6 (3%)	4	15
1	Cu	187/242 (77%)	159 (85%)	22 (12%)	6 (3%)	4	16
1	Cv	215/242 (89%)	187 (87%)	20 (9%)	8 (4%)	3	13
1	Cy	183/242 (76%)	165 (90%)	14 (8%)	4 (2%)	6	24
1	Cz	187/242 (77%)	158 (84%)	23 (12%)	6 (3%)	4	16
1	D1	215/242 (89%)	189 (88%)	16 (7%)	10 (5%)	2	8
1	D4	183/242 (76%)	165 (90%)	13 (7%)	5 (3%)	5	19
1	D5	187/242 (77%)	159 (85%)	22 (12%)	6 (3%)	4	16
1	D6	215/242 (89%)	190 (88%)	16 (7%)	9 (4%)	3	10
1	DA	183/242 (76%)	163 (89%)	15 (8%)	5 (3%)	5	19
1	DB	187/242 (77%)	163 (87%)	16 (9%)	8 (4%)	2	10
1	DC	215/242 (89%)	186 (86%)	20 (9%)	9 (4%)	3	10
1	DF	183/242 (76%)	166 (91%)	13 (7%)	4 (2%)	6	24
1	DG	187/242 (77%)	161 (86%)	18 (10%)	8 (4%)	2	10
1	DH	215/242 (89%)	186 (86%)	19 (9%)	10 (5%)	2	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DK	183/242 (76%)	161 (88%)	17 (9%)	5 (3%)	5	19
1	DL	187/242 (77%)	157 (84%)	24 (13%)	6 (3%)	4	16
1	DM	215/242 (89%)	188 (87%)	18 (8%)	9 (4%)	3	10
1	DP	183/242 (76%)	163 (89%)	16 (9%)	4 (2%)	6	24
1	DQ	187/242 (77%)	159 (85%)	22 (12%)	6 (3%)	4	16
1	DR	215/242 (89%)	188 (87%)	19 (9%)	8 (4%)	3	13
1	DU	183/242 (76%)	167 (91%)	12 (7%)	4 (2%)	6	24
1	DV	187/242 (77%)	159 (85%)	19 (10%)	9 (5%)	2	8
1	DW	215/242 (89%)	187 (87%)	18 (8%)	10 (5%)	2	8
1	DZ	183/242 (76%)	165 (90%)	13 (7%)	5 (3%)	5	19
1	Da	187/242 (77%)	160 (86%)	19 (10%)	8 (4%)	2	10
1	Db	215/242 (89%)	186 (86%)	20 (9%)	9 (4%)	3	10
1	De	183/242 (76%)	168 (92%)	11 (6%)	4 (2%)	6	24
1	Df	187/242 (77%)	161 (86%)	20 (11%)	6 (3%)	4	16
1	Dg	215/242 (89%)	191 (89%)	15 (7%)	9 (4%)	3	10
1	Dj	183/242 (76%)	166 (91%)	13 (7%)	4 (2%)	6	24
1	Dk	187/242 (77%)	161 (86%)	21 (11%)	5 (3%)	5	19
1	Dl	215/242 (89%)	189 (88%)	18 (8%)	8 (4%)	3	13
1	Do	183/242 (76%)	167 (91%)	12 (7%)	4 (2%)	6	24
1	Dp	187/242 (77%)	161 (86%)	19 (10%)	7 (4%)	3	13
1	Dq	215/242 (89%)	187 (87%)	17 (8%)	11 (5%)	2	7
1	Dt	183/242 (76%)	166 (91%)	13 (7%)	4 (2%)	6	24
1	Du	187/242 (77%)	158 (84%)	23 (12%)	6 (3%)	4	16
1	Dv	215/242 (89%)	187 (87%)	19 (9%)	9 (4%)	3	10
1	Dy	183/242 (76%)	165 (90%)	12 (7%)	6 (3%)	4	15
1	Dz	187/242 (77%)	160 (86%)	20 (11%)	7 (4%)	3	13
1	E1	215/242 (89%)	189 (88%)	18 (8%)	8 (4%)	3	13
1	E4	183/242 (76%)	164 (90%)	15 (8%)	4 (2%)	6	24
1	E5	187/242 (77%)	159 (85%)	22 (12%)	6 (3%)	4	16
1	E6	215/242 (89%)	189 (88%)	18 (8%)	8 (4%)	3	13
1	EA	183/242 (76%)	165 (90%)	14 (8%)	4 (2%)	6	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EB	187/242 (77%)	160 (86%)	19 (10%)	8 (4%)	2	10
1	EC	215/242 (89%)	185 (86%)	20 (9%)	10 (5%)	2	8
1	EF	183/242 (76%)	166 (91%)	13 (7%)	4 (2%)	6	24
1	EG	187/242 (77%)	159 (85%)	22 (12%)	6 (3%)	4	16
1	EH	215/242 (89%)	189 (88%)	17 (8%)	9 (4%)	3	10
1	EK	183/242 (76%)	163 (89%)	16 (9%)	4 (2%)	6	24
1	EL	187/242 (77%)	158 (84%)	23 (12%)	6 (3%)	4	16
1	EM	215/242 (89%)	188 (87%)	18 (8%)	9 (4%)	3	10
1	EP	183/242 (76%)	165 (90%)	14 (8%)	4 (2%)	6	24
1	EQ	187/242 (77%)	160 (86%)	20 (11%)	7 (4%)	3	13
1	ER	215/242 (89%)	186 (86%)	18 (8%)	11 (5%)	2	7
1	EU	183/242 (76%)	166 (91%)	13 (7%)	4 (2%)	6	24
1	EV	187/242 (77%)	160 (86%)	19 (10%)	8 (4%)	2	10
1	EW	215/242 (89%)	187 (87%)	19 (9%)	9 (4%)	3	10
1	EZ	183/242 (76%)	166 (91%)	13 (7%)	4 (2%)	6	24
1	Ea	187/242 (77%)	159 (85%)	21 (11%)	7 (4%)	3	13
1	Eb	215/242 (89%)	186 (86%)	21 (10%)	8 (4%)	3	13
1	Ee	183/242 (76%)	165 (90%)	13 (7%)	5 (3%)	5	19
1	Ef	187/242 (77%)	159 (85%)	22 (12%)	6 (3%)	4	16
1	Eg	215/242 (89%)	187 (87%)	19 (9%)	9 (4%)	3	10
1	Ej	183/242 (76%)	165 (90%)	14 (8%)	4 (2%)	6	24
1	Ek	187/242 (77%)	160 (86%)	21 (11%)	6 (3%)	4	16
1	El	215/242 (89%)	189 (88%)	18 (8%)	8 (4%)	3	13
1	Eo	183/242 (76%)	164 (90%)	15 (8%)	4 (2%)	6	24
1	Ep	187/242 (77%)	157 (84%)	25 (13%)	5 (3%)	5	19
1	Eq	215/242 (89%)	189 (88%)	17 (8%)	9 (4%)	3	10
1	Et	183/242 (76%)	165 (90%)	13 (7%)	5 (3%)	5	19
1	Eu	187/242 (77%)	161 (86%)	20 (11%)	6 (3%)	4	16
1	Ev	215/242 (89%)	187 (87%)	20 (9%)	8 (4%)	3	13
1	Ey	183/242 (76%)	164 (90%)	14 (8%)	5 (3%)	5	19
1	Ez	187/242 (77%)	162 (87%)	19 (10%)	6 (3%)	4	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F1	215/242 (89%)	186 (86%)	21 (10%)	8 (4%)	3	13
1	F4	183/242 (76%)	154 (84%)	24 (13%)	5 (3%)	5	19
1	F5	187/242 (77%)	160 (86%)	21 (11%)	6 (3%)	4	16
1	F6	215/242 (89%)	184 (86%)	21 (10%)	10 (5%)	2	8
1	FA	183/242 (76%)	155 (85%)	24 (13%)	4 (2%)	6	24
1	FB	187/242 (77%)	164 (88%)	20 (11%)	3 (2%)	9	32
1	FC	215/242 (89%)	182 (85%)	24 (11%)	9 (4%)	3	10
1	FF	183/242 (76%)	156 (85%)	22 (12%)	5 (3%)	5	19
1	FG	187/242 (77%)	161 (86%)	21 (11%)	5 (3%)	5	19
1	FH	215/242 (89%)	186 (86%)	21 (10%)	8 (4%)	3	13
1	FK	183/242 (76%)	154 (84%)	25 (14%)	4 (2%)	6	24
1	FL	187/242 (77%)	160 (86%)	21 (11%)	6 (3%)	4	16
1	FM	215/242 (89%)	188 (87%)	19 (9%)	8 (4%)	3	13
1	FP	183/242 (76%)	156 (85%)	22 (12%)	5 (3%)	5	19
1	FQ	187/242 (77%)	161 (86%)	20 (11%)	6 (3%)	4	16
1	FR	215/242 (89%)	185 (86%)	21 (10%)	9 (4%)	3	10
1	FU	183/242 (76%)	156 (85%)	22 (12%)	5 (3%)	5	19
1	FV	187/242 (77%)	159 (85%)	24 (13%)	4 (2%)	7	26
1	FW	215/242 (89%)	182 (85%)	22 (10%)	11 (5%)	2	7
1	FZ	183/242 (76%)	153 (84%)	25 (14%)	5 (3%)	5	19
1	Fa	187/242 (77%)	162 (87%)	19 (10%)	6 (3%)	4	16
1	Fb	215/242 (89%)	183 (85%)	24 (11%)	8 (4%)	3	13
1	Fe	183/242 (76%)	155 (85%)	23 (13%)	5 (3%)	5	19
1	Ff	187/242 (77%)	159 (85%)	22 (12%)	6 (3%)	4	16
1	Fg	215/242 (89%)	186 (86%)	21 (10%)	8 (4%)	3	13
1	Fj	183/242 (76%)	158 (86%)	20 (11%)	5 (3%)	5	19
1	Fk	187/242 (77%)	159 (85%)	23 (12%)	5 (3%)	5	19
1	Fl	215/242 (89%)	183 (85%)	24 (11%)	8 (4%)	3	13
1	Fo	183/242 (76%)	158 (86%)	22 (12%)	3 (2%)	9	32
1	Fp	187/242 (77%)	160 (86%)	23 (12%)	4 (2%)	7	26
1	Fq	215/242 (89%)	184 (86%)	20 (9%)	11 (5%)	2	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ft	183/242 (76%)	159 (87%)	19 (10%)	5 (3%)	5	19
1	Fu	187/242 (77%)	162 (87%)	20 (11%)	5 (3%)	5	19
1	Fv	215/242 (89%)	184 (86%)	23 (11%)	8 (4%)	3	13
1	Fy	183/242 (76%)	159 (87%)	20 (11%)	4 (2%)	6	24
1	Fz	187/242 (77%)	160 (86%)	24 (13%)	3 (2%)	9	32
1	G1	215/242 (89%)	187 (87%)	20 (9%)	8 (4%)	3	13
1	G4	183/242 (76%)	154 (84%)	25 (14%)	4 (2%)	6	24
1	G5	187/242 (77%)	159 (85%)	21 (11%)	7 (4%)	3	13
1	G6	215/242 (89%)	180 (84%)	27 (13%)	8 (4%)	3	13
1	GA	183/242 (76%)	158 (86%)	21 (12%)	4 (2%)	6	24
1	GB	187/242 (77%)	162 (87%)	21 (11%)	4 (2%)	7	26
1	GC	215/242 (89%)	183 (85%)	23 (11%)	9 (4%)	3	10
1	GF	183/242 (76%)	158 (86%)	20 (11%)	5 (3%)	5	19
1	GG	187/242 (77%)	161 (86%)	21 (11%)	5 (3%)	5	19
1	GH	215/242 (89%)	188 (87%)	19 (9%)	8 (4%)	3	13
1	GK	183/242 (76%)	159 (87%)	17 (9%)	7 (4%)	3	13
1	GL	187/242 (77%)	158 (84%)	23 (12%)	6 (3%)	4	16
1	GM	215/242 (89%)	187 (87%)	20 (9%)	8 (4%)	3	13
1	GP	183/242 (76%)	158 (86%)	20 (11%)	5 (3%)	5	19
1	GQ	187/242 (77%)	162 (87%)	21 (11%)	4 (2%)	7	26
1	GR	215/242 (89%)	185 (86%)	22 (10%)	8 (4%)	3	13
1	GU	183/242 (76%)	155 (85%)	23 (13%)	5 (3%)	5	19
1	GV	187/242 (77%)	162 (87%)	21 (11%)	4 (2%)	7	26
1	GW	215/242 (89%)	188 (87%)	18 (8%)	9 (4%)	3	10
1	GZ	183/242 (76%)	157 (86%)	20 (11%)	6 (3%)	4	15
