



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 05:43 PM BST

PDB ID : 4CTG
EMDB ID: : EMD-2390
Title : The limits of structural plasticity in a picornavirus capsid revealed by a massively expanded equine rhinitis A virus particle
Authors : Bakker, S.E.; Groppelli, E.; Pearson, A.R.; Stockley, P.G.; Rowlands, D.J.; Ranson, N.A.
Deposited on : 2014-05-21
Resolution : 17.00 Å(reported)
Based on PDB ID : 2WFF

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

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

A user guide is available at

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

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

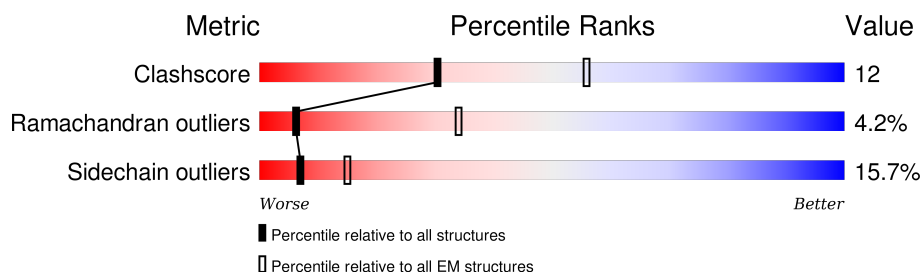
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 17.00 Å.

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
















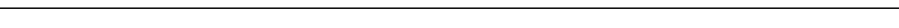











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A0	246	
1	A1	246	
1	A2	246	
1	A3	246	
1	A4	246	
1	A5	246	
1	A6	246	
1	A7	246	
1	A8	246	


























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Mol	Chain	Length	Quality of chain
1	A9	246	 60% 28% 10% •
1	AA	246	 61% 27% 10% •
1	AB	246	 61% 27% 10% •
1	AC	246	 61% 27% 10% •
1	AD	246	 60% 28% 10% •
1	AE	246	 60% 28% 10% •
1	AF	246	 60% 28% 10% •
1	AG	246	 60% 28% 9% •
1	AH	246	 60% 28% 10% •
1	AI	246	 61% 27% 10% •
1	AJ	246	 60% 28% 9% •
1	AK	246	 60% 28% 10% •
1	AL	246	 59% 28% 10% •
1	AM	246	 61% 27% 10% •
1	AN	246	 60% 28% 10% •
1	AO	246	 60% 28% 10% •
1	AP	246	 60% 28% 10% •
1	AQ	246	 61% 28% 9% •
1	AR	246	 60% 28% 10% •
1	AS	246	 61% 28% 9% •
1	AT	246	 61% 27% 10% •
1	AU	246	 61% 27% 10% •
1	AV	246	 61% 28% 9% •
1	AW	246	 60% 28% 10% •
1	AX	246	 60% 28% 10% •


























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Mol	Chain	Length	Quality of chain
1	AY	246	
1	AZ	246	
1	Aa	246	
1	Ab	246	
1	Ac	246	
1	Ad	246	
1	Ae	246	
1	Af	246	
1	Ag	246	
1	Ah	246	
1	Ai	246	
1	Aj	246	
1	Ak	246	
1	Al	246	
1	Am	246	
1	An	246	
1	Ao	246	
1	DC	246	
1	DD	246	
1	DE	246	
1	DF	246	
1	DG	246	
1	DH	246	
1	DI	246	
1	DJ	246	












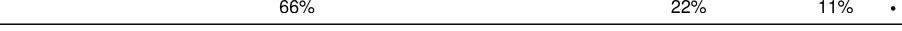







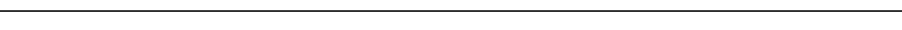

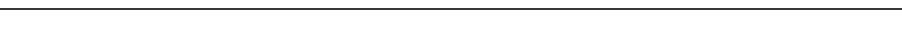
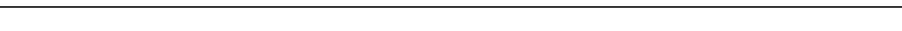


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Mol	Chain	Length	Quality of chain
1	DK	246	 60% 28% 10% .
2	B0	200	 66% 23% 11% .
2	B1	200	 66% 22% 11% .
2	B2	200	 66% 22% 11% .
2	B3	200	 65% 23% 11% .
2	B4	200	 64% 23% 12% .
2	B5	200	 67% 21% 11% .
2	B6	200	 66% 21% 12% .
2	B7	200	 67% 21% 11% .
2	B8	200	 65% 23% 11% .
2	B9	200	 67% 22% 11% .
2	BA	200	 65% 23% 11% .
2	BB	200	 66% 22% 12% .
2	BC	200	 66% 22% 11% .
2	BD	200	 66% 21% 12% .
2	BE	200	 65% 23% 12% .
2	BF	200	 65% 22% 12% .
2	BG	200	 65% 23% 11% .
2	BH	200	 65% 23% 11% .
2	BI	200	 65% 22% 12% .
2	BJ	200	 67% 21% 12% .
2	BK	200	 66% 22% 11% .
2	BL	200	 66% 23% 11% .
2	BM	200	 66% 22% 11% .
2	BN	200	 65% 23% 12% .











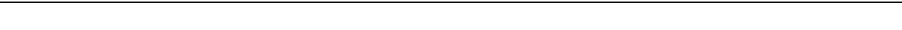

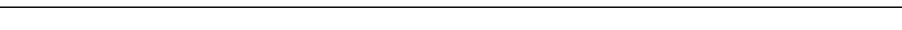
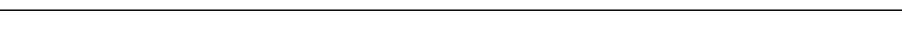











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Mol	Chain	Length	Quality of chain
2	BO	200	 64% 24% 11% .
2	BP	200	 66% 22% 11% .
2	BQ	200	 66% 22% 12% .
2	BR	200	 65% 23% 11% .
2	BS	200	 66% 22% 11% .
2	BT	200	 66% 21% 12% .
2	BU	200	 66% 22% 11% .
2	BV	200	 66% 22% 11% .
2	BW	200	 66% 23% 11% .
2	BX	200	 66% 22% 11% .
2	BY	200	 67% 21% 11% .
2	BZ	200	 66% 22% 11% .
2	Ba	200	 81% 17% ..
2	Bb	200	 81% 17% ..
2	Bc	200	 81% 17% ..
2	Bd	200	 81% 17% ..
2	Be	200	 81% 17% ..
2	Bf	200	 81% 17% ..
2	Bg	200	 81% 17% ..
2	Bh	200	 81% 17% ..
2	Bi	200	 81% 17% ..
2	Bj	200	 81% 17% ..
2	Bk	200	 81% 17% ..
2	Bl	200	 81% 17% ..
2	Bm	200	 81% 17% ..














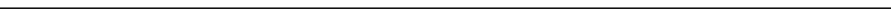











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Mol	Chain	Length	Quality of chain
2	Bn	200	 81% 17% ..
2	Bo	200	 81% 17% ..
2	Bp	200	 81% 17% ..
2	Bq	200	 81% 17% ..
2	Br	200	 81% 17% ..
2	Bs	200	 81% 17% ..
2	Bt	200	 81% 17% ..
2	Bu	200	 81% 17% ..
2	Bv	200	 81% 17% ..
2	Bw	200	 81% 17% ..
2	Bx	200	 81% 17% ..
3	C0	226	 64% 26% 9% .
3	C1	226	 62% 28% 8% .
3	C2	226	 62% 28% 9% .
3	C3	226	 64% 26% 9% .
3	C4	226	 62% 28% 8% .
3	C5	226	 62% 28% 9% .
3	C6	226	 63% 27% 9% .
3	C7	226	 63% 27% 9% .
3	C8	226	 62% 28% 9% .
3	C9	226	 62% 28% 8% .
3	CA	226	 62% 28% 8% .
3	CB	226	 62% 27% 9% .
3	CC	226	 62% 28% 9% .
3	CD	226	 62% 28% 9% .













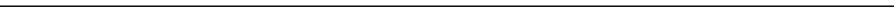
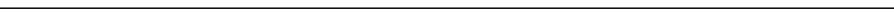







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Mol	Chain	Length	Quality of chain
3	CE	226	 62% 27% 9% .
3	CF	226	 62% 28% 8% .
3	CG	226	 62% 29% 8% .
3	CH	226	 62% 28% 8% .
3	CI	226	 62% 27% 9% .
3	CJ	226	 62% 28% 8% .
3	CK	226	 62% 27% 9% .
3	CL	226	 62% 27% 9% .
3	CM	226	 62% 27% 9% .
3	CN	226	 62% 28% 8% .
3	CO	226	 62% 28% 8% .
3	CP	226	 62% 28% 9% .
3	CQ	226	 62% 28% 9% .
3	CR	226	 62% 28% 8% .
3	CS	226	 62% 27% 9% .
3	CT	226	 62% 28% 9% .
3	CU	226	 62% 28% 8% .
3	CV	226	 62% 28% 9% .
3	CW	226	 62% 27% 9% .
3	CX	226	 62% 27% 9% .
3	CY	226	 62% 28% 9% .
3	CZ	226	 64% 27% 9% .
3	Cc	226	 80% 16% .
3	Cd	226	 80% 16% .
3	Ce	226	 80% 16% .