1	Ga	187/242 (77%)	161 (86%)	21 (11%)	5 (3%)	5	19
1	Gb	215/242 (89%)	187 (87%)	20 (9%)	8 (4%)	3	13
1	Ge	183/242 (76%)	156 (85%)	23 (13%)	4 (2%)	6	24
1	Gf	187/242 (77%)	159 (85%)	22 (12%)	6 (3%)	4	16
1	Gg	215/242 (89%)	185 (86%)	22 (10%)	8 (4%)	3	13
1	Gj	183/242 (76%)	153 (84%)	24 (13%)	6 (3%)	4	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Gk	187/242 (77%)	159 (85%)	24 (13%)	4 (2%)	7	26
1	Gl	215/242 (89%)	188 (87%)	19 (9%)	8 (4%)	3	13
1	Go	183/242 (76%)	158 (86%)	21 (12%)	4 (2%)	6	24
1	Gp	187/242 (77%)	160 (86%)	23 (12%)	4 (2%)	7	26
1	Gq	215/242 (89%)	188 (87%)	19 (9%)	8 (4%)	3	13
1	Gt	183/242 (76%)	158 (86%)	20 (11%)	5 (3%)	5	19
1	Gu	187/242 (77%)	159 (85%)	23 (12%)	5 (3%)	5	19
1	Gv	215/242 (89%)	187 (87%)	20 (9%)	8 (4%)	3	13
1	Gy	183/242 (76%)	159 (87%)	18 (10%)	6 (3%)	4	15
1	Gz	187/242 (77%)	163 (87%)	20 (11%)	4 (2%)	7	26
1	H1	215/242 (89%)	187 (87%)	18 (8%)	10 (5%)	2	8
1	H4	183/242 (76%)	157 (86%)	21 (12%)	5 (3%)	5	19
1	H5	187/242 (77%)	160 (86%)	22 (12%)	5 (3%)	5	19
1	H6	215/242 (89%)	186 (86%)	21 (10%)	8 (4%)	3	13
1	HA	183/242 (76%)	159 (87%)	19 (10%)	5 (3%)	5	19
1	HB	187/242 (77%)	160 (86%)	23 (12%)	4 (2%)	7	26
1	HC	215/242 (89%)	184 (86%)	21 (10%)	10 (5%)	2	8
1	HF	183/242 (76%)	155 (85%)	23 (13%)	5 (3%)	5	19
1	HG	187/242 (77%)	159 (85%)	23 (12%)	5 (3%)	5	19
1	HH	215/242 (89%)	189 (88%)	18 (8%)	8 (4%)	3	13
1	HK	183/242 (76%)	159 (87%)	19 (10%)	5 (3%)	5	19
1	HL	187/242 (77%)	159 (85%)	24 (13%)	4 (2%)	7	26
1	HM	215/242 (89%)	184 (86%)	23 (11%)	8 (4%)	3	13
1	HP	183/242 (76%)	159 (87%)	19 (10%)	5 (3%)	5	19
1	HQ	187/242 (77%)	162 (87%)	19 (10%)	6 (3%)	4	16
1	HR	215/242 (89%)	185 (86%)	21 (10%)	9 (4%)	3	10
1	HU	183/242 (76%)	155 (85%)	24 (13%)	4 (2%)	6	24
1	HV	187/242 (77%)	161 (86%)	20 (11%)	6 (3%)	4	16
1	HW	215/242 (89%)	185 (86%)	19 (9%)	11 (5%)	2	7
1	HZ	183/242 (76%)	159 (87%)	18 (10%)	6 (3%)	4	15
1	Ha	187/242 (77%)	163 (87%)	20 (11%)	4 (2%)	7	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Hb	215/242 (89%)	184 (86%)	22 (10%)	9 (4%)	3	10
1	He	183/242 (76%)	156 (85%)	21 (12%)	6 (3%)	4	15
1	Hf	187/242 (77%)	160 (86%)	22 (12%)	5 (3%)	5	19
1	Hg	215/242 (89%)	188 (87%)	18 (8%)	9 (4%)	3	10
1	Hj	183/242 (76%)	157 (86%)	22 (12%)	4 (2%)	6	24
1	Hk	187/242 (77%)	159 (85%)	23 (12%)	5 (3%)	5	19
1	Hl	215/242 (89%)	185 (86%)	21 (10%)	9 (4%)	3	10
1	Ho	183/242 (76%)	159 (87%)	19 (10%)	5 (3%)	5	19
1	Hp	187/242 (77%)	161 (86%)	21 (11%)	5 (3%)	5	19
1	Hq	215/242 (89%)	185 (86%)	22 (10%)	8 (4%)	3	13
1	Ht	183/242 (76%)	155 (85%)	23 (13%)	5 (3%)	5	19
1	Hu	187/242 (77%)	160 (86%)	21 (11%)	6 (3%)	4	16
1	Hv	215/242 (89%)	184 (86%)	22 (10%)	9 (4%)	3	10
1	Hy	183/242 (76%)	153 (84%)	26 (14%)	4 (2%)	6	24
1	Hz	187/242 (77%)	161 (86%)	21 (11%)	5 (3%)	5	19
1	I1	215/242 (89%)	185 (86%)	22 (10%)	8 (4%)	3	13
1	I4	183/242 (76%)	155 (85%)	21 (12%)	7 (4%)	3	13
1	I5	187/242 (77%)	158 (84%)	22 (12%)	7 (4%)	3	13
1	I6	215/242 (89%)	187 (87%)	18 (8%)	10 (5%)	2	8
1	IA	183/242 (76%)	156 (85%)	23 (13%)	4 (2%)	6	24
1	IB	187/242 (77%)	160 (86%)	22 (12%)	5 (3%)	5	19
1	IC	215/242 (89%)	188 (87%)	18 (8%)	9 (4%)	3	10
1	IF	183/242 (76%)	158 (86%)	21 (12%)	4 (2%)	6	24
1	IG	187/242 (77%)	162 (87%)	20 (11%)	5 (3%)	5	19
1	IH	215/242 (89%)	187 (87%)	19 (9%)	9 (4%)	3	10
1	IK	183/242 (76%)	156 (85%)	22 (12%)	5 (3%)	5	19
1	IL	187/242 (77%)	160 (86%)	20 (11%)	7 (4%)	3	13
1	IM	215/242 (89%)	183 (85%)	23 (11%)	9 (4%)	3	10
1	IP	183/242 (76%)	155 (85%)	23 (13%)	5 (3%)	5	19
1	IQ	187/242 (77%)	161 (86%)	22 (12%)	4 (2%)	7	26
1	IR	215/242 (89%)	188 (87%)	19 (9%)	8 (4%)	3	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	IU	183/242 (76%)	158 (86%)	20 (11%)	5 (3%)	5	19
1	IV	187/242 (77%)	160 (86%)	22 (12%)	5 (3%)	5	19
1	IW	215/242 (89%)	187 (87%)	20 (9%)	8 (4%)	3	13
1	IZ	183/242 (76%)	155 (85%)	24 (13%)	4 (2%)	6	24
1	Ia	187/242 (77%)	161 (86%)	22 (12%)	4 (2%)	7	26
1	Ib	215/242 (89%)	188 (87%)	18 (8%)	9 (4%)	3	10
1	Ie	183/242 (76%)	158 (86%)	20 (11%)	5 (3%)	5	19
1	If	187/242 (77%)	162 (87%)	22 (12%)	3 (2%)	9	32
1	Ig	215/242 (89%)	185 (86%)	21 (10%)	9 (4%)	3	10
1	Ij	183/242 (76%)	156 (85%)	21 (12%)	6 (3%)	4	15
1	Ik	187/242 (77%)	159 (85%)	23 (12%)	5 (3%)	5	19
1	Il	215/242 (89%)	180 (84%)	26 (12%)	9 (4%)	3	10
1	Io	183/242 (76%)	157 (86%)	21 (12%)	5 (3%)	5	19
1	Ip	187/242 (77%)	161 (86%)	21 (11%)	5 (3%)	5	19
1	Iq	215/242 (89%)	186 (86%)	21 (10%)	8 (4%)	3	13
1	It	183/242 (76%)	156 (85%)	23 (13%)	4 (2%)	6	24
1	Iu	187/242 (77%)	158 (84%)	25 (13%)	4 (2%)	7	26
1	Iv	215/242 (89%)	188 (87%)	19 (9%)	8 (4%)	3	13
1	Iy	183/242 (76%)	156 (85%)	22 (12%)	5 (3%)	5	19
1	Iz	187/242 (77%)	162 (87%)	20 (11%)	5 (3%)	5	19
1	J1	215/242 (89%)	185 (86%)	22 (10%)	8 (4%)	3	13
1	J4	183/242 (76%)	156 (85%)	22 (12%)	5 (3%)	5	19
1	J5	187/242 (77%)	158 (84%)	23 (12%)	6 (3%)	4	16
1	J6	215/242 (89%)	185 (86%)	20 (9%)	10 (5%)	2	8
1	JA	183/242 (76%)	158 (86%)	19 (10%)	6 (3%)	4	15
1	JB	187/242 (77%)	159 (85%)	23 (12%)	5 (3%)	5	19
1	JC	215/242 (89%)	186 (86%)	21 (10%)	8 (4%)	3	13
1	JF	183/242 (76%)	157 (86%)	22 (12%)	4 (2%)	6	24
1	JG	187/242 (77%)	161 (86%)	19 (10%)	7 (4%)	3	13
1	JH	215/242 (89%)	188 (87%)	18 (8%)	9 (4%)	3	10
1	JK	183/242 (76%)	158 (86%)	21 (12%)	4 (2%)	6	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	JL	187/242 (77%)	162 (87%)	21 (11%)	4 (2%)	7	26
1	JM	215/242 (89%)	184 (86%)	23 (11%)	8 (4%)	3	13
1	JP	183/242 (76%)	156 (85%)	22 (12%)	5 (3%)	5	19
1	JQ	187/242 (77%)	163 (87%)	20 (11%)	4 (2%)	7	26
1	JR	215/242 (89%)	189 (88%)	18 (8%)	8 (4%)	3	13
1	JU	183/242 (76%)	157 (86%)	22 (12%)	4 (2%)	6	24
1	JV	187/242 (77%)	158 (84%)	22 (12%)	7 (4%)	3	13
1	JW	215/242 (89%)	184 (86%)	22 (10%)	9 (4%)	3	10
1	JZ	183/242 (76%)	155 (85%)	24 (13%)	4 (2%)	6	24
1	Ja	187/242 (77%)	159 (85%)	23 (12%)	5 (3%)	5	19
1	Jb	215/242 (89%)	184 (86%)	23 (11%)	8 (4%)	3	13
1	Je	183/242 (76%)	161 (88%)	18 (10%)	4 (2%)	6	24
1	Jf	187/242 (77%)	164 (88%)	19 (10%)	4 (2%)	7	26
1	Jg	215/242 (89%)	186 (86%)	21 (10%)	8 (4%)	3	13
1	Jj	183/242 (76%)	156 (85%)	23 (13%)	4 (2%)	6	24
1	Jk	187/242 (77%)	160 (86%)	23 (12%)	4 (2%)	7	26
1	Jl	215/242 (89%)	188 (87%)	19 (9%)	8 (4%)	3	13
1	Jo	183/242 (76%)	153 (84%)	26 (14%)	4 (2%)	6	24
1	Jp	187/242 (77%)	160 (86%)	22 (12%)	5 (3%)	5	19
1	Jq	215/242 (89%)	190 (88%)	17 (8%)	8 (4%)	3	13
1	Jt	183/242 (76%)	157 (86%)	21 (12%)	5 (3%)	5	19
1	Ju	187/242 (77%)	161 (86%)	23 (12%)	3 (2%)	9	32
1	Jv	215/242 (89%)	187 (87%)	20 (9%)	8 (4%)	3	13
1	Jy	183/242 (76%)	157 (86%)	19 (10%)	7 (4%)	3	13
1	Jz	187/242 (77%)	161 (86%)	19 (10%)	7 (4%)	3	13
All	All	70200/87120 (81%)	60905 (87%)	6970 (10%)	2325 (3%)	4	15

5 of 2325 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AC	28	LYS
1	AC	29	SER
1	AH	28	LYS

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Mol	Chain	Res	Type
1	AH	29	SER
1	AM	28	LYS

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 X-ray entries followed by that with respect to entries of similar resolution.

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	A1	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	A4	160/204 (78%)	151 (94%)	9 (6%)	21	52
1	A5	162/204 (79%)	151 (93%)	11 (7%)	16	42
1	A6	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	AA	160/204 (78%)	152 (95%)	8 (5%)	24	57
1	AB	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	AC	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	AF	160/204 (78%)	153 (96%)	7 (4%)	28	61
1	AG	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	AH	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	AK	160/204 (78%)	150 (94%)	10 (6%)	18	46
1	AL	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	AM	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	AP	160/204 (78%)	150 (94%)	10 (6%)	18	46
1	AQ	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	AR	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	AU	160/204 (78%)	153 (96%)	7 (4%)	28	61
1	AV	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	AW	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	AZ	160/204 (78%)	152 (95%)	8 (5%)	24	57
1	Aa	162/204 (79%)	153 (94%)	9 (6%)	21	52
1	Ab	186/204 (91%)	179 (96%)	7 (4%)	33	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ae	160/204 (78%)	152 (95%)	8 (5%)	24	57
1	Af	162/204 (79%)	150 (93%)	12 (7%)	13	38
1	Ag	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	Aj	160/204 (78%)	152 (95%)	8 (5%)	24	57
1	Ak	162/204 (79%)	150 (93%)	12 (7%)	13	38
1	Al	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	Ao	160/204 (78%)	151 (94%)	9 (6%)	21	52
1	Ap	162/204 (79%)	149 (92%)	13 (8%)	12	33
1	Aq	186/204 (91%)	176 (95%)	10 (5%)	22	54
1	At	160/204 (78%)	153 (96%)	7 (4%)	28	61
1	Au	162/204 (79%)	153 (94%)	9 (6%)	21	52
1	Av	186/204 (91%)	176 (95%)	10 (5%)	22	54
1	Ay	160/204 (78%)	150 (94%)	10 (6%)	18	46
1	Az	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	B1	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	B4	160/204 (78%)	153 (96%)	7 (4%)	28	61
1	B5	162/204 (79%)	153 (94%)	9 (6%)	21	52
1	B6	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	BA	160/204 (78%)	152 (95%)	8 (5%)	24	57
1	BB	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	BC	186/204 (91%)	176 (95%)	10 (5%)	22	54
1	BF	160/204 (78%)	150 (94%)	10 (6%)	18	46
1	BG	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	BH	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	BK	160/204 (78%)	152 (95%)	8 (5%)	24	57
1	BL	162/204 (79%)	153 (94%)	9 (6%)	21	52
1	BM	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	BP	160/204 (78%)	151 (94%)	9 (6%)	21	52
1	BQ	162/204 (79%)	151 (93%)	11 (7%)	16	42
1	BR	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	BU	160/204 (78%)	152 (95%)	8 (5%)	24	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BV	162/204 (79%)	153 (94%)	9 (6%)	21	52
1	BW	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	BZ	160/204 (78%)	152 (95%)	8 (5%)	24	57
1	Ba	162/204 (79%)	153 (94%)	9 (6%)	21	52
1	Bb	186/204 (91%)	175 (94%)	11 (6%)	19	49
1	Be	160/204 (78%)	152 (95%)	8 (5%)	24	57
1	Bf	162/204 (79%)	153 (94%)	9 (6%)	21	52
1	Bg	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	Bj	160/204 (78%)	152 (95%)	8 (5%)	24	57
1	Bk	162/204 (79%)	153 (94%)	9 (6%)	21	52
1	Bl	186/204 (91%)	176 (95%)	10 (5%)	22	54
1	Bo	160/204 (78%)	151 (94%)	9 (6%)	21	52
1	Bp	162/204 (79%)	151 (93%)	11 (7%)	16	42
1	Bq	186/204 (91%)	175 (94%)	11 (6%)	19	49
1	Bt	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	Bu	162/204 (79%)	153 (94%)	9 (6%)	21	52
1	Bv	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	By	160/204 (78%)	150 (94%)	10 (6%)	18	46
1	Bz	162/204 (79%)	151 (93%)	11 (7%)	16	42
1	C1	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	C4	160/204 (78%)	151 (94%)	9 (6%)	21	52
1	C5	162/204 (79%)	151 (93%)	11 (7%)	16	42
1	C6	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	CA	160/204 (78%)	150 (94%)	10 (6%)	18	46
1	CB	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	CC	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	CF	160/204 (78%)	152 (95%)	8 (5%)	24	57
1	CG	162/204 (79%)	153 (94%)	9 (6%)	21	52
1	CH	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	CK	160/204 (78%)	152 (95%)	8 (5%)	24	57
1	CL	162/204 (79%)	152 (94%)	10 (6%)	18	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CM	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	CP	160/204 (78%)	153 (96%)	7 (4%)	28	61
1	CQ	162/204 (79%)	154 (95%)	8 (5%)	25	57
1	CR	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	CU	160/204 (78%)	151 (94%)	9 (6%)	21	52
1	CV	162/204 (79%)	150 (93%)	12 (7%)	13	38
1	CW	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	CZ	160/204 (78%)	148 (92%)	12 (8%)	13	37
1	Ca	162/204 (79%)	151 (93%)	11 (7%)	16	42
1	Cb	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	Ce	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	Cf	162/204 (79%)	151 (93%)	11 (7%)	16	42
1	Cg	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	Cj	160/204 (78%)	152 (95%)	8 (5%)	24	57
1	Ck	162/204 (79%)	150 (93%)	12 (7%)	13	38
1	Cl	186/204 (91%)	176 (95%)	10 (5%)	22	54
1	Co	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	Cp	162/204 (79%)	153 (94%)	9 (6%)	21	52
1	Cq	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	Ct	160/204 (78%)	153 (96%)	7 (4%)	28	61
1	Cu	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	Cv	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	Cy	160/204 (78%)	151 (94%)	9 (6%)	21	52
1	Cz	162/204 (79%)	151 (93%)	11 (7%)	16	42
1	D1	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	D4	160/204 (78%)	151 (94%)	9 (6%)	21	52
1	D5	162/204 (79%)	153 (94%)	9 (6%)	21	52
1	D6	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	DA	160/204 (78%)	152 (95%)	8 (5%)	24	57
1	DB	162/204 (79%)	150 (93%)	12 (7%)	13	38
1	DC	186/204 (91%)	175 (94%)	11 (6%)	19	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DF	160/204 (78%)	153 (96%)	7 (4%)	28	61
1	DG	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	DH	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	DK	160/204 (78%)	151 (94%)	9 (6%)	21	52
1	DL	162/204 (79%)	153 (94%)	9 (6%)	21	52
1	DM	186/204 (91%)	176 (95%)	10 (5%)	22	54
1	DP	160/204 (78%)	153 (96%)	7 (4%)	28	61
1	DQ	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	DR	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	DU	160/204 (78%)	151 (94%)	9 (6%)	21	52
1	DV	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	DW	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	DZ	160/204 (78%)	151 (94%)	9 (6%)	21	52
1	Da	162/204 (79%)	151 (93%)	11 (7%)	16	42
1	Db	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	De	160/204 (78%)	152 (95%)	8 (5%)	24	57
1	Df	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	Dg	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	Dj	160/204 (78%)	149 (93%)	11 (7%)	15	41
1	Dk	162/204 (79%)	154 (95%)	8 (5%)	25	57
1	Dl	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	Do	160/204 (78%)	153 (96%)	7 (4%)	28	61
1	Dp	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	Dq	186/204 (91%)	176 (95%)	10 (5%)	22	54
1	Dt	160/204 (78%)	151 (94%)	9 (6%)	21	52
1	Du	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	Dv	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	Dy	160/204 (78%)	150 (94%)	10 (6%)	18	46
1	Dz	162/204 (79%)	151 (93%)	11 (7%)	16	42
1	E1	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	E4	160/204 (78%)	152 (95%)	8 (5%)	24	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E5	162/204 (79%)	153 (94%)	9 (6%)	21	52
1	E6	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	EA	160/204 (78%)	152 (95%)	8 (5%)	24	57
1	EB	162/204 (79%)	151 (93%)	11 (7%)	16	42
1	EC	186/204 (91%)	175 (94%)	11 (6%)	19	49
1	EF	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	EG	162/204 (79%)	153 (94%)	9 (6%)	21	52
1	EH	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	EK	160/204 (78%)	153 (96%)	7 (4%)	28	61
1	EL	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	EM	186/204 (91%)	176 (95%)	10 (5%)	22	54
1	EP	160/204 (78%)	152 (95%)	8 (5%)	24	57
1	EQ	162/204 (79%)	154 (95%)	8 (5%)	25	57
1	ER	186/204 (91%)	176 (95%)	10 (5%)	22	54
1	EU	160/204 (78%)	151 (94%)	9 (6%)	21	52
1	EV	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	EW	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	EZ	160/204 (78%)	151 (94%)	9 (6%)	21	52
1	Ea	162/204 (79%)	153 (94%)	9 (6%)	21	52
1	Eb	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	Ee	160/204 (78%)	153 (96%)	7 (4%)	28	61
1	Ef	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	Eg	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	Ej	160/204 (78%)	152 (95%)	8 (5%)	24	57
1	Ek	162/204 (79%)	153 (94%)	9 (6%)	21	52
1	El	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	Eo	160/204 (78%)	151 (94%)	9 (6%)	21	52
1	Ep	162/204 (79%)	152 (94%)	10 (6%)	18	47
1	Eq	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	Et	160/204 (78%)	153 (96%)	7 (4%)	28	61
1	Eu	162/204 (79%)	152 (94%)	10 (6%)	18	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ev	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	Ey	160/204 (78%)	152 (95%)	8 (5%)	24	57
1	Ez	162/204 (79%)	151 (93%)	11 (7%)	16	42
1	F1	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	F4	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	F5	162/204 (79%)	155 (96%)	7 (4%)	29	62
1	F6	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	FA	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	FB	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	FC	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	FF	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	FG	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	FH	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	FK	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	FL	162/204 (79%)	155 (96%)	7 (4%)	29	62