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Mol	Chain	Length	Quality of chain
3	Cf	226	 80% 16% .
3	Cg	226	 80% 16% .
3	Ch	226	 80% 16% .
3	Ci	226	 80% 16% .
3	Cj	226	 80% 16% .
3	Ck	226	 80% 16% .
3	Cl	226	 80% 16% .
3	Cm	226	 80% 16% .
3	Cn	226	 80% 16% .
3	Co	226	 80% 16% .
3	Cp	226	 80% 16% .
3	Cq	226	 80% 16% .
3	Cr	226	 80% 16% .
3	Cs	226	 80% 16% .
3	Ct	226	 80% 16% .
3	Cu	226	 80% 16% .
3	Cv	226	 80% 16% .
3	Cw	226	 80% 16% .
3	Cx	226	 80% 16% .
3	DA	226	 63% 27% 8% .
3	DB	226	 62% 28% 9% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 311940 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AB	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AC	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AD	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AE	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AF	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AG	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AH	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AI	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AJ	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AK	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AL	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AM	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AN	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AO	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AP	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AQ	246	Total 1928	C 1240	N 329	O 351	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AR	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AS	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AT	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AU	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AV	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AW	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AX	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AY	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	AZ	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	A0	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	A1	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	A2	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	A3	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	A4	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	A5	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	A6	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	A7	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	A8	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	A9	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	Aa	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	Ab	246	Total 1928	C 1240	N 329	O 351	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ac	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	Ad	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	Ae	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	Af	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	Ag	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	Ah	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	Ai	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	Aj	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	Ak	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	Al	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	Am	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	An	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	Ao	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	DC	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	DD	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	DE	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	DF	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	DG	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	DH	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	DI	246	Total 1928	C 1240	N 329	O 351	S 8	0	0
1	DJ	246	Total 1928	C 1240	N 329	O 351	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	DK	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		

- Molecule 2 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BA	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BB	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BC	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BD	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BE	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BF	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BG	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BH	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BI	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BJ	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BK	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BL	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BM	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BN	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BR	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BO	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BS	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BP	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BQ	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BT	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BU	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BV	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BW	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BX	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BY	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BZ	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B0	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B1	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B2	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B3	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B4	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B5	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B6	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B7	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B8	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B9	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Ba	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bb	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bc	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Bd	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Be	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bf	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bg	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bh	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bi	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bj	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bk	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bl	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bm	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bn	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bo	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bp	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bq	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Br	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bs	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bt	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bu	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bv	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bw	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bx	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B0	85	SER	GLY	CONFLICT	UNP Q91B42
B1	85	SER	GLY	CONFLICT	UNP Q91B42
B2	85	SER	GLY	CONFLICT	UNP Q91B42
B3	85	SER	GLY	CONFLICT	UNP Q91B42
B4	85	SER	GLY	CONFLICT	UNP Q91B42
B5	85	SER	GLY	CONFLICT	UNP Q91B42
B6	85	SER	GLY	CONFLICT	UNP Q91B42
B7	85	SER	GLY	CONFLICT	UNP Q91B42
B8	85	SER	GLY	CONFLICT	UNP Q91B42
B9	85	SER	GLY	CONFLICT	UNP Q91B42
BA	85	SER	GLY	CONFLICT	UNP Q91B42
BB	85	SER	GLY	CONFLICT	UNP Q91B42
BC	85	SER	GLY	CONFLICT	UNP Q91B42
BD	85	SER	GLY	CONFLICT	UNP Q91B42
BE	85	SER	GLY	CONFLICT	UNP Q91B42
BF	85	SER	GLY	CONFLICT	UNP Q91B42
BG	85	SER	GLY	CONFLICT	UNP Q91B42
BH	85	SER	GLY	CONFLICT	UNP Q91B42
BI	85	SER	GLY	CONFLICT	UNP Q91B42
BJ	85	SER	GLY	CONFLICT	UNP Q91B42
BK	85	SER	GLY	CONFLICT	UNP Q91B42
BL	85	SER	GLY	CONFLICT	UNP Q91B42
BM	85	SER	GLY	CONFLICT	UNP Q91B42
BN	85	SER	GLY	CONFLICT	UNP Q91B42
BO	85	SER	GLY	CONFLICT	UNP Q91B42
BP	85	SER	GLY	CONFLICT	UNP Q91B42
BQ	85	SER	GLY	CONFLICT	UNP Q91B42
BR	85	SER	GLY	CONFLICT	UNP Q91B42
BS	85	SER	GLY	CONFLICT	UNP Q91B42
BT	85	SER	GLY	CONFLICT	UNP Q91B42
BU	85	SER	GLY	CONFLICT	UNP Q91B42
BV	85	SER	GLY	CONFLICT	UNP Q91B42
BW	85	SER	GLY	CONFLICT	UNP Q91B42
BX	85	SER	GLY	CONFLICT	UNP Q91B42
BY	85	SER	GLY	CONFLICT	UNP Q91B42
BZ	85	SER	GLY	CONFLICT	UNP Q91B42
Ba	85	SER	GLY	CONFLICT	UNP Q91B42
Bb	85	SER	GLY	CONFLICT	UNP Q91B42
Bc	85	SER	GLY	CONFLICT	UNP Q91B42
Bd	85	SER	GLY	CONFLICT	UNP Q91B42
Be	85	SER	GLY	CONFLICT	UNP Q91B42
Bf	85	SER	GLY	CONFLICT	UNP Q91B42

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Chain	Residue	Modelled	Actual	Comment	Reference
Bg	85	SER	GLY	CONFLICT	UNP Q91B42
Bh	85	SER	GLY	CONFLICT	UNP Q91B42
Bi	85	SER	GLY	CONFLICT	UNP Q91B42
Bj	85	SER	GLY	CONFLICT	UNP Q91B42
Bk	85	SER	GLY	CONFLICT	UNP Q91B42
Bl	85	SER	GLY	CONFLICT	UNP Q91B42
Bm	85	SER	GLY	CONFLICT	UNP Q91B42
Bn	85	SER	GLY	CONFLICT	UNP Q91B42
Bo	85	SER	GLY	CONFLICT	UNP Q91B42
Bp	85	SER	GLY	CONFLICT	UNP Q91B42
Bq	85	SER	GLY	CONFLICT	UNP Q91B42
Br	85	SER	GLY	CONFLICT	UNP Q91B42
Bs	85	SER	GLY	CONFLICT	UNP Q91B42
Bt	85	SER	GLY	CONFLICT	UNP Q91B42
Bu	85	SER	GLY	CONFLICT	UNP Q91B42
Bv	85	SER	GLY	CONFLICT	UNP Q91B42
Bw	85	SER	GLY	CONFLICT	UNP Q91B42
Bx	85	SER	GLY	CONFLICT	UNP Q91B42

- Molecule 3 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	CA	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CB	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CC	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CD	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CE	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CF	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CG	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CH	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CI	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CJ	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	CK	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CL	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CM	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CN	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CO	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CP	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CQ	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CR	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CS	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CT	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CU	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CV	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CW	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CX	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CY	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CZ	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	C0	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	C1	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	C2	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	C3	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	C4	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	C5	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	C6	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	C7	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	C8	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	C9	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cc	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cd	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Ce	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cf	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cg	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Ch	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Ci	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cj	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Ck	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cl	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cm	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cn	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Co	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cp	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cq	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cr	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		

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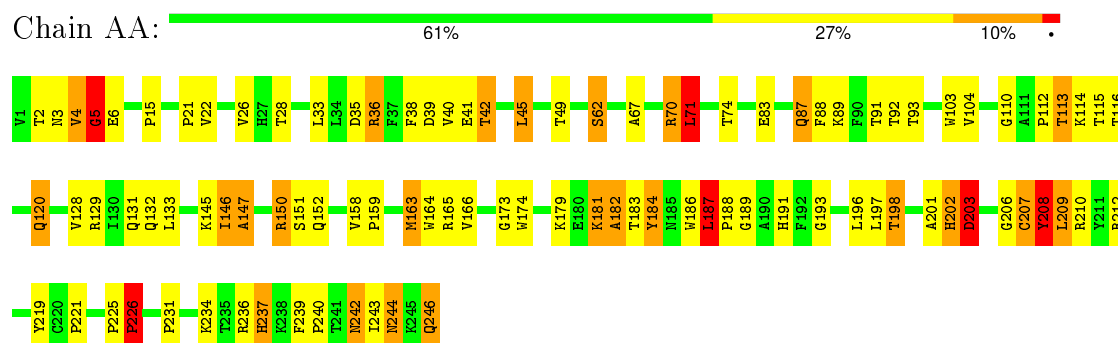
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Cs	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Ct	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cu	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cv	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cw	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cx	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	DA	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	DB	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		