1	FM	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	FP	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	FQ	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	FR	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	FU	160/204 (78%)	152 (95%)	8 (5%)	24	57
1	FV	162/204 (79%)	154 (95%)	8 (5%)	25	57
1	FW	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	FZ	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	Fa	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	Fb	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	Fe	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	Ff	162/204 (79%)	155 (96%)	7 (4%)	29	62
1	Fg	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	Fj	160/204 (78%)	153 (96%)	7 (4%)	28	61
1	Fk	162/204 (79%)	157 (97%)	5 (3%)	40	74
1	Fl	186/204 (91%)	179 (96%)	7 (4%)	33	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Fo	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	Fp	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	Fq	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	Ft	160/204 (78%)	153 (96%)	7 (4%)	28	61
1	Fu	162/204 (79%)	154 (95%)	8 (5%)	25	57
1	Fv	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	Fy	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	Fz	162/204 (79%)	155 (96%)	7 (4%)	29	62
1	G1	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	G4	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	G5	162/204 (79%)	157 (97%)	5 (3%)	40	74
1	G6	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	GA	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	GB	162/204 (79%)	154 (95%)	8 (5%)	25	57
1	GC	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	GF	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	GG	162/204 (79%)	155 (96%)	7 (4%)	29	62
1	GH	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	GK	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	GL	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	GM	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	GP	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	GQ	162/204 (79%)	154 (95%)	8 (5%)	25	57
1	GR	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	GU	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	GV	162/204 (79%)	155 (96%)	7 (4%)	29	62
1	GW	186/204 (91%)	177 (95%)	9 (5%)	25	58
1	GZ	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	Ga	162/204 (79%)	154 (95%)	8 (5%)	25	57
1	Gb	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	Ge	160/204 (78%)	155 (97%)	5 (3%)	40	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Gf	162/204 (79%)	155 (96%)	7 (4%)	29	62
1	Gg	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	Gj	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	Gk	162/204 (79%)	155 (96%)	7 (4%)	29	62
1	Gl	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	Go	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	Gp	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	Gq	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	Gt	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	Gu	162/204 (79%)	155 (96%)	7 (4%)	29	62
1	Gv	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	Gy	160/204 (78%)	153 (96%)	7 (4%)	28	61
1	Gz	162/204 (79%)	157 (97%)	5 (3%)	40	74
1	H1	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	H4	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	H5	162/204 (79%)	154 (95%)	8 (5%)	25	57
1	H6	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	HA	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	HB	162/204 (79%)	155 (96%)	7 (4%)	29	62
1	HC	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	HF	160/204 (78%)	156 (98%)	4 (2%)	47	78
1	HG	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	HH	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	HK	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	HL	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	HM	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	HP	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	HQ	162/204 (79%)	155 (96%)	7 (4%)	29	62
1	HR	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	HU	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	HV	162/204 (79%)	156 (96%)	6 (4%)	34	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	HW	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	HZ	160/204 (78%)	153 (96%)	7 (4%)	28	61
1	Ha	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	Hb	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	He	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	Hf	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	Hg	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	Hj	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	Hk	162/204 (79%)	155 (96%)	7 (4%)	29	62
1	Hl	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	Ho	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	Hp	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	Hq	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	Ht	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	Hu	162/204 (79%)	157 (97%)	5 (3%)	40	74
1	Hv	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	Hy	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	Hz	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	I1	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	I4	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	I5	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	I6	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	IA	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	IB	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	IC	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	IF	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	IG	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	IH	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	IK	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	IL	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	IM	186/204 (91%)	180 (97%)	6 (3%)	39	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	IP	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	IQ	162/204 (79%)	155 (96%)	7 (4%)	29	62
1	IR	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	IU	160/204 (78%)	153 (96%)	7 (4%)	28	61
1	IV	162/204 (79%)	154 (95%)	8 (5%)	25	57
1	IW	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	IZ	160/204 (78%)	153 (96%)	7 (4%)	28	61
1	Ia	162/204 (79%)	154 (95%)	8 (5%)	25	57
1	Ib	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	Ie	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	If	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	Ig	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	Ij	160/204 (78%)	156 (98%)	4 (2%)	47	78
1	Ik	162/204 (79%)	155 (96%)	7 (4%)	29	62
1	Il	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	Io	160/204 (78%)	156 (98%)	4 (2%)	47	78
1	Ip	162/204 (79%)	155 (96%)	7 (4%)	29	62
1	Iq	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	It	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	Iu	162/204 (79%)	155 (96%)	7 (4%)	29	62
1	Iv	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	Iy	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	Iz	162/204 (79%)	155 (96%)	7 (4%)	29	62
1	J1	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	J4	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	J5	162/204 (79%)	154 (95%)	8 (5%)	25	57
1	J6	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	JA	160/204 (78%)	156 (98%)	4 (2%)	47	78
1	JB	162/204 (79%)	155 (96%)	7 (4%)	29	62
1	JC	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	JF	160/204 (78%)	154 (96%)	6 (4%)	33	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	JG	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	JH	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	JK	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	JL	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	JM	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	JP	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	JQ	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	JR	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	JU	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	JV	162/204 (79%)	154 (95%)	8 (5%)	25	57
1	JW	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	JZ	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	Ja	162/204 (79%)	157 (97%)	5 (3%)	40	74
1	Jb	186/204 (91%)	178 (96%)	8 (4%)	29	62
1	Je	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	Jf	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	Jg	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	Jj	160/204 (78%)	154 (96%)	6 (4%)	33	67
1	Jk	162/204 (79%)	154 (95%)	8 (5%)	25	57
1	Jl	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	Jo	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	Jp	162/204 (79%)	154 (95%)	8 (5%)	25	57
1	Jq	186/204 (91%)	179 (96%)	7 (4%)	33	67
1	Jt	160/204 (78%)	153 (96%)	7 (4%)	28	61
1	Ju	162/204 (79%)	155 (96%)	7 (4%)	29	62
1	Jv	186/204 (91%)	180 (97%)	6 (3%)	39	73
1	Jy	160/204 (78%)	155 (97%)	5 (3%)	40	74
1	Jz	162/204 (79%)	154 (95%)	8 (5%)	25	57
All	All	60960/73440 (83%)	58192 (96%)	2768 (4%)	27	61

5 of 2768 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F6	131	PRO
1	H1	189	THR
1	GM	76	THR
1	F6	72	THR
1	G6	76	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1669 such sidechains are listed below:

Mol	Chain	Res	Type
1	FV	67	GLN
1	Gp	113	HIS
1	Jg	69	ASN
1	Fg	52	GLN
1	FV	52	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A2	16/17 (94%)	3 (18%)	3 (18%)
2	A7	16/17 (94%)	3 (18%)	3 (18%)
2	AD	16/17 (94%)	3 (18%)	3 (18%)
2	AI	16/17 (94%)	3 (18%)	3 (18%)
2	AN	16/17 (94%)	3 (18%)	3 (18%)
2	AS	16/17 (94%)	3 (18%)	3 (18%)
2	AX	16/17 (94%)	3 (18%)	3 (18%)
2	Ac	16/17 (94%)	3 (18%)	0
2	Ah	16/17 (94%)	3 (18%)	0
2	Am	16/17 (94%)	3 (18%)	0
2	Ar	16/17 (94%)	3 (18%)	0
2	Aw	16/17 (94%)	3 (18%)	0
2	B2	16/17 (94%)	3 (18%)	3 (18%)
2	B7	16/17 (94%)	3 (18%)	3 (18%)
2	BD	16/17 (94%)	3 (18%)	3 (18%)
2	BI	16/17 (94%)	3 (18%)	3 (18%)
2	BN	16/17 (94%)	3 (18%)	3 (18%)
2	BS	16/17 (94%)	3 (18%)	3 (18%)
2	BX	16/17 (94%)	3 (18%)	3 (18%)
2	Bc	16/17 (94%)	3 (18%)	0
2	Bh	16/17 (94%)	3 (18%)	0
2	Bm	16/17 (94%)	3 (18%)	0
2	Br	16/17 (94%)	3 (18%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Bw	16/17 (94%)	3 (18%)	0
2	C2	16/17 (94%)	3 (18%)	3 (18%)
2	C7	16/17 (94%)	3 (18%)	3 (18%)
2	CD	16/17 (94%)	3 (18%)	3 (18%)
2	CI	16/17 (94%)	3 (18%)	3 (18%)
2	CN	16/17 (94%)	3 (18%)	3 (18%)
2	CS	16/17 (94%)	3 (18%)	3 (18%)
2	CX	16/17 (94%)	3 (18%)	3 (18%)
2	Cc	16/17 (94%)	3 (18%)	0
2	Ch	16/17 (94%)	3 (18%)	0
2	Cm	16/17 (94%)	3 (18%)	0
2	Cr	16/17 (94%)	3 (18%)	0
2	Cw	16/17 (94%)	3 (18%)	0
2	D2	16/17 (94%)	3 (18%)	3 (18%)
2	D7	16/17 (94%)	3 (18%)	3 (18%)
2	DD	16/17 (94%)	3 (18%)	3 (18%)
2	DI	16/17 (94%)	3 (18%)	3 (18%)
2	DN	16/17 (94%)	3 (18%)	3 (18%)
2	DS	16/17 (94%)	3 (18%)	3 (18%)
2	DX	16/17 (94%)	3 (18%)	3 (18%)
2	Dc	16/17 (94%)	3 (18%)	0
2	Dh	16/17 (94%)	3 (18%)	0
2	Dm	16/17 (94%)	3 (18%)	0
2	Dr	16/17 (94%)	3 (18%)	0
2	Dw	16/17 (94%)	3 (18%)	0
2	E2	16/17 (94%)	3 (18%)	3 (18%)
2	E7	16/17 (94%)	3 (18%)	3 (18%)
2	ED	16/17 (94%)	3 (18%)	3 (18%)
2	EI	16/17 (94%)	3 (18%)	3 (18%)
2	EN	16/17 (94%)	3 (18%)	3 (18%)
2	ES	16/17 (94%)	3 (18%)	3 (18%)
2	EX	16/17 (94%)	3 (18%)	3 (18%)
2	Ec	16/17 (94%)	3 (18%)	0
2	Eh	16/17 (94%)	3 (18%)	0
2	Em	16/17 (94%)	3 (18%)	0
2	Er	16/17 (94%)	3 (18%)	0
2	Ew	16/17 (94%)	3 (18%)	0
2	F2	16/17 (94%)	3 (18%)	3 (18%)
2	F7	16/17 (94%)	3 (18%)	3 (18%)
2	FD	16/17 (94%)	3 (18%)	3 (18%)
2	FI	16/17 (94%)	3 (18%)	3 (18%)
2	FN	16/17 (94%)	3 (18%)	3 (18%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	FS	16/17 (94%)	3 (18%)	3 (18%)
2	FX	16/17 (94%)	3 (18%)	3 (18%)
2	Fc	16/17 (94%)	3 (18%)	0
2	Fh	16/17 (94%)	3 (18%)	0
2	Fm	16/17 (94%)	3 (18%)	0
2	Fr	16/17 (94%)	3 (18%)	0
2	Fw	16/17 (94%)	3 (18%)	0
2	G2	16/17 (94%)	3 (18%)	3 (18%)
2	G7	16/17 (94%)	3 (18%)	3 (18%)
2	GD	16/17 (94%)	3 (18%)	3 (18%)
2	GI	16/17 (94%)	3 (18%)	3 (18%)
2	GN	16/17 (94%)	3 (18%)	3 (18%)
2	GS	16/17 (94%)	3 (18%)	3 (18%)
2	GX	16/17 (94%)	3 (18%)	3 (18%)
2	Gc	16/17 (94%)	3 (18%)	0
2	Gh	16/17 (94%)	3 (18%)	0
2	Gm	16/17 (94%)	3 (18%)	0
2	Gr	16/17 (94%)	3 (18%)	0
2	Gw	16/17 (94%)	3 (18%)	0
2	H2	16/17 (94%)	3 (18%)	3 (18%)
2	H7	16/17 (94%)	3 (18%)	3 (18%)
2	HD	16/17 (94%)	3 (18%)	3 (18%)
2	HI	16/17 (94%)	3 (18%)	3 (18%)
2	HN	16/17 (94%)	3 (18%)	3 (18%)
2	HS	16/17 (94%)	3 (18%)	3 (18%)
2	HX	16/17 (94%)	3 (18%)	3 (18%)
2	Hc	16/17 (94%)	3 (18%)	0
2	Hh	16/17 (94%)	3 (18%)	0
2	Hm	16/17 (94%)	3 (18%)	0
2	Hr	16/17 (94%)	3 (18%)	0
2	Hw	16/17 (94%)	3 (18%)	0
2	I2	16/17 (94%)	3 (18%)	3 (18%)
2	I7	16/17 (94%)	3 (18%)	3 (18%)
2	ID	16/17 (94%)	3 (18%)	3 (18%)
2	II	16/17 (94%)	3 (18%)	3 (18%)
2	IN	16/17 (94%)	3 (18%)	3 (18%)
2	IS	16/17 (94%)	3 (18%)	3 (18%)
2	IX	16/17 (94%)	3 (18%)	3 (18%)
2	Ic	16/17 (94%)	3 (18%)	0
2	Ih	16/17 (94%)	3 (18%)	0
2	Im	16/17 (94%)	3 (18%)	0
2	Ir	16/17 (94%)	3 (18%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Iw	16/17 (94%)	3 (18%)	0
2	J2	16/17 (94%)	3 (18%)	3 (18%)
2	J7	16/17 (94%)	3 (18%)	3 (18%)
2	JD	16/17 (94%)	3 (18%)	3 (18%)
2	JI	16/17 (94%)	3 (18%)	3 (18%)
2	JN	16/17 (94%)	3 (18%)	3 (18%)
2	JS	16/17 (94%)	3 (18%)	3 (18%)
2	JX	16/17 (94%)	3 (18%)	3 (18%)
2	Jc	16/17 (94%)	3 (18%)	0
2	Jh	16/17 (94%)	3 (18%)	0
2	Jm	16/17 (94%)	3 (18%)	0
2	Jr	16/17 (94%)	3 (18%)	0
2	Jw	16/17 (94%)	3 (18%)	0
All	All	1920/2040 (94%)	360 (18%)	210 (10%)

5 of 360 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	AD	9	U
2	AD	10	U
2	AD	11	U
2	AI	9	U
2	AI	10	U

5 of 210 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	FS	9	U
2	G2	10	U
2	JS	9	U
2	FX	10	U
2	GI	9	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 120 ligands modelled in this entry, 120 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A1	217/242 (89%)	-0.14	5 (2%)	60	58	26, 56, 111, 194	0
1	A4	185/242 (76%)	-0.23	1 (0%)	91	91	23, 52, 88, 132	0
1	A5	189/242 (78%)	-0.31	2 (1%)	80	80	18, 52, 92, 153	0
1	A6	217/242 (89%)	-0.15	8 (3%)	41	37	20, 53, 107, 200	0
1	AA	185/242 (76%)	-0.38	0	100	100	29, 54, 87, 113	0
1	AB	189/242 (78%)	-0.38	2 (1%)	80	80	25, 49, 90, 154	0
1	AC	217/242 (89%)	-0.16	7 (3%)	47	43	21, 50, 108, 201	0
1	AF	185/242 (76%)	-0.43	0	100	100	22, 48, 85, 115	0
1	AG	189/242 (78%)	-0.50	1 (0%)	91	91	17, 42, 85, 140	0
1	AH	217/242 (89%)	-0.23	7 (3%)	47	43	21, 50, 114, 203	0
1	AK	185/242 (76%)	-0.34	1 (0%)	91	91	17, 51, 88, 123	0
1	AL	189/242 (78%)	-0.39	2 (1%)	80	80	24, 47, 91, 137	0
1	AM	217/242 (89%)	-0.24	6 (2%)	53	49	19, 48, 106, 200	0
1	AP	185/242 (76%)	-0.40	0	100	100	21, 47, 87, 124	0
1	AQ	189/242 (78%)	-0.45	2 (1%)	80	80	17, 47, 87, 127	0
1	AR	217/242 (89%)	-0.24	6 (2%)	53	49	17, 48, 103, 199	0
1	AU	185/242 (76%)	-0.29	0	100	100	36, 61, 96, 124	0
1	AV	189/242 (78%)	-0.36	3 (1%)	72	71	35, 58, 91, 153	0
1	AW	217/242 (89%)	-0.07	8 (3%)	41	37	27, 58, 108, 201	0
1	AZ	185/242 (76%)	-0.54	0	100	100	14, 38, 69, 107	0
1	Aa	189/242 (78%)	-0.46	0	100	100	14, 37, 79, 138	0
1	Ab	217/242 (89%)	-0.17	6 (2%)	53	49	16, 43, 107, 197	0
1	Ae	185/242 (76%)	-0.47	0	100	100	17, 48, 92, 113	0
1	Af	189/242 (78%)	-0.38	2 (1%)	80	80	19, 44, 87, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	Ag	217/242 (89%)	-0.26	6 (2%)	53	49	18, 48, 95, 199	0
1	Aj	185/242 (76%)	-0.44	0	100	100	15, 48, 82, 114	0
1	Ak	189/242 (78%)	-0.39	0	100	100	21, 47, 85, 136	0
1	Al	217/242 (89%)	-0.19	6 (2%)	53	49	19, 44, 104, 191	0
1	Ao	185/242 (76%)	-0.28	3 (1%)	72	71	20, 46, 79, 105	0
1	Ap	189/242 (78%)	-0.50	0	100	100	19, 44, 80, 137	0
1	Aq	217/242 (89%)	-0.19	6 (2%)	53	49	16, 46, 100, 197	0
1	At	185/242 (76%)	-0.49	0	100	100	19, 45, 81, 112	0
1	Au	189/242 (78%)	-0.47	0	100	100	9, 41, 85, 128	0
1	Av	217/242 (89%)	-0.10	6 (2%)	53	49	10, 45, 106, 196	0
1	Ay	185/242 (76%)	-0.30	0	100	100	26, 57, 89, 119	0
1	Az	189/242 (78%)	-0.40	0	100	100	27, 54, 96, 132	0
1	B1	217/242 (89%)	-0.31	6 (2%)	53	49	18, 44, 101, 188	0
1	B4	185/242 (76%)	-0.30	0	100	100	36, 61, 85, 117	0
1	B5	189/242 (78%)	-0.30	2 (1%)	80	80	29, 55, 93, 145	0
1	B6	217/242 (89%)	-0.13	7 (3%)	47	43	26, 54, 116, 209	0
1	BA	185/242 (76%)	-0.31	1 (0%)	91	91	17, 56, 91, 116	0
1	BB	189/242 (78%)	-0.36	1 (0%)	91	91	22, 50, 92, 146	0
1	BC	217/242 (89%)	-0.18	7 (3%)	47	43	8, 50, 108, 193	0
1	BF	185/242 (76%)	-0.42	0	100	100	18, 45, 81, 116	0
1	BG	189/242 (78%)	-0.55	2 (1%)	80	80	10, 38, 85, 127	0
1	BH	217/242 (89%)	-0.18	6 (2%)	53	49	13, 40, 95, 200	0
1	BK	185/242 (76%)	-0.33	0	100	100	12, 48, 87, 133	0
1	BL	189/242 (78%)	-0.40	0	100	100	17, 47, 86, 130	0
1	BM	217/242 (89%)	-0.18	7 (3%)	47	43	21, 48, 107, 209	0
1	BP	185/242 (76%)	-0.44	0	100	100	22, 48, 84, 109	0
1	BQ	189/242 (78%)	-0.44	0	100	100	27, 48, 84, 139	0
1	BR	217/242 (89%)	-0.30	6 (2%)	53	49	15, 46, 101, 202	0
1	BU	185/242 (76%)	-0.27	2 (1%)	80	80	29, 59, 97, 130	0
1	BV	189/242 (78%)	-0.42	0	100	100	26, 54, 93, 137	0
1	BW	217/242 (89%)	-0.12	7 (3%)	47	43	27, 59, 110, 219	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	BZ	185/242 (76%)	-0.46	0	100	100	15, 43, 81, 120	0
1	Ba	189/242 (78%)	-0.48	0	100	100	22, 46, 88, 121	0
1	Bb	217/242 (89%)	-0.27	6 (2%)	53	49	19, 45, 111, 192	0
1	Be	185/242 (76%)	-0.44	0	100	100	17, 44, 83, 112	0
1	Bf	189/242 (78%)	-0.46	0	100	100	14, 41, 86, 119	0
1	Bg	217/242 (89%)	-0.29	7 (3%)	47	43	18, 45, 105, 176	0
1	Bj	185/242 (76%)	-0.42	0	100	100	19, 46, 79, 117	0
1	Bk	189/242 (78%)	-0.46	0	100	100	18, 47, 88, 127	0
1	Bl	217/242 (89%)	-0.21	7 (3%)	47	43	16, 48, 101, 206	0
1	Bo	185/242 (76%)	-0.36	0	100	100	20, 50, 77, 121	0
1	Bp	189/242 (78%)	-0.40	0	100	100	21, 46, 92, 129	0
1	Bq	217/242 (89%)	-0.22	6 (2%)	53	49	26, 48, 106, 189	0
1	Bt	185/242 (76%)	-0.19	2 (1%)	80	80	33, 60, 94, 120	0
1	Bu	189/242 (78%)	-0.33	0	100	100	20, 51, 94, 133	0
1	Bv	217/242 (89%)	-0.09	8 (3%)	41	37	25, 56, 111, 187	0
1	By	185/242 (76%)	-0.41	0	100	100	14, 46, 84, 123	0
1	Bz	189/242 (78%)	-0.54	1 (0%)	91	91	14, 40, 80, 139	0
1	C1	217/242 (89%)	-0.12	6 (2%)	53	49	12, 39, 104, 212	0
1	C4	185/242 (76%)	-0.36	0	100	100	19, 55, 92, 112	0
1	C5	189/242 (78%)	-0.42	1 (0%)	91	91	23, 51, 89, 164	0
1	C6	217/242 (89%)	-0.16	6 (2%)	53	49	24, 52, 109, 189	0
1	CA	185/242 (76%)	-0.28	1 (0%)	91	91	28, 52, 94, 114	0
1	CB	189/242 (78%)	-0.38	1 (0%)	91	91	18, 50, 81, 123	0
1	CC	217/242 (89%)	-0.12	7 (3%)	47	43	22, 51, 107, 181	0
1	CF	185/242 (76%)	-0.52	1 (0%)	91	91	15, 37, 79, 119	0
1	CG	189/242 (78%)	-0.53	1 (0%)	91	91	9, 36, 82, 131	0
1	CH	217/242 (89%)	-0.27	6 (2%)	53	49	15, 35, 90, 195	0
1	CK	185/242 (76%)	-0.27	2 (1%)	80	80	23, 53, 82, 125	0
1	CL	189/242 (78%)	-0.37	1 (0%)	91	91	13, 47, 84, 149	0
1	CM	217/242 (89%)	-0.12	6 (2%)	53	49	16, 50, 108, 206	0
1	CP	185/242 (76%)	-0.36	1 (0%)	91	91	23, 49, 77, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	CQ	189/242 (78%)	-0.42	1 (0%)	91	91	16, 44, 92, 126	0
1	CR	217/242 (89%)	-0.20	6 (2%)	53	49	24, 50, 106, 195	0