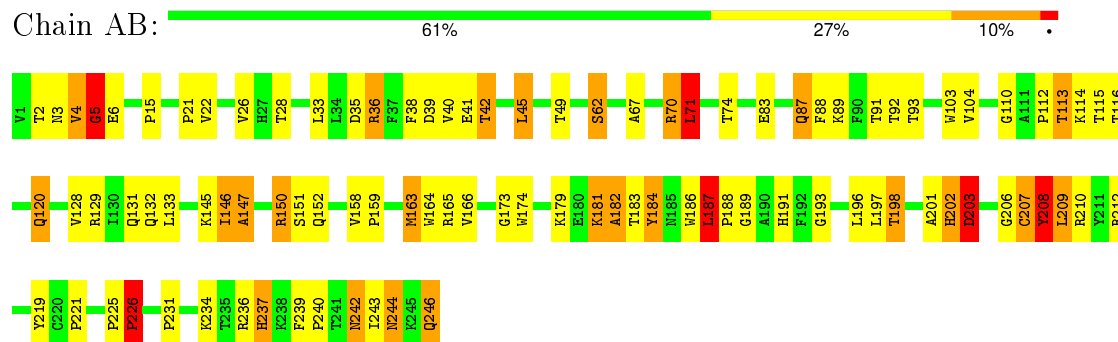
3 Residue-property plots

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

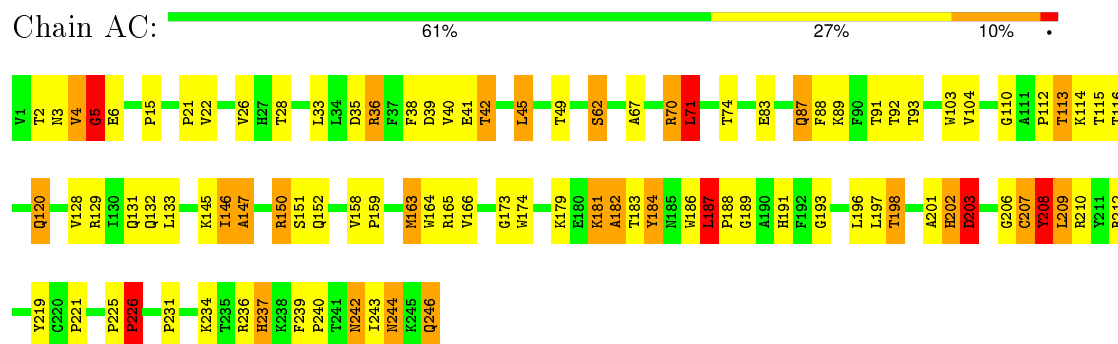
- Molecule 1: P1



- Molecule 1: P1

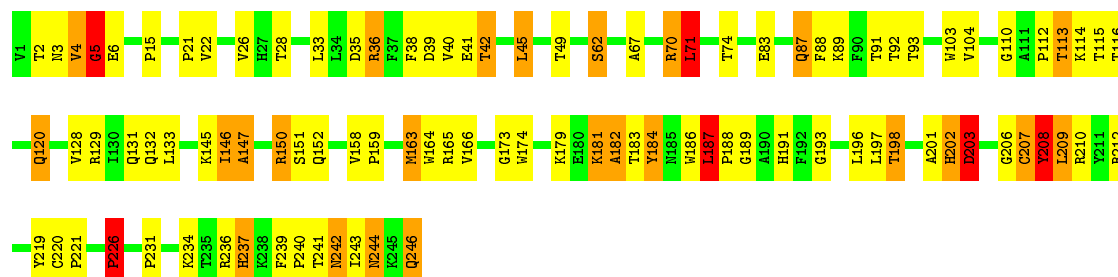


- Molecule 1: P1



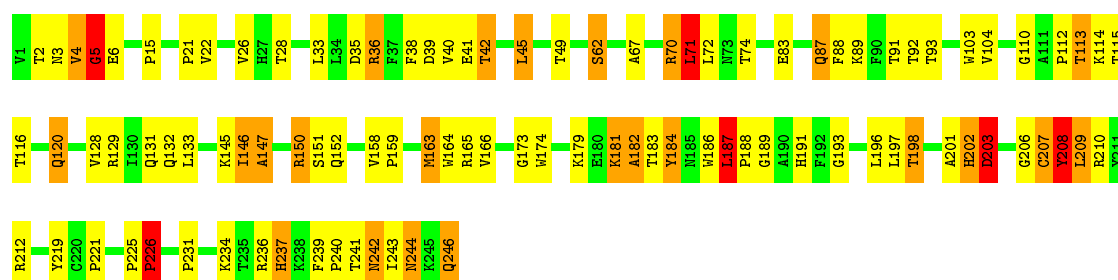
- Molecule 1: P1

Chain AD:



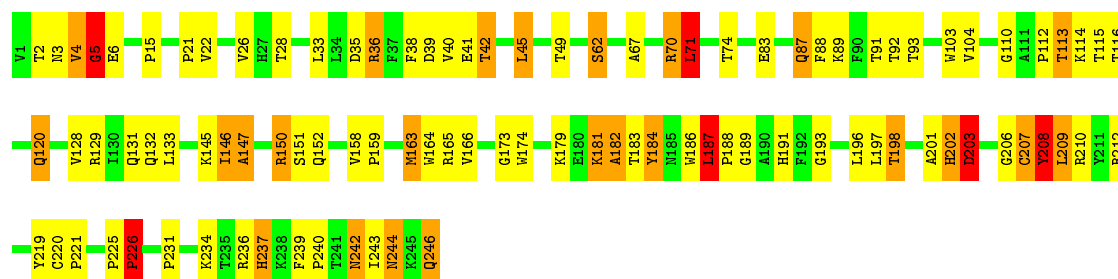
- Molecule 1: P1

Chain AE:



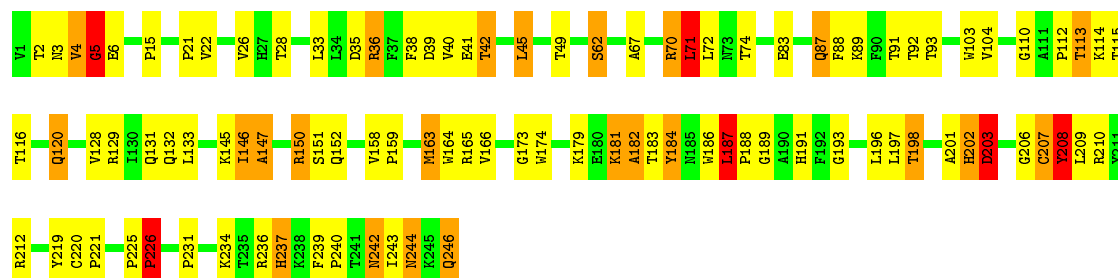
- Molecule 1: P1

Chain AF:



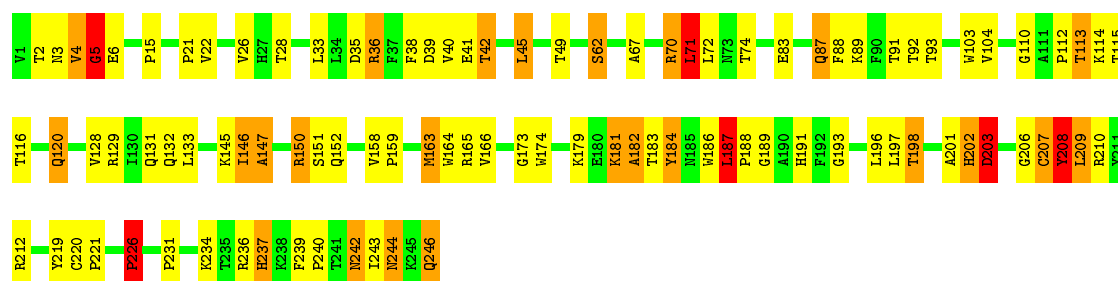
- Molecule 1: P1

Chain AG:



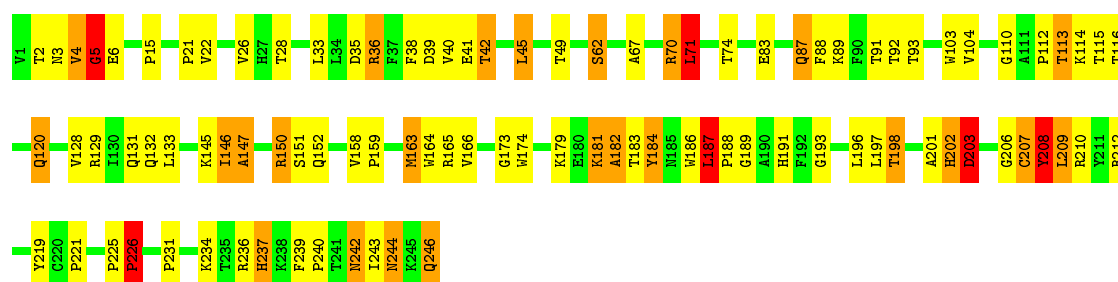
- Molecule 1: P1

Chain AH: 



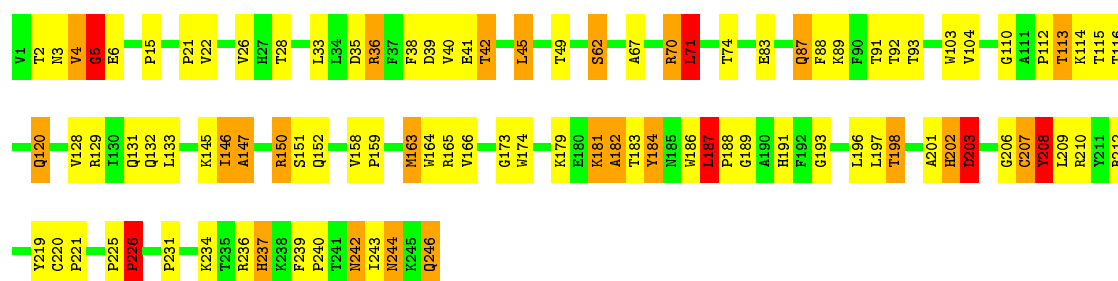
- Molecule 1: P1

Chain AI:  61% 27% 10% •



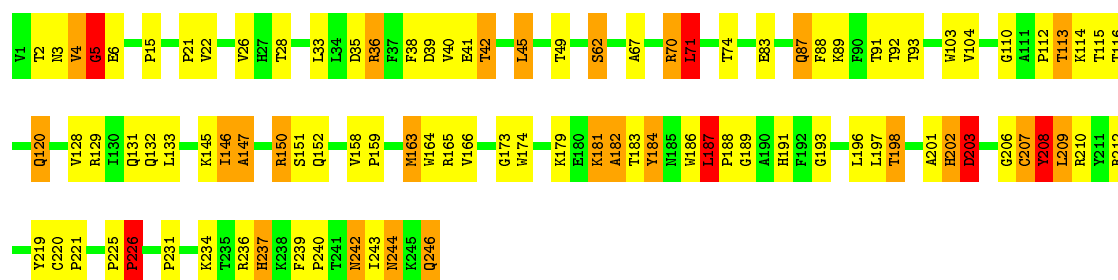
- Molecule 1: P1

Chain AJ:  60% 28% 9% •



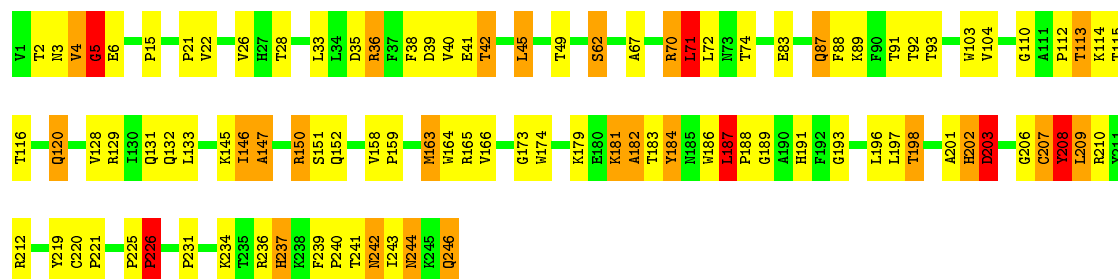
- Molecule 1: P1

Chain AK: 



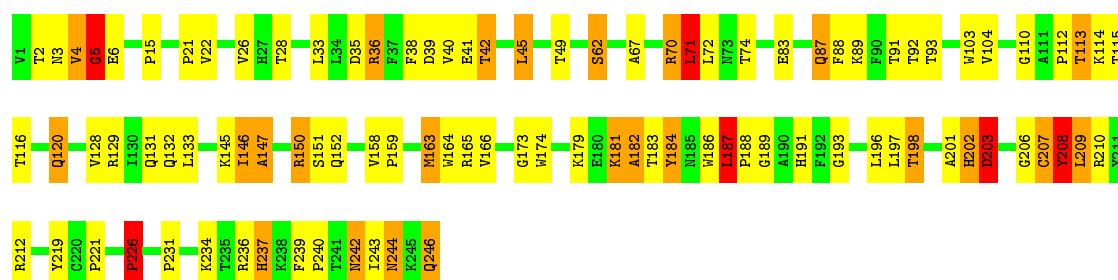
- Molecule 1: P1

Chain AL:



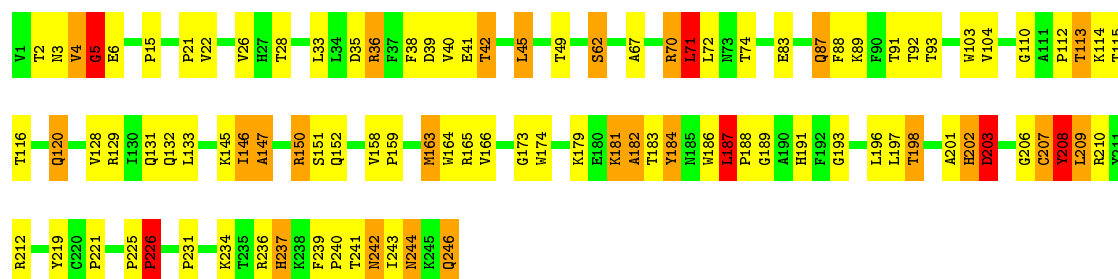
- Molecule 1: P1

Chain AM:



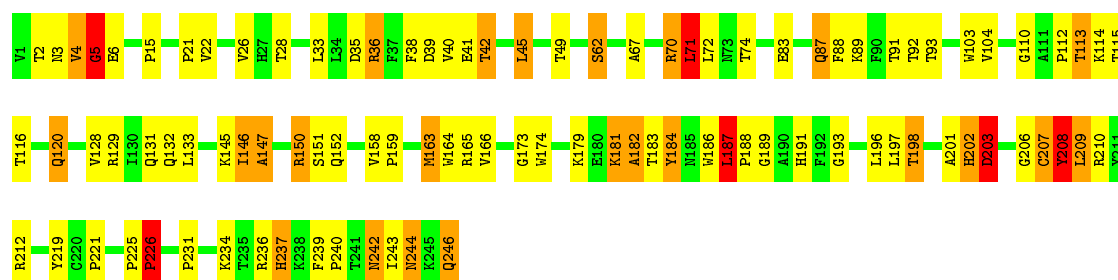
- Molecule 1: P1

Chain AN:



- Molecule 1: P1

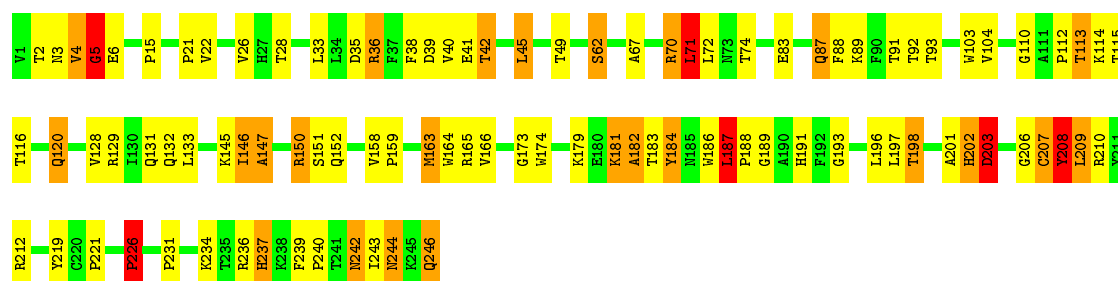
Chain AO:



- Molecule 1: P1

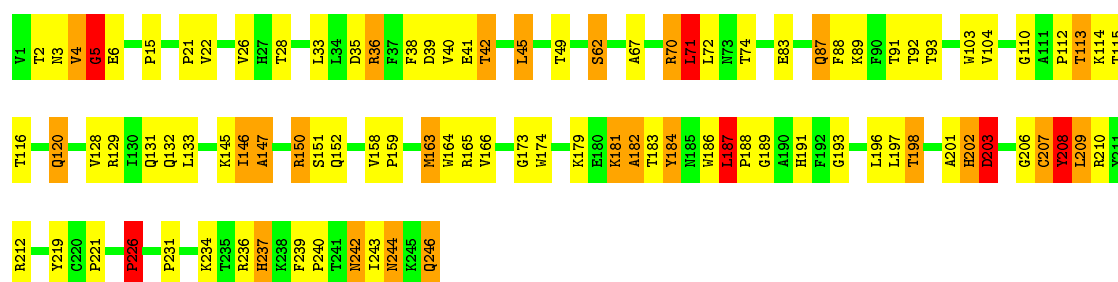


Chain AT:



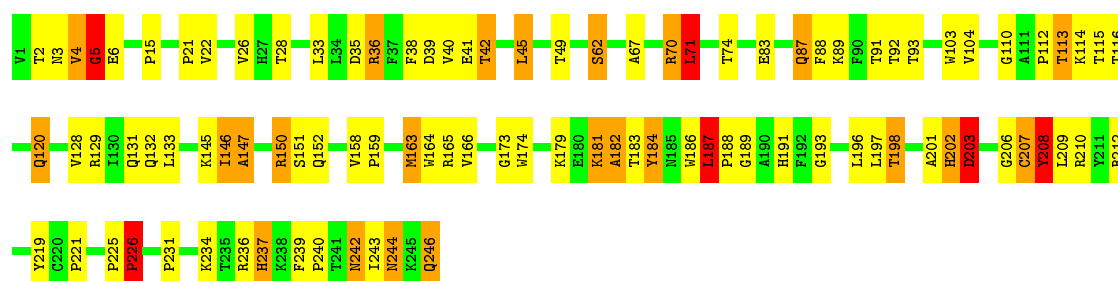
- Molecule 1: P1

Chain AU:



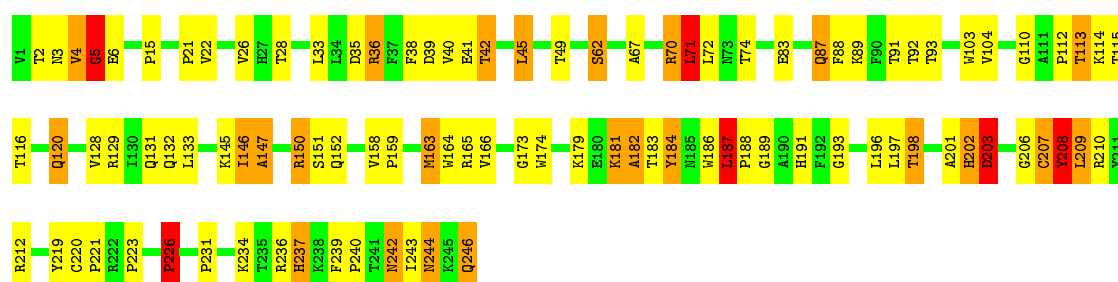
- Molecule 1: P1

Chain AV:

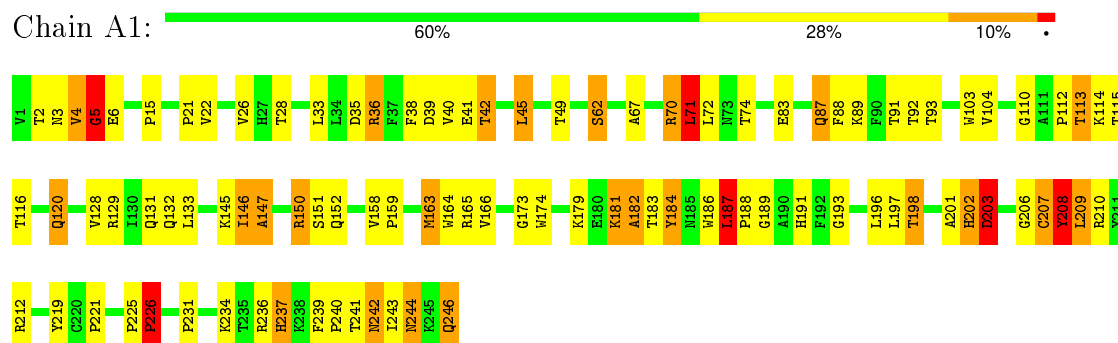


- Molecule 1: P1

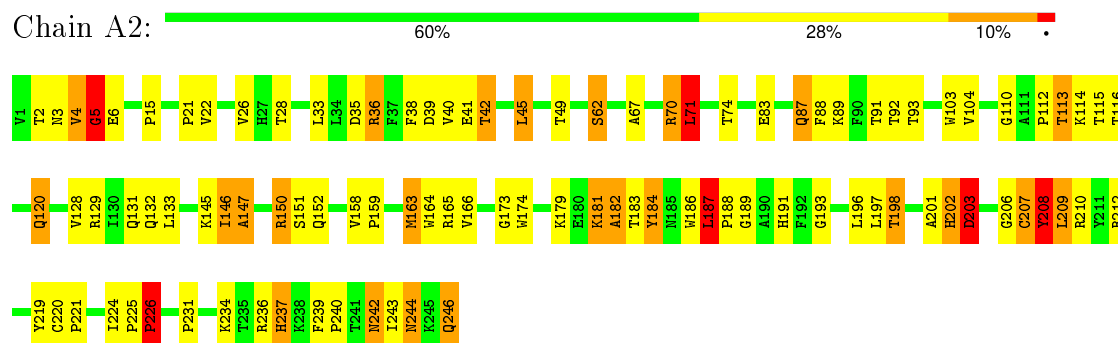
Chain AW:



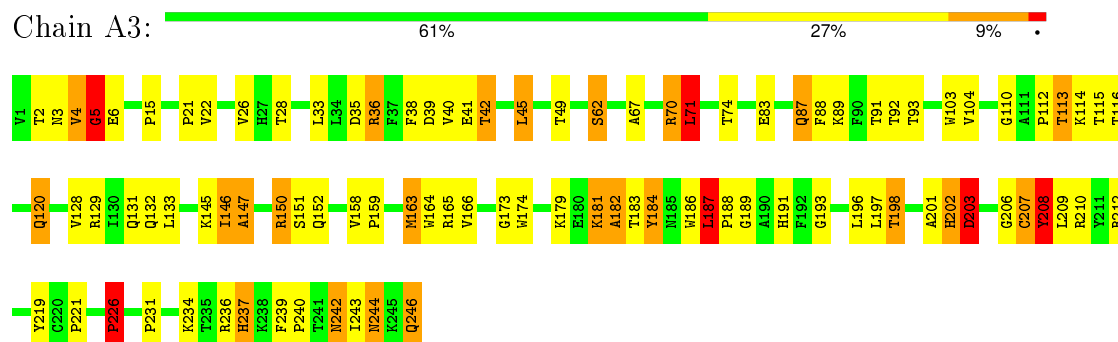
- Molecule 1: P1



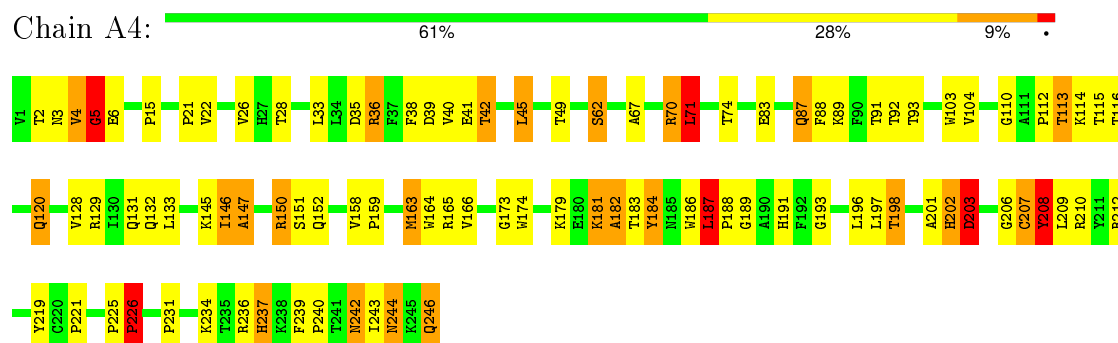
- Molecule 1: P1



- Molecule 1: P1

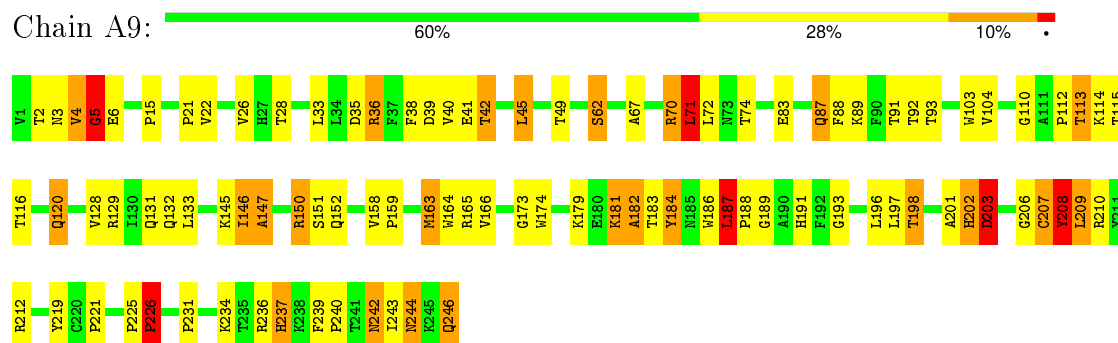


- Molecule 1: P1

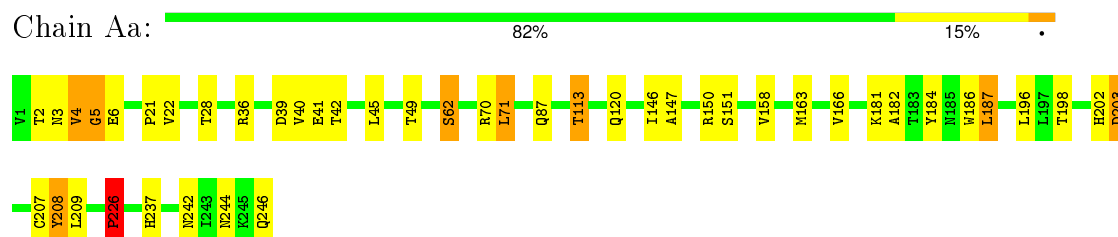


- Molecule 1: P1

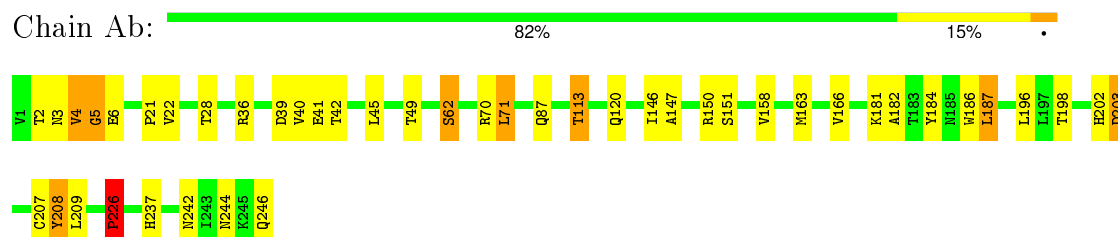
- Molecule 1: P1



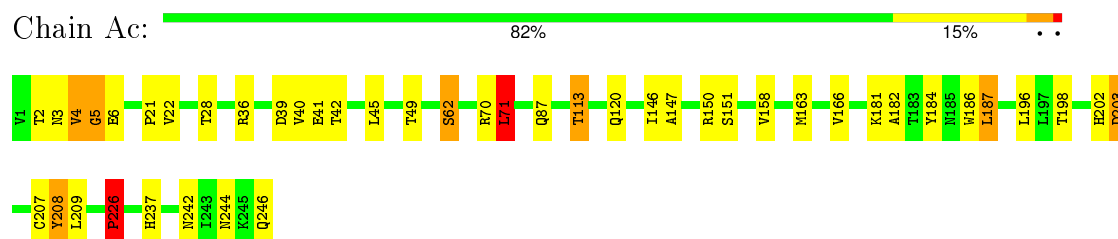
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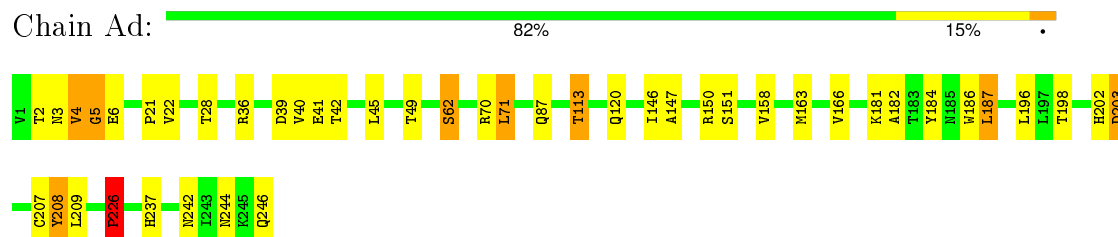
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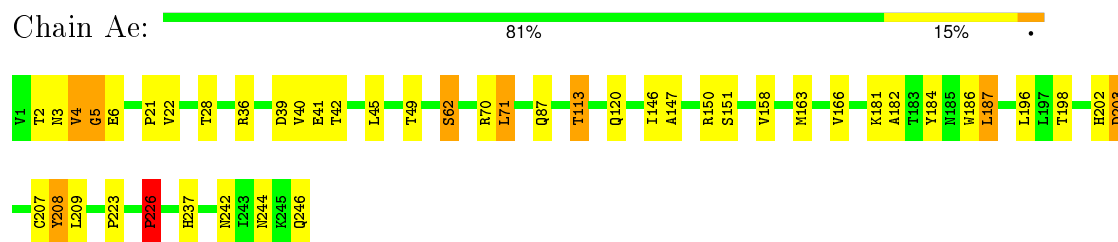
- Molecule 1: P1