1	CU	185/242 (76%)	-0.31	0	100	100	28, 56, 91, 117	0
1	CV	189/242 (78%)	-0.36	3 (1%)	72	71	21, 52, 92, 144	0
1	CW	217/242 (89%)	-0.22	6 (2%)	53	49	21, 51, 107, 194	0
1	CZ	185/242 (76%)	-0.37	0	100	100	26, 55, 91, 108	0
1	Ca	189/242 (78%)	-0.44	2 (1%)	80	80	22, 53, 93, 141	0
1	Cb	217/242 (89%)	-0.23	7 (3%)	47	43	15, 50, 106, 197	0
1	Ce	185/242 (76%)	-0.45	0	100	100	17, 49, 82, 117	0
1	Cf	189/242 (78%)	-0.40	1 (0%)	91	91	20, 46, 96, 130	0
1	Cg	217/242 (89%)	-0.09	6 (2%)	53	49	16, 50, 104, 215	0
1	Cj	185/242 (76%)	-0.43	0	100	100	20, 48, 84, 109	0
1	Ck	189/242 (78%)	-0.43	1 (0%)	91	91	20, 49, 98, 146	0
1	Cl	217/242 (89%)	-0.18	6 (2%)	53	49	20, 46, 105, 204	0
1	Co	185/242 (76%)	-0.43	0	100	100	24, 49, 77, 110	0
1	Cp	189/242 (78%)	-0.45	2 (1%)	80	80	16, 47, 90, 145	0
1	Cq	217/242 (89%)	-0.14	5 (2%)	60	58	27, 52, 109, 204	0
1	Ct	185/242 (76%)	-0.44	1 (0%)	91	91	21, 45, 78, 116	0
1	Cu	189/242 (78%)	-0.55	0	100	100	11, 39, 89, 136	0
1	Cv	217/242 (89%)	-0.24	9 (4%)	37	32	19, 42, 99, 199	0
1	Cy	185/242 (76%)	-0.52	0	100	100	13, 38, 78, 107	0
1	Cz	189/242 (78%)	-0.55	4 (2%)	63	61	12, 34, 82, 123	0
1	D1	217/242 (89%)	-0.18	6 (2%)	53	49	14, 42, 106, 203	0
1	D4	185/242 (76%)	-0.44	0	100	100	19, 41, 85, 110	0
1	D5	189/242 (78%)	-0.56	1 (0%)	91	91	12, 35, 78, 121	0
1	D6	217/242 (89%)	-0.24	7 (3%)	47	43	15, 38, 95, 205	0
1	DA	185/242 (76%)	-0.32	1 (0%)	91	91	20, 49, 83, 111	0
1	DB	189/242 (78%)	-0.34	1 (0%)	91	91	16, 47, 85, 130	0
1	DC	217/242 (89%)	-0.19	6 (2%)	53	49	17, 48, 103, 188	0
1	DF	185/242 (76%)	-0.30	1 (0%)	91	91	25, 54, 85, 123	0
1	DG	189/242 (78%)	-0.45	1 (0%)	91	91	25, 51, 89, 164	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB($Å^2$)	Q<0.9
1	DH	217/242 (89%)	-0.19	6 (2%) 53 49	22, 53, 106, 186	0
1	DK	185/242 (76%)	-0.40	1 (0%) 91 91	18, 45, 78, 105	0
1	DL	189/242 (78%)	-0.45	1 (0%) 91 91	13, 40, 84, 129	0
1	DM	217/242 (89%)	-0.27	7 (3%) 47 43	15, 43, 105, 207	0
1	DP	185/242 (76%)	-0.35	0 100 100	26, 52, 91, 123	0
1	DQ	189/242 (78%)	-0.40	0 100 100	19, 47, 86, 137	0
1	DR	217/242 (89%)	-0.22	6 (2%) 53 49	17, 46, 102, 190	0
1	DU	185/242 (76%)	-0.24	3 (1%) 72 71	26, 63, 95, 128	0
1	DV	189/242 (78%)	-0.40	2 (1%) 80 80	27, 57, 94, 149	0
1	DW	217/242 (89%)	-0.08	9 (4%) 37 32	32, 60, 111, 195	0
1	DZ	185/242 (76%)	-0.40	0 100 100	22, 50, 94, 123	0
1	Da	189/242 (78%)	-0.47	0 100 100	18, 46, 89, 134	0
1	Db	217/242 (89%)	-0.01	8 (3%) 41 37	19, 49, 102, 207	0
1	De	185/242 (76%)	-0.31	0 100 100	31, 62, 93, 116	0
1	Df	189/242 (78%)	-0.43	0 100 100	22, 54, 92, 139	0
1	Dg	217/242 (89%)	-0.14	6 (2%) 53 49	24, 56, 108, 184	0
1	Dj	185/242 (76%)	-0.40	0 100 100	22, 48, 84, 115	0
1	Dk	189/242 (78%)	-0.49	3 (1%) 72 71	14, 41, 88, 147	0
1	Dl	217/242 (89%)	-0.21	6 (2%) 53 49	21, 47, 102, 192	0
1	Do	185/242 (76%)	-0.27	0 100 100	32, 59, 96, 120	0
1	Dp	189/242 (78%)	-0.33	2 (1%) 80 80	26, 57, 97, 164	0
1	Dq	217/242 (89%)	-0.12	7 (3%) 47 43	24, 56, 111, 193	0
1	Dt	185/242 (76%)	-0.31	2 (1%) 80 80	16, 48, 80, 132	0
1	Du	189/242 (78%)	-0.38	2 (1%) 80 80	23, 47, 90, 143	0
1	Dv	217/242 (89%)	-0.22	6 (2%) 53 49	18, 50, 101, 190	0
1	Dy	185/242 (76%)	-0.45	0 100 100	7, 38, 76, 98	0
1	Dz	189/242 (78%)	-0.48	2 (1%) 80 80	16, 38, 75, 130	0
1	E1	217/242 (89%)	-0.28	6 (2%) 53 49	14, 43, 102, 207	0
1	E4	185/242 (76%)	-0.46	0 100 100	18, 46, 87, 114	0
1	E5	189/242 (78%)	-0.44	1 (0%) 91 91	15, 43, 84, 124	0
1	E6	217/242 (89%)	-0.32	6 (2%) 53 49	16, 44, 106, 194	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	EA	185/242 (76%)	-0.35	1 (0%)	91	91	12, 43, 74, 108	0
1	EB	189/242 (78%)	-0.46	1 (0%)	91	91	12, 41, 81, 122	0
1	EC	217/242 (89%)	-0.21	6 (2%)	53	49	18, 43, 98, 186	0
1	EF	185/242 (76%)	-0.35	1 (0%)	91	91	22, 52, 90, 126	0
1	EG	189/242 (78%)	-0.42	1 (0%)	91	91	21, 51, 92, 151	0
1	EH	217/242 (89%)	-0.17	7 (3%)	47	43	24, 55, 114, 189	0
1	EK	185/242 (76%)	-0.34	0	100	100	25, 54, 89, 122	0
1	EL	189/242 (78%)	-0.32	1 (0%)	91	91	27, 53, 95, 126	0
1	EM	217/242 (89%)	-0.21	7 (3%)	47	43	21, 52, 108, 195	0
1	EP	185/242 (76%)	-0.41	0	100	100	17, 45, 86, 118	0
1	EQ	189/242 (78%)	-0.50	0	100	100	15, 43, 78, 131	0
1	ER	217/242 (89%)	-0.22	6 (2%)	53	49	15, 46, 105, 192	0
1	EU	185/242 (76%)	-0.40	1 (0%)	91	91	22, 52, 83, 128	0
1	EV	189/242 (78%)	-0.47	1 (0%)	91	91	16, 46, 89, 135	0
1	EW	217/242 (89%)	-0.17	6 (2%)	53	49	21, 50, 103, 200	0
1	EZ	185/242 (76%)	-0.31	2 (1%)	80	80	30, 53, 85, 118	0
1	Ea	189/242 (78%)	-0.37	0	100	100	20, 48, 90, 143	0
1	Eb	217/242 (89%)	-0.16	7 (3%)	47	43	16, 50, 105, 190	0
1	Ee	185/242 (76%)	-0.36	0	100	100	33, 59, 88, 116	0
1	Ef	189/242 (78%)	-0.39	0	100	100	21, 54, 93, 136	0
1	Eg	217/242 (89%)	0.01	8 (3%)	41	37	24, 60, 113, 203	0
1	Ej	185/242 (76%)	-0.16	2 (1%)	80	80	22, 58, 90, 113	0
1	Ek	189/242 (78%)	-0.38	4 (2%)	63	61	29, 57, 94, 139	0
1	El	217/242 (89%)	-0.06	5 (2%)	60	58	30, 56, 107, 191	0
1	Eo	185/242 (76%)	-0.36	0	100	100	25, 54, 84, 113	0
1	Ep	189/242 (78%)	-0.38	4 (2%)	63	61	20, 46, 89, 162	0
1	Eq	217/242 (89%)	-0.27	5 (2%)	60	58	23, 52, 112, 190	0
1	Et	185/242 (76%)	-0.46	0	100	100	17, 38, 77, 114	0
1	Eu	189/242 (78%)	-0.50	1 (0%)	91	91	13, 37, 80, 134	0
1	Ev	217/242 (89%)	-0.22	8 (3%)	41	37	12, 38, 97, 197	0
1	Ey	185/242 (76%)	-0.47	0	100	100	24, 48, 79, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	Ez	189/242 (78%)	-0.54	0	100	100	19, 43, 84, 139	0
1	F1	217/242 (89%)	0.25	10 (4%)	32	29	49, 80, 118, 186	0
1	F4	185/242 (76%)	-0.34	0	100	100	26, 57, 86, 112	0
1	F5	189/242 (78%)	-0.31	3 (1%)	72	71	28, 57, 94, 140	0
1	F6	217/242 (89%)	-0.06	9 (4%)	37	32	31, 64, 117, 195	0
1	FA	185/242 (76%)	-0.26	1 (0%)	91	91	22, 59, 95, 134	0
1	FB	189/242 (78%)	-0.46	1 (0%)	91	91	20, 47, 90, 148	0
1	FC	217/242 (89%)	0.15	10 (4%)	32	29	29, 62, 110, 205	0
1	FF	185/242 (76%)	-0.29	0	100	100	30, 55, 92, 114	0
1	FG	189/242 (78%)	-0.36	1 (0%)	91	91	20, 51, 92, 133	0
1	FH	217/242 (89%)	-0.11	6 (2%)	53	49	24, 60, 106, 197	0
1	FK	185/242 (76%)	-0.24	0	100	100	28, 59, 90, 131	0
1	FL	189/242 (78%)	-0.19	4 (2%)	63	61	24, 59, 100, 150	0
1	FM	217/242 (89%)	-0.11	6 (2%)	53	49	22, 54, 101, 200	0
1	FP	185/242 (76%)	-0.11	2 (1%)	80	80	24, 62, 101, 112	0
1	FQ	189/242 (78%)	-0.11	3 (1%)	72	71	23, 61, 94, 134	0
1	FR	217/242 (89%)	0.03	9 (4%)	37	32	26, 55, 118, 222	0
1	FU	185/242 (76%)	-0.37	0	100	100	32, 55, 86, 119	0
1	FV	189/242 (78%)	-0.41	1 (0%)	91	91	21, 48, 87, 130	0
1	FW	217/242 (89%)	-0.08	7 (3%)	47	43	19, 52, 105, 190	0
1	FZ	185/242 (76%)	-0.05	3 (1%)	72	71	42, 78, 106, 129	0
1	Fa	189/242 (78%)	-0.17	5 (2%)	56	52	34, 70, 104, 157	0
1	Fb	217/242 (89%)	0.09	7 (3%)	47	43	41, 70, 117, 212	0
1	Fe	185/242 (76%)	0.41	13 (7%)	16	12	63, 97, 124, 151	0
1	Ff	189/242 (78%)	0.25	14 (7%)	14	11	52, 93, 121, 163	0
1	Fg	217/242 (89%)	0.61	19 (8%)	10	7	58, 92, 134, 190	0
1	Fj	185/242 (76%)	0.06	3 (1%)	72	71	38, 74, 107, 128	0
1	Fk	189/242 (78%)	0.07	8 (4%)	36	32	35, 75, 111, 141	0
1	Fl	217/242 (89%)	0.30	8 (3%)	41	37	41, 79, 127, 203	0
1	Fo	185/242 (76%)	-0.23	5 (2%)	54	50	26, 54, 92, 120	0
1	Fp	189/242 (78%)	-0.28	0	100	100	14, 49, 93, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^{2})	Q<0.9
1	Fq	217/242 (89%)	-0.19	6 (2%) 53 49	11, 50, 103, 203	0
1	Ft	185/242 (76%)	-0.30	0 100 100	27, 55, 92, 127	0
1	Fu	189/242 (78%)	-0.40	1 (0%) 91 91	24, 51, 88, 140	0
1	Fv	217/242 (89%)	-0.18	6 (2%) 53 49	20, 53, 102, 187	0
1	Fy	185/242 (76%)	0.10	0 100 100	59, 90, 117, 135	0
1	Fz	189/242 (78%)	-0.16	5 (2%) 56 52	40, 76, 113, 150	0
1	G1	217/242 (89%)	0.08	10 (4%) 32 29	34, 66, 116, 201	0
1	G4	185/242 (76%)	0.12	6 (3%) 47 43	57, 89, 114, 148	0
1	G5	189/242 (78%)	0.16	10 (5%) 26 22	45, 83, 114, 159	0
1	G6	217/242 (89%)	0.22	12 (5%) 25 21	38, 73, 126, 187	0
1	GA	185/242 (76%)	-0.21	1 (0%) 91 91	20, 57, 92, 118	0
1	GB	189/242 (78%)	-0.29	0 100 100	28, 59, 96, 125	0
1	GC	217/242 (89%)	-0.02	10 (4%) 32 29	23, 58, 113, 202	0
1	GF	185/242 (76%)	-0.28	0 100 100	20, 56, 83, 116	0
1	GG	189/242 (78%)	-0.31	2 (1%) 80 80	22, 53, 94, 132	0
1	GH	217/242 (89%)	-0.14	6 (2%) 53 49	25, 54, 105, 188	0
1	GK	185/242 (76%)	0.27	7 (3%) 40 36	61, 90, 117, 142	0
1	GL	189/242 (78%)	0.12	10 (5%) 26 22	52, 84, 119, 165	0
1	GM	217/242 (89%)	0.22	8 (3%) 41 37	42, 77, 118, 205	0
1	GP	185/242 (76%)	-0.31	0 100 100	20, 55, 91, 125	0
1	GQ	189/242 (78%)	-0.21	2 (1%) 80 80	26, 58, 93, 117	0
1	GR	217/242 (89%)	-0.07	6 (2%) 53 49	25, 55, 106, 199	0
1	GU	185/242 (76%)	-0.34	2 (1%) 80 80	26, 55, 87, 128	0
1	GV	189/242 (78%)	-0.44	2 (1%) 80 80	15, 46, 88, 131	0
1	GW	217/242 (89%)	-0.09	6 (2%) 53 49	23, 48, 102, 194	0
1	GZ	185/242 (76%)	0.02	0 100 100	26, 67, 96, 131	0
1	Ga	189/242 (78%)	-0.27	2 (1%) 80 80	20, 55, 99, 172	0
1	Gb	217/242 (89%)	0.08	10 (4%) 32 29	32, 61, 109, 200	0
1	Ge	185/242 (76%)	0.10	6 (3%) 47 43	33, 67, 100, 126	0
1	Gf	189/242 (78%)	-0.03	3 (1%) 72 71	28, 70, 108, 147	0
1	Gg	217/242 (89%)	0.22	9 (4%) 37 32	34, 69, 117, 199	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	Gj	185/242 (76%)	0.26	7 (3%) 40 36	51, 89, 118, 144	0
1	Gk	189/242 (78%)	0.08	5 (2%) 56 52	53, 82, 114, 143	0
1	Gl	217/242 (89%)	0.27	15 (6%) 16 13	38, 75, 119, 194	0
1	Go	185/242 (76%)	0.49	15 (8%) 12 9	62, 92, 120, 144	0
1	Gp	189/242 (78%)	0.32	12 (6%) 20 16	56, 95, 124, 162	0
1	Gq	217/242 (89%)	0.23	10 (4%) 32 29	57, 91, 129, 191	0
1	Gt	185/242 (76%)	-0.24	2 (1%) 80 80	25, 56, 90, 118	0
1	Gu	189/242 (78%)	-0.32	0 100 100	24, 51, 89, 145	0
1	Gv	217/242 (89%)	-0.13	6 (2%) 53 49	24, 53, 105, 199	0
1	Gy	185/242 (76%)	-0.07	2 (1%) 80 80	35, 64, 98, 129	0
1	Gz	189/242 (78%)	-0.30	2 (1%) 80 80	34, 63, 97, 153	0