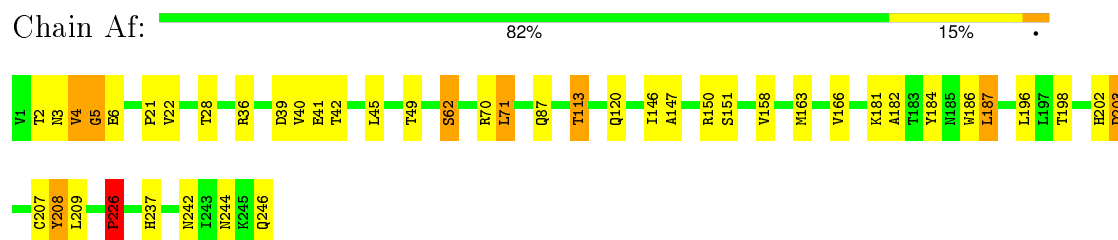
- Molecule 1: P1



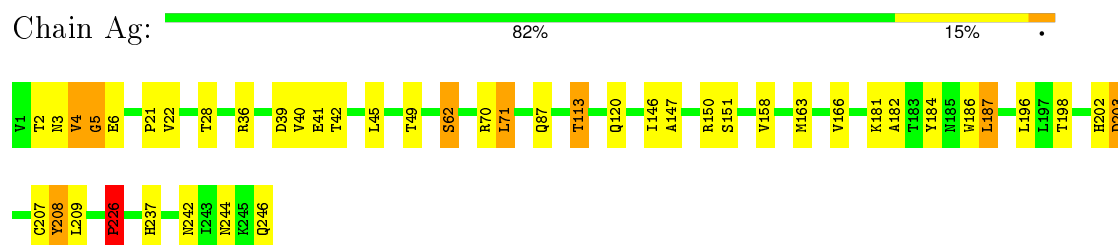
- Molecule 1: P1



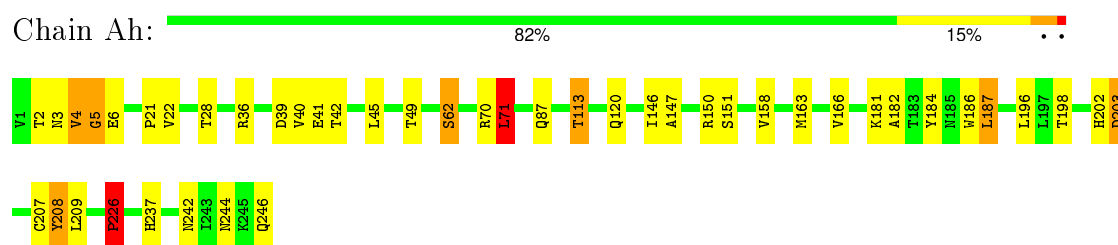
- Molecule 1: P1



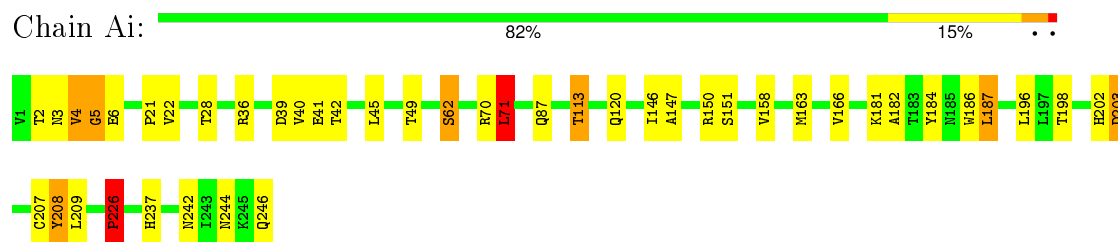
- Molecule 1: P1



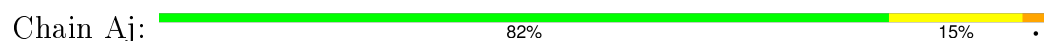
- Molecule 1: P1

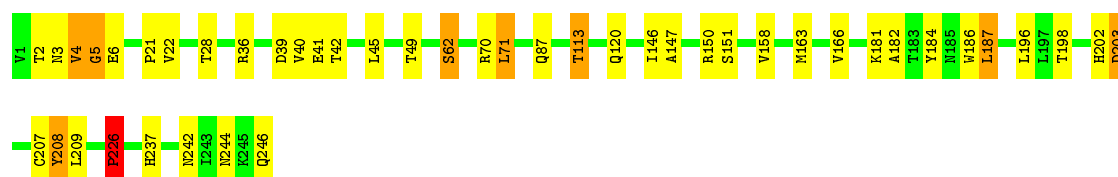


- Molecule 1: P1



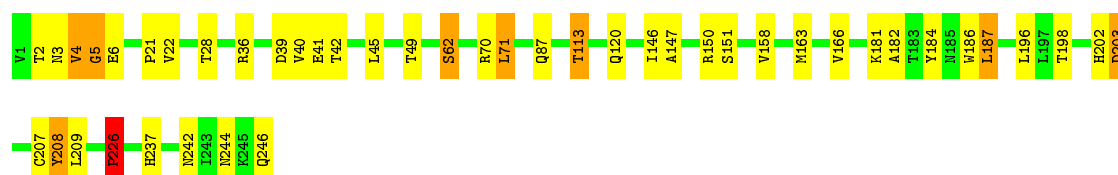
- Molecule 1: P1





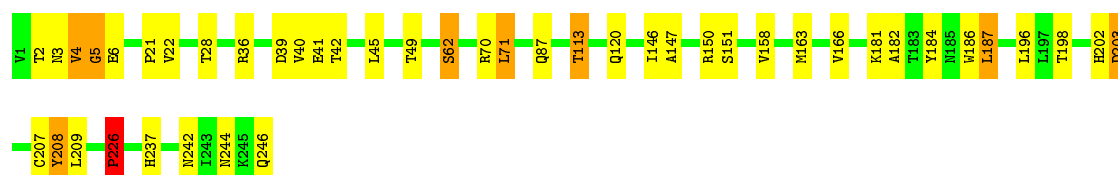
- Molecule 1: P1

Chain Ak: 82% 15% •



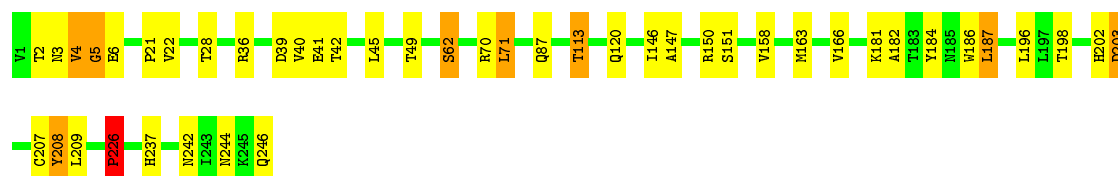
- Molecule 1: P1

Chain Al: 82% 15% •



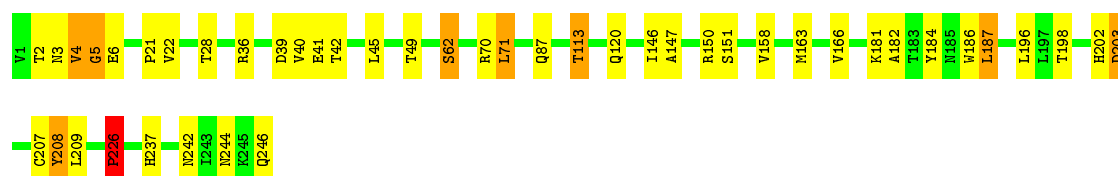
- Molecule 1: P1

Chain Am: 82% 15% •



- Molecule 1: P1

Chain An: 82% 15% •



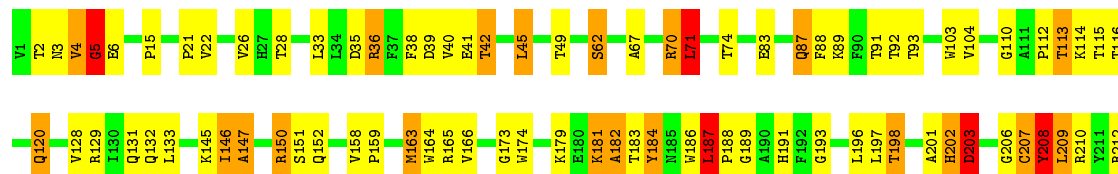
- Molecule 1: P1

Chain Ao: 82% 15% •

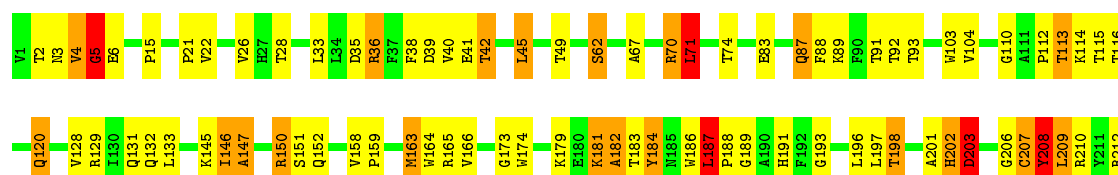




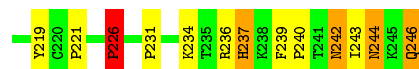
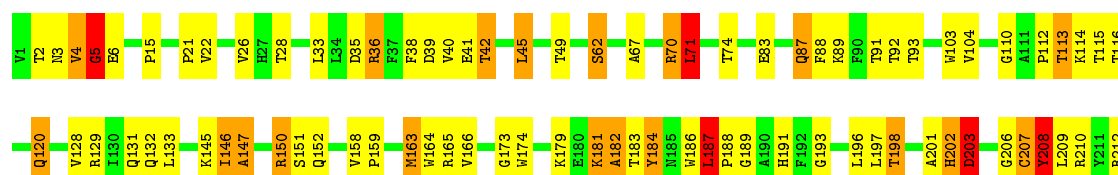
- Molecule 1: P1



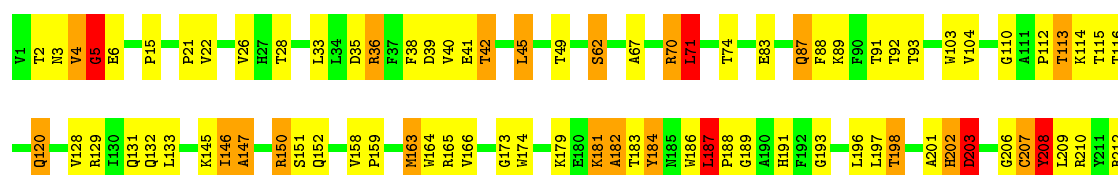
- Molecule 1: P1

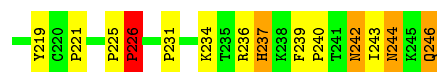


- Molecule 1: P1



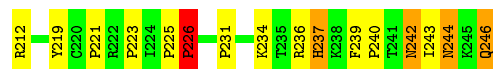
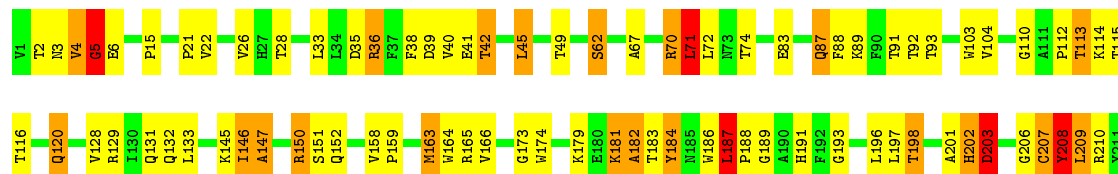
- Molecule 1: P1