1	H1	217/242 (89%)	0.09	9 (4%) 37 32	32, 69, 116, 189	0
1	H4	185/242 (76%)	0.32	12 (6%) 18 14	56, 91, 125, 144	0
1	H5	189/242 (78%)	0.32	8 (4%) 36 32	57, 93, 122, 143	0
1	H6	217/242 (89%)	0.41	15 (6%) 16 13	55, 92, 133, 193	0
1	HA	185/242 (76%)	-0.22	2 (1%) 80 80	41, 71, 100, 130	0
1	HB	189/242 (78%)	-0.23	2 (1%) 80 80	34, 67, 106, 131	0
1	HC	217/242 (89%)	0.19	10 (4%) 32 29	46, 78, 133, 205	0
1	HF	185/242 (76%)	-0.03	1 (0%) 91 91	40, 70, 98, 130	0
1	HG	189/242 (78%)	-0.25	2 (1%) 80 80	32, 58, 99, 136	0
1	HH	217/242 (89%)	-0.05	7 (3%) 47 43	26, 60, 105, 206	0
1	HK	185/242 (76%)	-0.26	1 (0%) 91 91	30, 62, 97, 119	0
1	HL	189/242 (78%)	-0.24	1 (0%) 91 91	24, 52, 93, 141	0
1	HM	217/242 (89%)	0.02	6 (2%) 53 49	25, 64, 112, 190	0
1	HP	185/242 (76%)	-0.18	0 100 100	23, 66, 103, 127	0
1	HQ	189/242 (78%)	-0.35	0 100 100	21, 54, 99, 137	0
1	HR	217/242 (89%)	0.09	10 (4%) 32 29	24, 62, 118, 186	0
1	HU	185/242 (76%)	-0.20	2 (1%) 80 80	27, 60, 89, 126	0
1	HV	189/242 (78%)	-0.30	1 (0%) 91 91	31, 60, 104, 142	0
1	HW	217/242 (89%)	0.09	11 (5%) 28 24	38, 67, 112, 183	0
1	HZ	185/242 (76%)	-0.11	2 (1%) 80 80	36, 66, 93, 130	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB($Å^2$)	Q<0.9
1	Ha	189/242 (78%)	-0.30	3 (1%) 72 71	26, 57, 95, 154	0
1	Hb	217/242 (89%)	0.14	7 (3%) 47 43	33, 65, 107, 199	0
1	He	185/242 (76%)	0.30	8 (4%) 35 31	55, 96, 127, 153	0
1	Hf	189/242 (78%)	0.34	12 (6%) 20 16	50, 88, 122, 171	0
1	Hg	217/242 (89%)	0.50	18 (8%) 11 8	54, 94, 131, 203	0
1	Hj	185/242 (76%)	0.12	7 (3%) 40 36	51, 88, 110, 134	0
1	Hk	189/242 (78%)	-0.18	1 (0%) 91 91	35, 73, 112, 169	0
1	Hl	217/242 (89%)	0.16	9 (4%) 37 32	39, 71, 121, 178	0
1	Ho	185/242 (76%)	-0.24	1 (0%) 91 91	37, 65, 100, 127	0
1	Hp	189/242 (78%)	-0.28	1 (0%) 91 91	32, 61, 96, 139	0
1	Hq	217/242 (89%)	-0.07	7 (3%) 47 43	31, 62, 106, 201	0
1	Ht	185/242 (76%)	-0.02	4 (2%) 62 59	27, 67, 98, 131	0
1	Hu	189/242 (78%)	-0.10	5 (2%) 56 52	23, 62, 106, 162	0
1	Hv	217/242 (89%)	-0.06	8 (3%) 41 37	25, 57, 111, 205	0
1	Hy	185/242 (76%)	-0.16	0 100 100	37, 68, 108, 132	0
1	Hz	189/242 (78%)	-0.19	4 (2%) 63 61	25, 62, 101, 141	0
1	I1	217/242 (89%)	0.10	11 (5%) 28 24	23, 63, 112, 193	0
1	I4	185/242 (76%)	-0.05	4 (2%) 62 59	29, 67, 97, 116	0
1	I5	189/242 (78%)	-0.26	4 (2%) 63 61	31, 58, 97, 146	0
1	I6	217/242 (89%)	0.10	6 (2%) 53 49	30, 69, 117, 212	0
1	IA	185/242 (76%)	0.40	14 (7%) 13 10	67, 98, 122, 151	0
1	IB	189/242 (78%)	0.23	9 (4%) 30 27	53, 89, 127, 196	0
1	IC	217/242 (89%)	0.63	22 (10%) 7 5	56, 98, 138, 201	0
1	IF	185/242 (76%)	-0.06	5 (2%) 54 50	34, 68, 102, 130	0
1	IG	189/242 (78%)	-0.02	3 (1%) 72 71	46, 73, 104, 142	0
1	IH	217/242 (89%)	0.11	9 (4%) 37 32	42, 71, 118, 184	0
1	IK	185/242 (76%)	-0.28	0 100 100	35, 60, 90, 127	0
1	IL	189/242 (78%)	-0.38	1 (0%) 91 91	22, 50, 90, 138	0
1	IM	217/242 (89%)	-0.13	6 (2%) 53 49	27, 58, 112, 188	0
1	IP	185/242 (76%)	-0.11	3 (1%) 72 71	36, 68, 101, 128	0
1	IQ	189/242 (78%)	-0.22	3 (1%) 72 71	39, 65, 102, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	IR	217/242 (89%)	-0.03	7 (3%)	47	43	40, 69, 111, 186	0
1	IU	185/242 (76%)	-0.27	0	100	100	21, 55, 88, 116	0
1	IV	189/242 (78%)	-0.47	0	100	100	18, 48, 81, 134	0
1	IW	217/242 (89%)	-0.03	6 (2%)	53	49	21, 52, 107, 195	0
1	IZ	185/242 (76%)	-0.29	1 (0%)	91	91	21, 58, 87, 123	0
1	Ia	189/242 (78%)	-0.42	0	100	100	17, 46, 86, 144	0
1	Ib	217/242 (89%)	-0.15	7 (3%)	47	43	23, 50, 105, 194	0
1	Ie	185/242 (76%)	0.10	4 (2%)	62	59	53, 85, 115, 136	0
1	If	189/242 (78%)	-0.03	3 (1%)	72	71	37, 71, 116, 154	0
1	Ig	217/242 (89%)	0.09	9 (4%)	37	32	34, 70, 116, 193	0
1	Ij	185/242 (76%)	0.44	15 (8%)	12	9	56, 89, 121, 143	0
1	Ik	189/242 (78%)	0.12	4 (2%)	63	61	34, 76, 114, 152	0
1	Il	217/242 (89%)	0.44	13 (5%)	21	18	40, 85, 123, 212	0
1	Io	185/242 (76%)	-0.29	2 (1%)	80	80	26, 56, 94, 123	0
1	Ip	189/242 (78%)	-0.42	0	100	100	21, 51, 90, 140	0
1	Iq	217/242 (89%)	-0.06	7 (3%)	47	43	26, 58, 112, 189	0
1	It	185/242 (76%)	-0.22	1 (0%)	91	91	29, 59, 94, 132	0
1	Iu	189/242 (78%)	-0.32	2 (1%)	80	80	21, 53, 102, 135	0
1	Iv	217/242 (89%)	-0.14	5 (2%)	60	58	26, 54, 103, 186	0
1	Iy	185/242 (76%)	-0.11	3 (1%)	72	71	44, 73, 104, 132	0
1	Iz	189/242 (78%)	-0.26	3 (1%)	72	71	37, 67, 105, 162	0
1	J1	217/242 (89%)	0.14	6 (2%)	53	49	23, 66, 107, 195	0
1	J4	185/242 (76%)	0.32	11 (5%)	22	18	43, 83, 113, 139	0
1	J5	189/242 (78%)	0.06	6 (3%)	47	43	27, 73, 118, 145	0
1	J6	217/242 (89%)	0.32	9 (4%)	37	32	34, 74, 126, 198	0
1	JA	185/242 (76%)	0.09	4 (2%)	62	59	35, 70, 105, 127	0
1	JB	189/242 (78%)	-0.04	2 (1%)	80	80	32, 65, 110, 139	0
1	JC	217/242 (89%)	0.28	10 (4%)	32	29	31, 74, 118, 188	0
1	JF	185/242 (76%)	-0.03	3 (1%)	72	71	39, 73, 109, 134	0
1	JG	189/242 (78%)	-0.09	2 (1%)	80	80	24, 70, 109, 153	0
1	JH	217/242 (89%)	0.31	8 (3%)	41	37	42, 77, 115, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	JK	185/242 (76%)	0.49	19 (10%)	6	5	63, 97, 126, 150	0
1	JL	189/242 (78%)	0.03	4 (2%)	63	61	52, 87, 125, 168	0
1	JM	217/242 (89%)	0.53	14 (6%)	18	14	62, 98, 136, 192	0
1	JP	185/242 (76%)	0.26	9 (4%)	29	26	58, 90, 114, 148	0
1	JQ	189/242 (78%)	-0.09	2 (1%)	80	80	44, 77, 116, 137	0
1	JR	217/242 (89%)	0.34	13 (5%)	21	18	47, 85, 125, 215	0
1	JU	185/242 (76%)	-0.03	6 (3%)	47	43	38, 69, 105, 133	0
1	JV	189/242 (78%)	-0.18	1 (0%)	91	91	35, 67, 102, 152	0
1	JW	217/242 (89%)	0.18	13 (5%)	21	18	42, 79, 121, 215	0
1	JZ	185/242 (76%)	-0.13	4 (2%)	62	59	38, 68, 101, 131	0
1	Ja	189/242 (78%)	-0.06	4 (2%)	63	61	41, 76, 108, 163	0
1	Jb	217/242 (89%)	0.00	7 (3%)	47	43	36, 69, 115, 195	0
1	Je	185/242 (76%)	-0.27	0	100	100	29, 57, 92, 124	0
1	Jf	189/242 (78%)	-0.31	0	100	100	28, 58, 98, 135	0
1	Jg	217/242 (89%)	-0.14	6 (2%)	53	49	19, 51, 99, 197	0
1	Jj	185/242 (76%)	-0.40	0	100	100	22, 49, 80, 117	0
1	Jk	189/242 (78%)	-0.46	1 (0%)	91	91	14, 44, 91, 123	0
1	Jl	217/242 (89%)	-0.16	6 (2%)	53	49	17, 44, 92, 208	0
1	Jo	185/242 (76%)	-0.27	0	100	100	31, 59, 91, 124	0
1	Jp	189/242 (78%)	-0.20	1 (0%)	91	91	31, 62, 101, 130	0
1	Jq	217/242 (89%)	-0.12	8 (3%)	41	37	24, 54, 108, 199	0
1	Jt	185/242 (76%)	-0.07	1 (0%)	91	91	36, 73, 106, 129	0
1	Ju	189/242 (78%)	-0.04	5 (2%)	56	52	34, 69, 102, 152	0
1	Jv	217/242 (89%)	0.11	6 (2%)	53	49	34, 68, 121, 185	0
1	Jy	185/242 (76%)	0.07	3 (1%)	72	71	36, 71, 108, 126	0
1	Jz	189/242 (78%)	0.05	5 (2%)	56	52	34, 73, 110, 141	0
2	A2	17/17 (100%)	4.80	14 (82%)	0	0	159, 199, 279, 304	0
2	A7	17/17 (100%)	4.93	17 (100%)	0	0	154, 204, 269, 286	0
2	AD	17/17 (100%)	5.47	15 (88%)	0	0	157, 204, 281, 286	0
2	AI	17/17 (100%)	4.65	16 (94%)	0	0	164, 188, 256, 267	0
2	AN	17/17 (100%)	4.27	16 (94%)	0	0	159, 190, 274, 277	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
2	AS	17/17 (100%)	3.86	12 (70%)	0	0	154, 202, 274, 275	0
2	AX	17/17 (100%)	4.06	13 (76%)	0	0	164, 193, 269, 273	0
2	Ac	17/17 (100%)	4.29	15 (88%)	0	0	141, 188, 262, 275	0
2	Ah	17/17 (100%)	5.02	16 (94%)	0	0	154, 193, 271, 272	0
2	Am	17/17 (100%)	4.49	16 (94%)	0	0	137, 213, 264, 277	0
2	Ar	17/17 (100%)	5.11	15 (88%)	0	0	149, 198, 271, 283	0
2	Aw	17/17 (100%)	4.75	17 (100%)	0	0	163, 197, 284, 286	0
2	B2	17/17 (100%)	5.12	16 (94%)	0	0	162, 190, 261, 267	0
2	B7	17/17 (100%)	4.42	15 (88%)	0	0	177, 200, 254, 265	0
2	BD	17/17 (100%)	5.58	17 (100%)	0	0	160, 209, 274, 279	0
2	BI	17/17 (100%)	4.85	16 (94%)	0	0	156, 207, 280, 280	0
2	BN	17/17 (100%)	4.37	11 (64%)	0	0	156, 200, 262, 264	0
2	BS	17/17 (100%)	4.93	15 (88%)	0	0	159, 208, 260, 270	0
2	BX	17/17 (100%)	4.80	16 (94%)	0	0	174, 199, 274, 277	0
2	Bc	17/17 (100%)	4.66	14 (82%)	0	0	165, 199, 272, 280	0
2	Bh	17/17 (100%)	4.40	16 (94%)	0	0	163, 199, 271, 273	0
2	Bm	17/17 (100%)	4.59	16 (94%)	0	0	154, 202, 276, 289	0
2	Br	17/17 (100%)	4.91	16 (94%)	0	0	144, 200, 289, 290	0
2	Bw	17/17 (100%)	4.25	16 (94%)	0	0	154, 195, 277, 282	0
2	C2	17/17 (100%)	3.53	13 (76%)	0	0	144, 205, 267, 273	0
2	C7	17/17 (100%)	4.53	14 (82%)	0	0	164, 209, 267, 273	0
2	CD	17/17 (100%)	5.34	16 (94%)	0	0	158, 202, 277, 281	0
2	CI	17/17 (100%)	5.99	16 (94%)	0	0	159, 206, 278, 289	0
2	CN	17/17 (100%)	5.04	16 (94%)	0	0	168, 187, 268, 276	0
2	CS	17/17 (100%)	4.28	13 (76%)	0	0	157, 199, 273, 276	0
2	CX	17/17 (100%)	5.14	16 (94%)	0	0	162, 189, 274, 293	0
2	Cc	17/17 (100%)	5.33	16 (94%)	0	0	161, 205, 260, 270	0
2	Ch	17/17 (100%)	4.25	11 (64%)	0	0	151, 201, 273, 279	0
2	Cm	17/17 (100%)	5.39	17 (100%)	0	0	152, 201, 267, 268	0
2	Cr	17/17 (100%)	4.73	14 (82%)	0	0	152, 206, 261, 272	0
2	Cw	17/17 (100%)	4.94	15 (88%)	0	0	160, 193, 274, 284	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	D2	17/17 (100%)	4.31	17 (100%) 0 0	152, 201, 267, 269	0
2	D7	17/17 (100%)	4.96	15 (88%) 0 0	152, 194, 266, 269	0
2	DD	17/17 (100%)	4.80	16 (94%) 0 0	161, 204, 270, 283	0
2	DI	17/17 (100%)	4.53	13 (76%) 0 0	164, 212, 272, 278	0
2	DN	17/17 (100%)	5.20	17 (100%) 0 0	162, 207, 268, 275	0
2	DS	17/17 (100%)	4.49	14 (82%) 0 0	168, 199, 259, 264	0
2	DX	17/17 (100%)	5.43	17 (100%) 0 0	176, 203, 267, 271	0
2	Dc	17/17 (100%)	4.16	15 (88%) 0 0	159, 209, 267, 279	0
2	Dh	17/17 (100%)	5.72	17 (100%) 0 0	164, 208, 269, 280	0
2	Dm	17/17 (100%)	4.70	14 (82%) 0 0	148, 199, 269, 272	0
2	Dr	17/17 (100%)	5.90	17 (100%) 0 0	157, 207, 277, 281	0
2	Dw	17/17 (100%)	4.90	15 (88%) 0 0	152, 191, 275, 293	0
2	E2	17/17 (100%)	5.19	16 (94%) 0 0	156, 193, 283, 293	0
2	E7	17/17 (100%)	4.76	15 (88%) 0 0	156, 195, 271, 287	0
2	ED	17/17 (100%)	4.49	15 (88%) 0 0	152, 188, 275, 277	0
2	EI	17/17 (100%)	4.57	14 (82%) 0 0	160, 206, 260, 264	0
2	EN	17/17 (100%)	4.45	15 (88%) 0 0	156, 192, 258, 286	0
2	ES	17/17 (100%)	4.91	15 (88%) 0 0	162, 204, 265, 279	0
2	EX	17/17 (100%)	4.62	15 (88%) 0 0	158, 195, 272, 273	0
2	Ec	17/17 (100%)	4.09	14 (82%) 0 0	157, 196, 258, 270	0
2	Eh	17/17 (100%)	4.04	16 (94%) 0 0	172, 198, 263, 268	0
2	Em	17/17 (100%)	4.19	13 (76%) 0 0	147, 194, 261, 261	0
2	Er	17/17 (100%)	5.03	17 (100%) 0 0	159, 202, 272, 280	0
2	Ew	17/17 (100%)	5.15	17 (100%) 0 0	150, 183, 263, 264	0
2	F2	17/17 (100%)	5.40	17 (100%) 0 0	194, 214, 267, 274	0
2	F7	17/17 (100%)	4.10	15 (88%) 0 0	159, 205, 277, 288	0
2	FD	17/17 (100%)	3.84	13 (76%) 0 0	167, 208, 268, 288	0
2	FI	17/17 (100%)	3.93	15 (88%) 0 0	170, 198, 262, 266	0
2	FN	17/17 (100%)	5.26	17 (100%) 0 0	163, 208, 292, 304	0
2	FS	17/17 (100%)	4.06	13 (76%) 0 0	174, 204, 274, 289	0
2	FX	17/17 (100%)	5.25	16 (94%) 0 0	158, 198, 284, 293	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	Fc	17/17 (100%)	5.04	17 (100%) 0 0	179, 218, 269, 281	0
2	Fh	17/17 (100%)	4.01	13 (76%) 0 0	180, 240, 287, 293	0
2	Fm	17/17 (100%)	5.38	17 (100%) 0 0	181, 216, 278, 291	0
2	Fr	17/17 (100%)	5.66	16 (94%) 0 0	167, 200, 274, 280	0
2	Fw	17/17 (100%)	4.23	15 (88%) 0 0	165, 214, 286, 290	0
2	G2	17/17 (100%)	4.51	16 (94%) 0 0	170, 212, 259, 261	0
2	G7	17/17 (100%)	4.27	15 (88%) 0 0	189, 209, 259, 271	0
2	GD	17/17 (100%)	5.45	17 (100%) 0 0	168, 211, 280, 286	0
2	GI	17/17 (100%)	5.37	17 (100%) 0 0	163, 209, 263, 277	0
2	GN	17/17 (100%)	5.81	17 (100%) 0 0	185, 217, 288, 291	0
2	GS	17/17 (100%)	4.82	17 (100%) 0 0	184, 209, 263, 275	0
2	GX	17/17 (100%)	4.11	12 (70%) 0 0	166, 203, 273, 303	0
2	Gc	17/17 (100%)	4.21	13 (76%) 0 0	165, 211, 270, 276	0
2	Gh	17/17 (100%)	5.73	17 (100%) 0 0	162, 216, 260, 260	0
2	Gm	17/17 (100%)	6.02	17 (100%) 0 0	191, 213, 278, 289	0
2	Gr	17/17 (100%)	3.98	14 (82%) 0 0	192, 219, 275, 295	0
2	Gw	17/17 (100%)	5.79	16 (94%) 0 0	165, 218, 280, 284	0
2	H2	17/17 (100%)	5.56	17 (100%) 0 0	173, 207, 289, 293	0
2	H7	17/17 (100%)	5.47	17 (100%) 0 0	195, 214, 276, 279	0
2	HD	17/17 (100%)	4.92	15 (88%) 0 0	177, 229, 281, 286	0
2	HI	17/17 (100%)	4.61	16 (94%) 0 0	173, 194, 258, 289	0
2	HN	17/17 (100%)	5.18	17 (100%) 0 0	167, 214, 281, 292	0
2	HS	17/17 (100%)	4.14	15 (88%) 0 0	174, 213, 281, 294	0
2	HX	17/17 (100%)	3.92	11 (64%) 0 0	158, 206, 276, 283	0
2	Hc	17/17 (100%)	4.48	11 (64%) 0 0	173, 208, 274, 293	0
2	Hh	17/17 (100%)	5.60	16 (94%) 0 0	196, 227, 270, 292	0
2	Hm	17/17 (100%)	5.12	15 (88%) 0 0	191, 215, 278, 297	0
2	Hr	17/17 (100%)	4.63	16 (94%) 0 0	170, 214, 284, 291	0
2	Hw	17/17 (100%)	5.62	16 (94%) 0 0	170, 214, 272, 286	0
2	I2	17/17 (100%)	4.55	14 (82%) 0 0	173, 227, 265, 269	0
2	I7	17/17 (100%)	5.34	15 (88%) 0 0	169, 209, 277, 284	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
2	ID	17/17 (100%)	5.49	17 (100%)	0	0	197, 230, 270, 282	0
2	II	17/17 (100%)	5.36	17 (100%)	0	0	181, 209, 283, 298	0
2	IN	17/17 (100%)	4.78	14 (82%)	0	0	170, 195, 279, 286	0
2	IS	17/17 (100%)	5.82	17 (100%)	0	0	180, 207, 271, 276	0
2	IX	17/17 (100%)	4.48	16 (94%)	0	0	168, 215, 279, 286	0
2	Ic	17/17 (100%)	4.15	14 (82%)	0	0	165, 214, 265, 278	0
2	Ih	17/17 (100%)	5.42	17 (100%)	0	0	176, 208, 264, 275	0
2	Im	17/17 (100%)	4.53	14 (82%)	0	0	193, 215, 278, 294	0
2	Ir	17/17 (100%)	5.09	16 (94%)	0	0	175, 206, 269, 274	0
2	Iw	17/17 (100%)	4.69	16 (94%)	0	0	167, 208, 273, 276	0
2	J2	17/17 (100%)	5.61	17 (100%)	0	0	187, 220, 287, 302	0
2	J7	17/17 (100%)	4.60	17 (100%)	0	0	181, 227, 279, 294	0
2	JD	17/17 (100%)	3.84	12 (70%)	0	0	169, 211, 260, 265	0
2	JI	17/17 (100%)	5.86	16 (94%)	0	0	179, 213, 269, 274	0
2	JN	17/17 (100%)	4.88	15 (88%)	0	0	193, 227, 264, 264	0
2	JS	17/17 (100%)	5.36	16 (94%)	0	0	203, 222, 276, 276	0
2	JX	17/17 (100%)	5.35	17 (100%)	0	0	175, 221, 275, 281	0
2	Jc	17/17 (100%)	4.93	17 (100%)	0	0	177, 215, 290, 291	0
2	Jh	17/17 (100%)	4.52	13 (76%)	0	0	156, 200, 280, 285	0
2	Jm	17/17 (100%)	5.02	15 (88%)	0	0	165, 207, 294, 298	0
2	Jr	17/17 (100%)	4.49	17 (100%)	0	0	165, 208, 270, 278	0
2	Jw	17/17 (100%)	4.02	13 (76%)	0	0	180, 215, 280, 291	0
All	All	72960/89160 (81%)	-0.04	3296 (4%)	33	29	7, 58, 123, 304	0

The worst 5 of 3296 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	IW	25	ALA	25.7
1	DC	25	ALA	20.7
1	AC	25	ALA	20.2
1	Cg	25	ALA	19.6
1	Ab	25	ALA	19.3

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	CA	Ij	301	1/1	0.63	0.17	130,130,130,130	0
3	CA	Hy	301	1/1	0.65	0.21	138,138,138,138	0
3	CA	I4	301	1/1	0.69	0.22	147,147,147,147	0
3	CA	JL	301	1/1	0.73	0.11	141,141,141,141	0
3	CA	JF	301	1/1	0.74	0.09	103,103,103,103	0
3	CA	C4	301	1/1	0.77	0.12	127,127,127,127	0
3	CA	Ht	301	1/1	0.78	0.11	88,88,88,88	0
3	CA	Ce	301	1/1	0.78	0.16	113,113,113,113	0
3	CA	FA	301	1/1	0.78	0.14	94,94,94,94	0
3	CA	IR	301	1/1	0.80	0.10	119,119,119,119	0
3	CA	Io	301	1/1	0.81	0.09	85,85,85,85	0
3	CA	Jt	301	1/1	0.81	0.11	154,154,154,154	0
3	CA	IA	301	1/1	0.82	0.09	115,115,115,115	0
3	CA	Eo	301	1/1	0.82	0.13	105,105,105,105	0
3	CA	If	301	1/1	0.82	0.11	124,124,124,124	0
3	CA	F1	301	1/1	0.83	0.10	102,102,102,102	0
3	CA	Bt	301	1/1	0.83	0.08	90,90,90,90	0
3	CA	Ge	301	1/1	0.86	0.18	121,121,121,121	0
3	CA	Ee	301	1/1	0.86	0.11	102,102,102,102	0
3	CA	At	301	1/1	0.87	0.09	99,99,99,99	0
3	CA	JP	301	1/1	0.87	0.31	143,143,143,143	0
3	CA	CU	301	1/1	0.87	0.07	96,96,96,96	0
3	CA	Jo	301	1/1	0.88	0.11	105,105,105,105	0
3	CA	AF	301	1/1	0.88	0.11	92,92,92,92	0
3	CA	J4	301	1/1	0.88	0.07	110,110,110,110	0
3	CA	H4	301	1/1	0.89	0.11	115,115,115,115	0
3	CA	G1	301	1/1	0.89	0.12	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	CA	Jy	301	1/1	0.89	0.08	123,123,123,123	0
3	CA	JU	301	1/1	0.89	0.10	100,100,100,100	0
3	CA	Fe	301	1/1	0.90	0.09	123,123,123,123	0
3	CA	Do	301	1/1	0.90	0.10	87,87,87,87	0
3	CA	A1	301	1/1	0.90	0.09	106,106,106,106	0
3	CA	A4	301	1/1	0.90	0.13	81,81,81,81	0
3	CA	G4	301	1/1	0.90	0.07	109,109,109,109	0
3	CA	AP	301	1/1	0.90	0.09	81,81,81,81	0
3	CA	FZ	301	1/1	0.90	0.07	106,106,106,106	0
3	CA	JA	301	1/1	0.90	0.14	109,109,109,109	0
3	CA	IU	301	1/1	0.91	0.09	88,88,88,88	0
3	CA	DU	301	1/1	0.91	0.20	113,113,113,113	0
3	CA	Gt	301	1/1	0.91	0.09	92,92,92,92	0
3	CA	Je	301	1/1	0.91	0.12	112,112,112,112	0
3	CA	Fk	301	1/1	0.91	0.09	96,96,96,96	0
3	CA	E4	301	1/1	0.91	0.19	98,98,98,98	0
3	CA	IF	301	1/1	0.91	0.12	111,111,111,111	0
3	CA	HZ	301	1/1	0.91	0.11	88,88,88,88	0
3	CA	HF	301	1/1	0.92	0.11	101,101,101,101	0
3	CA	DZ	301	1/1	0.92	0.12	68,68,68,68	0
3	CA	GF	301	1/1	0.92	0.20	105,105,105,105	0
3	CA	Af	301	1/1	0.92	0.13	105,105,105,105	0
3	CA	EZ	301	1/1	0.92	0.08	88,88,88,88	0
3	CA	By	301	1/1	0.92	0.11	90,90,90,90	0
3	CA	BU	301	1/1	0.92	0.07	110,110,110,110	0
3	CA	IK	301	1/1	0.92	0.11	105,105,105,105	0
3	CA	I1	301	1/1	0.93	0.07	117,117,117,117	0
3	CA	Ft	301	1/1	0.93	0.05	88,88,88,88	0
3	CA	BQ	301	1/1	0.93	0.10	93,93,93,93	0
3	CA	It	301	1/1	0.93	0.07	102,102,102,102	0
3	CA	GP	301	1/1	0.94	0.04	91,91,91,91	0
3	CA	GU	301	1/1	0.94	0.09	84,84,84,84	0
3	CA	GZ	301	1/1	0.94	0.12	104,104,104,104	0
3	CA	BZ	301	1/1	0.94	0.14	97,97,97,97	0
3	CA	Gj	301	1/1	0.94	0.09	126,126,126,126	0
3	CA	Go	301	1/1	0.94	0.07	102,102,102,102	0
3	CA	DP	301	1/1	0.94	0.08	67,67,67,67	0
3	CA	CP	301	1/1	0.94	0.12	71,71,71,71	0
3	CA	Be	301	1/1	0.94	0.09	53,53,53,53	0
3	CA	HA	301	1/1	0.94	0.07	93,93,93,93	0
3	CA	Dj	301	1/1	0.94	0.11	86,86,86,86	0
3	CA	HK	301	1/1	0.94	0.08	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	BK	301	1/1	0.94	0.15	96,96,96,96	0
3	CA	Hg	301	1/1	0.94	0.07	102,102,102,102	0
3	CA	D4	301	1/1	0.94	0.15	77,77,77,77	0
3	CA	EK	301	1/1	0.94	0.10	89,89,89,89	0
3	CA	EP	301	1/1	0.94	0.17	84,84,84,84	0
3	CA	F4	301	1/1	0.94	0.06	95,95,95,95	0
3	CA	Cy	301	1/1	0.94	0.08	78,78,78,78	0
3	CA	Dt	301	1/1	0.95	0.08	76,76,76,76	0
3	CA	Hj	301	1/1	0.95	0.12	104,104,104,104	0
3	CA	Ho	301	1/1	0.95	0.16	95,95,95,95	0
3	CA	FF	301	1/1	0.95	0.09	100,100,100,100	0
3	CA	CG	301	1/1	0.95	0.07	79,79,79,79	0
3	CA	EC	301	1/1	0.95	0.16	90,90,90,90	0
3	CA	DK	301	1/1	0.95	0.10	101,101,101,101	0
3	CA	CK	301	1/1	0.95	0.09	105,105,105,105	0
3	CA	BB	301	1/1	0.95	0.15	114,114,114,114	0
3	CA	JZ	301	1/1	0.95	0.10	109,109,109,109	0
3	CA	Ao	301	1/1	0.95	0.05	93,93,93,93	0
3	CA	B5	301	1/1	0.95	0.10	95,95,95,95	0
3	CA	IZ	301	1/1	0.95	0.14	94,94,94,94	0
3	CA	Ey	301	1/1	0.95	0.24	95,95,95,95	0
3	CA	CA	301	1/1	0.95	0.04	93,93,93,93	0
3	CA	GA	301	1/1	0.96	0.07	90,90,90,90	0
3	CA	Et	301	1/1	0.96	0.07	71,71,71,71	0
3	CA	DF	301	1/1	0.96	0.05	94,94,94,94	0
3	CA	Dy	301	1/1	0.96	0.18	65,65,65,65	0
3	CA	CZ	301	1/1	0.96	0.07	84,84,84,84	0
3	CA	AU	301	1/1	0.96	0.11	102,102,102,102	0
3	CA	FU	301	1/1	0.96	0.11	91,91,91,91	0
3	CA	Cj	301	1/1	0.96	0.07	87,87,87,87	0
3	CA	Co	301	1/1	0.96	0.09	86,86,86,86	0
3	CA	EU	301	1/1	0.96	0.11	109,109,109,109	0
3	CA	Fo	301	1/1	0.96	0.07	96,96,96,96	0
3	CA	Df	301	1/1	0.96	0.05	74,74,74,74	0
3	CA	AA	301	1/1	0.96	0.13	75,75,75,75	0
3	CA	Aj	301	1/1	0.96	0.09	70,70,70,70	0
3	CA	HU	301	1/1	0.96	0.09	78,78,78,78	0
3	CA	EF	301	1/1	0.97	0.10	112,112,112,112	0
3	CA	GK	301	1/1	0.97	0.04	97,97,97,97	0
3	CA	Ct	301	1/1	0.97	0.11	79,79,79,79	0
3	CA	AL	301	1/1	0.97	0.13	85,85,85,85	0
3	CA	AZ	301	1/1	0.97	0.12	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	CA	Jj	301	1/1	0.97	0.13	74,74,74,74	0
3	CA	Bk	301	1/1	0.97	0.06	90,90,90,90	0
3	CA	Bo	301	1/1	0.97	0.11	74,74,74,74	0
3	CA	FK	301	1/1	0.97	0.11	91,91,91,91	0
3	CA	Ek	301	1/1	0.97	0.10	74,74,74,74	0
3	CA	FP	301	1/1	0.98	0.13	80,80,80,80	0
3	CA	BF	301	1/1	0.98	0.04	88,88,88,88	0
3	CA	DA	301	1/1	0.98	0.09	67,67,67,67	0
3	CA	HP	301	1/1	0.98	0.12	81,81,81,81	0

6.5 Other polymers

There are no such residues in this entry.