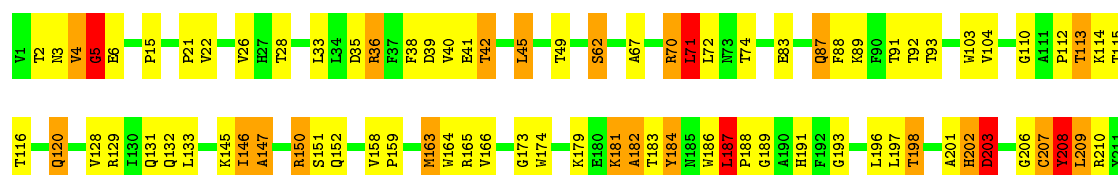
• Molecule 1: P1

Chain DG: 60% 28% 10%



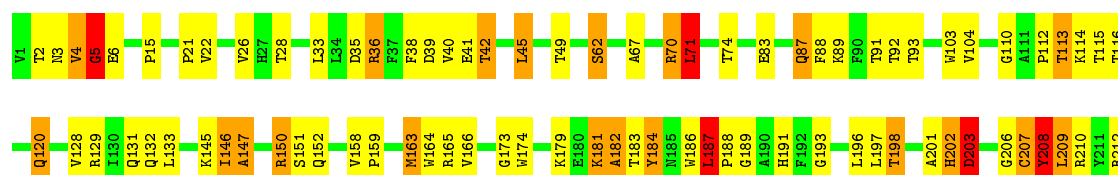
• Molecule 1: P1

Chain DH: 60% 28% 10%



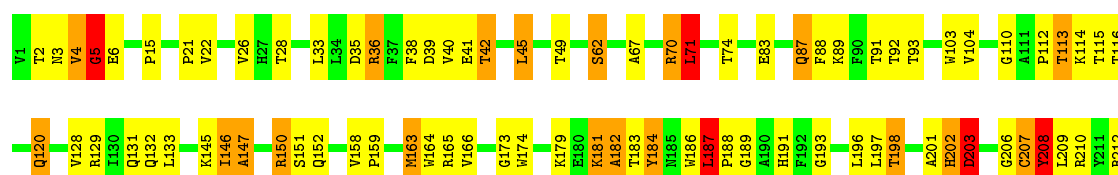
• Molecule 1: P1

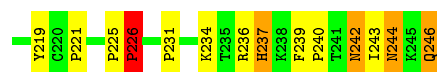
Chain DI: 61% 27% 10%



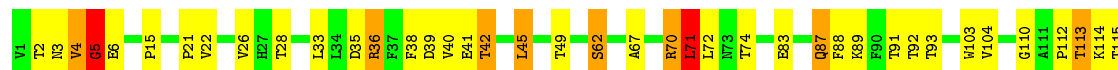
• Molecule 1: P1

Chain DJ: 61% 28% 9%

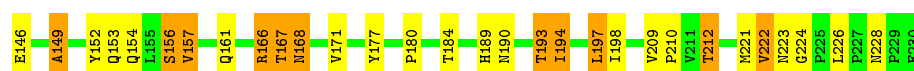




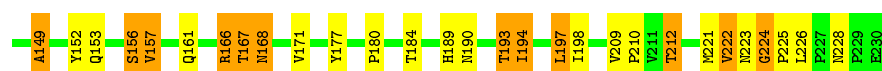
• Molecule 1: P1



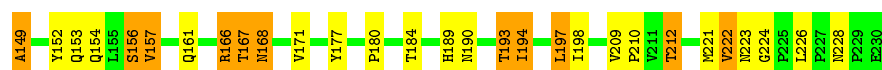
• Molecule 2: P1



• Molecule 2: P1



• Molecule 2: P1



• Molecule 2: P1





• Molecule 2: P1

Chain BE: 65% 23% 12%



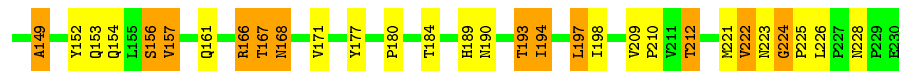
• Molecule 2: P1

Chain BF: 65% 22% 12%



• Molecule 2: P1

Chain BG: 65% 23% 11%



• Molecule 2: P1

Chain BH: 65% 23% 11%

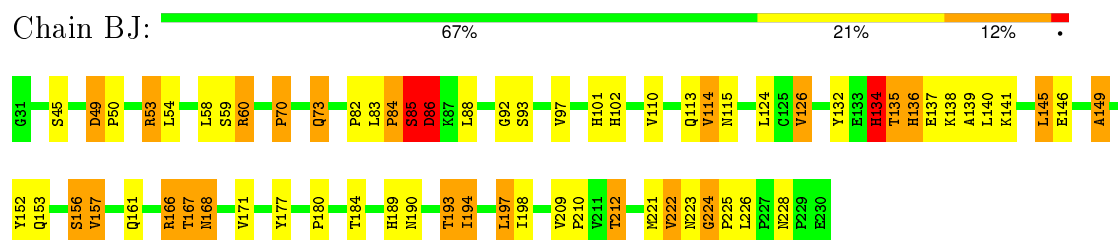


• Molecule 2: P1

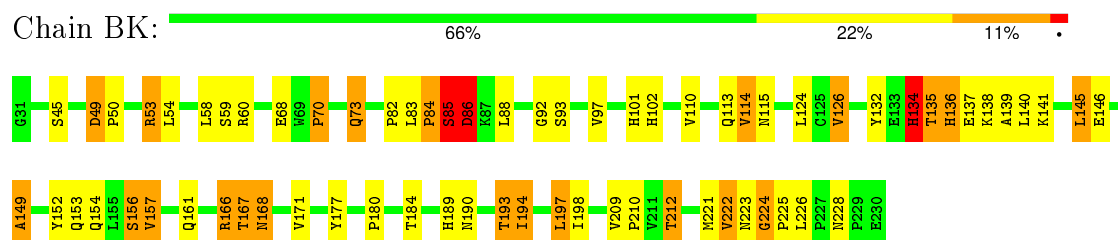
Chain BI: 65% 22% 12%



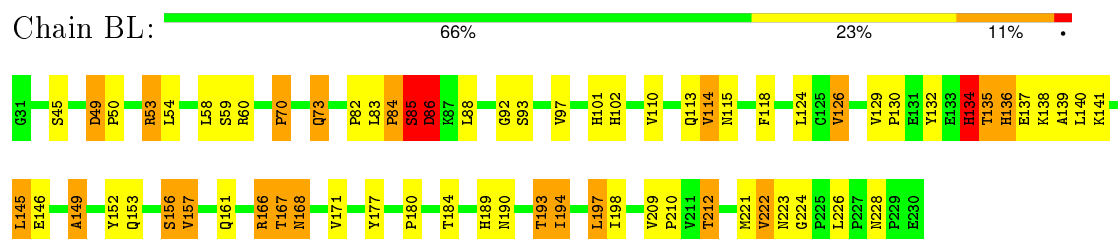
- Molecule 2: P1



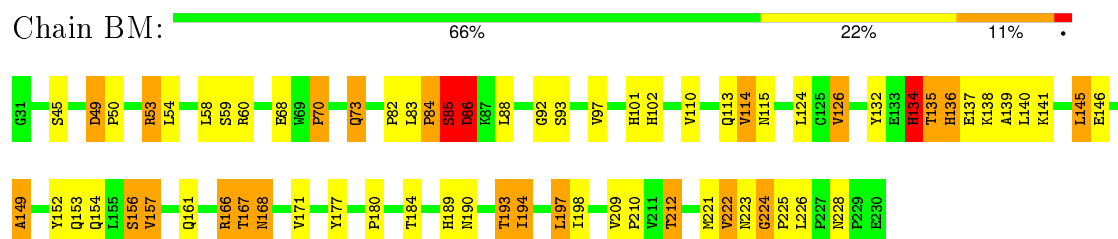
- Molecule 2: P1



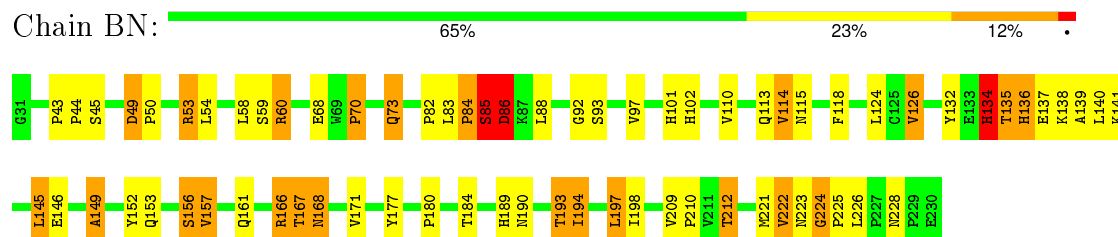
- Molecule 2: P1



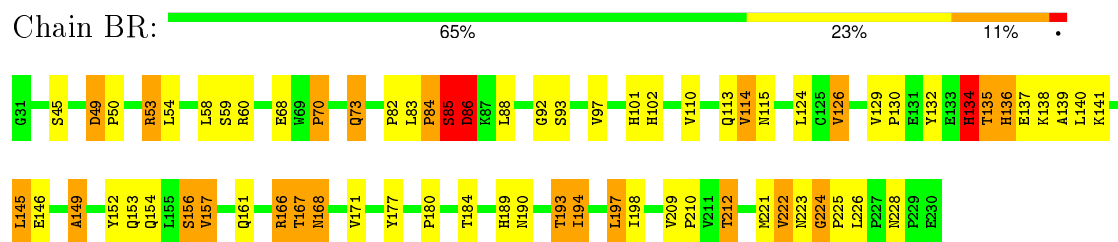
- Molecule 2: P1



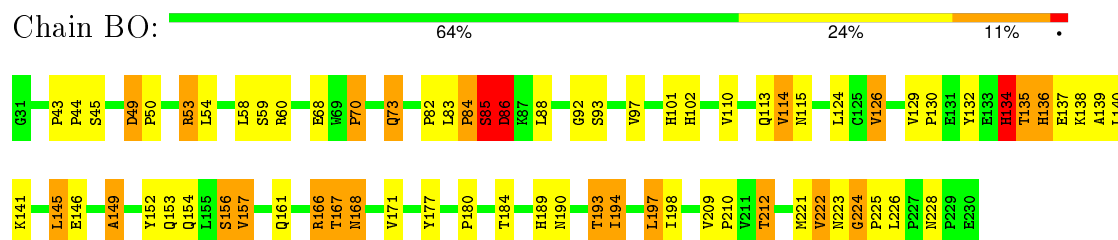
- Molecule 2: P1



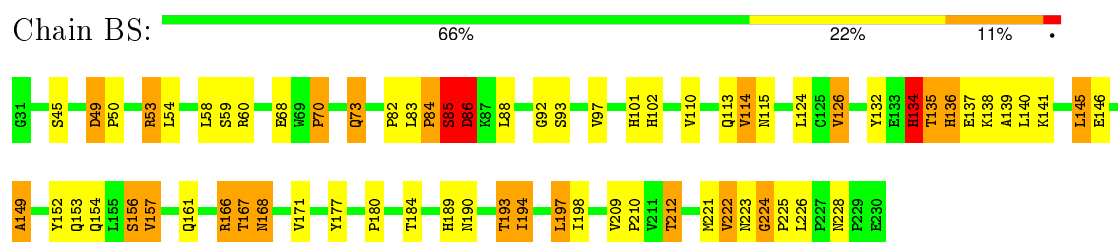
- Molecule 2: P1



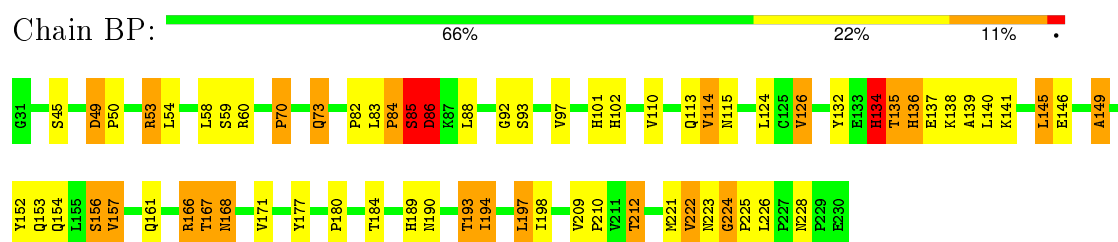
- Molecule 2: P1



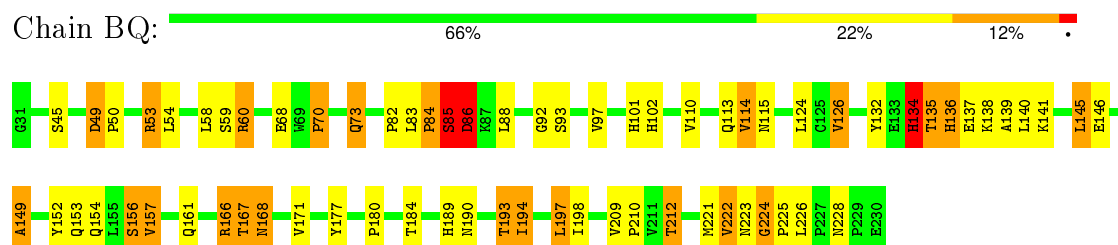
- Molecule 2: P1



- Molecule 2: P1

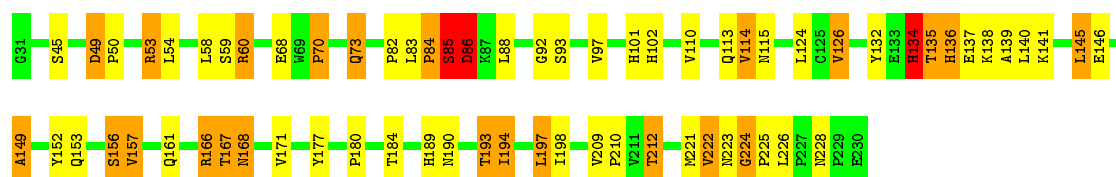


- Molecule 2: P1

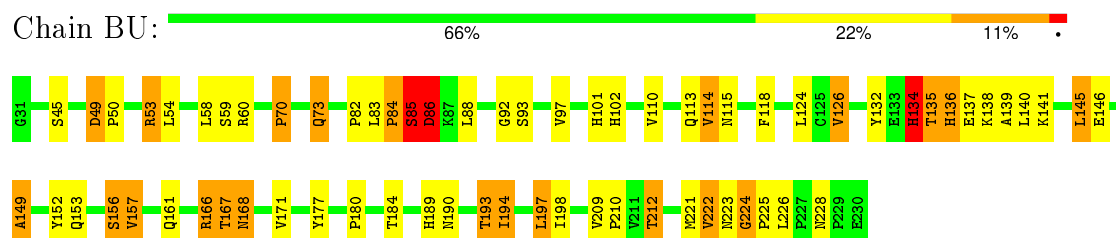


- Molecule 2: P1

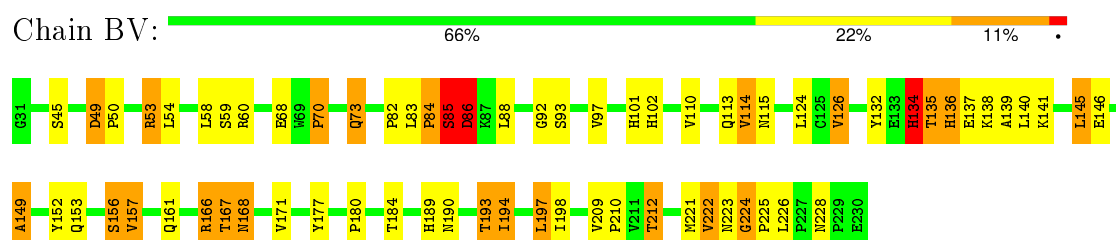




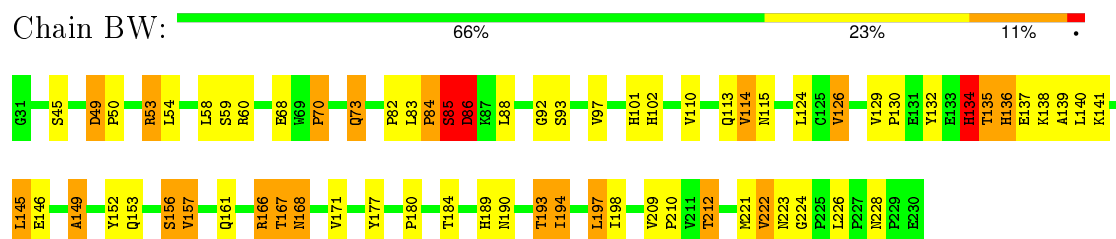
- Molecule 2: P1



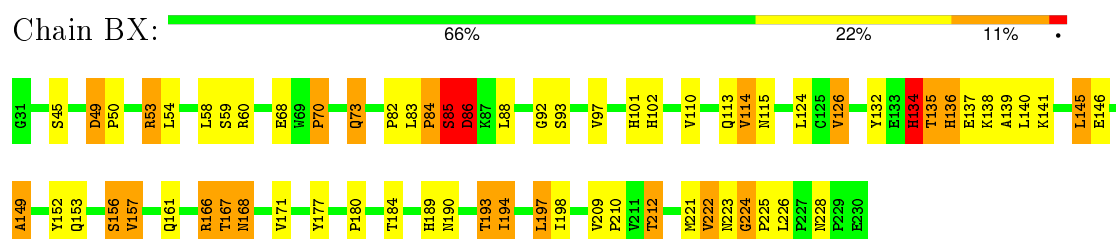
- Molecule 2: P1



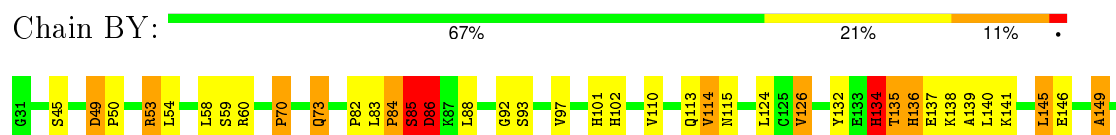
- Molecule 2: P1

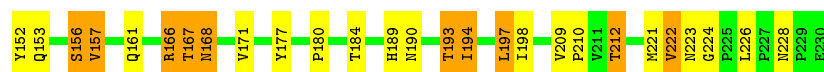


- Molecule 2: P1



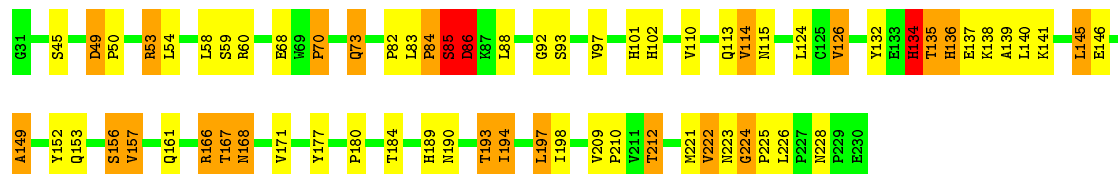
- Molecule 2: P1





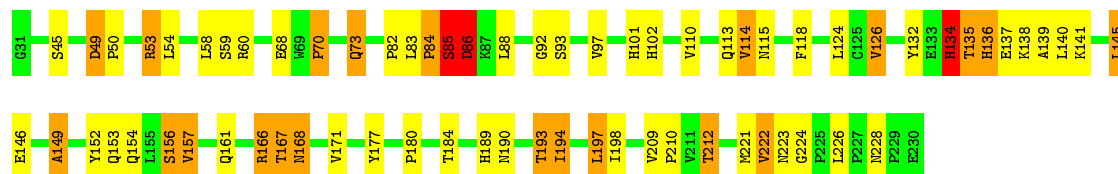
• Molecule 2: P1

Chain BZ: 66% 22% 11%



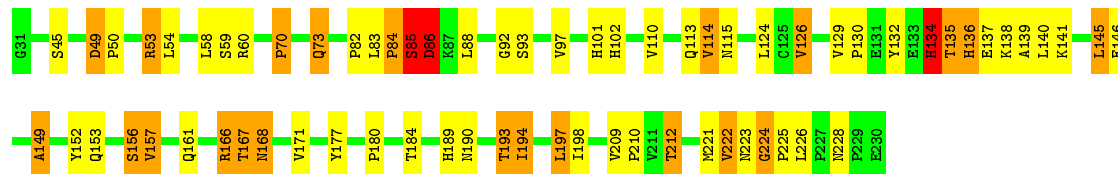
• Molecule 2: P1

Chain B0: 66% 23% 11%



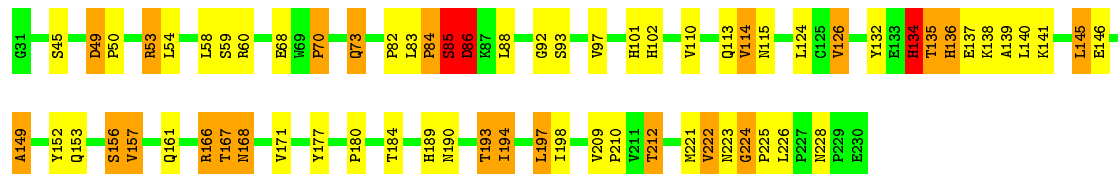
• Molecule 2: P1

Chain B1: 66% 22% 11%



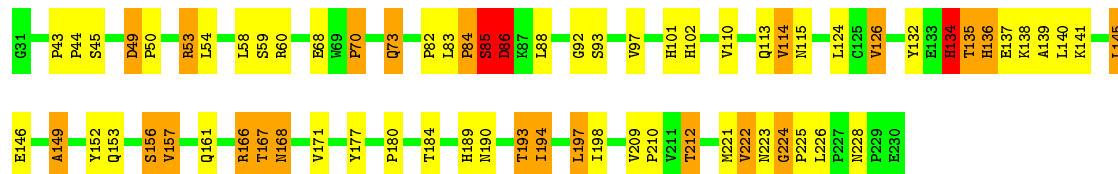
• Molecule 2: P1

Chain B2: 66% 22% 11%

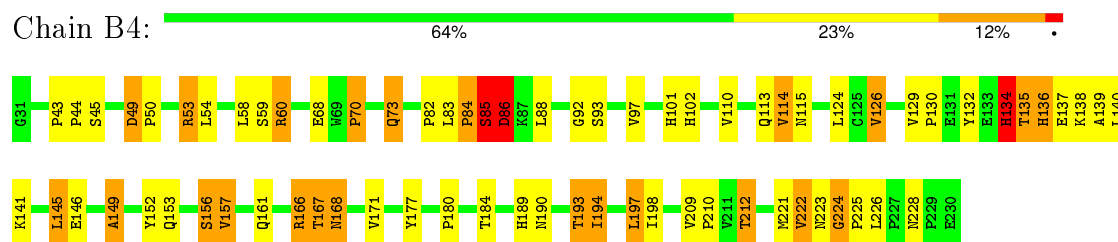


• Molecule 2: P1

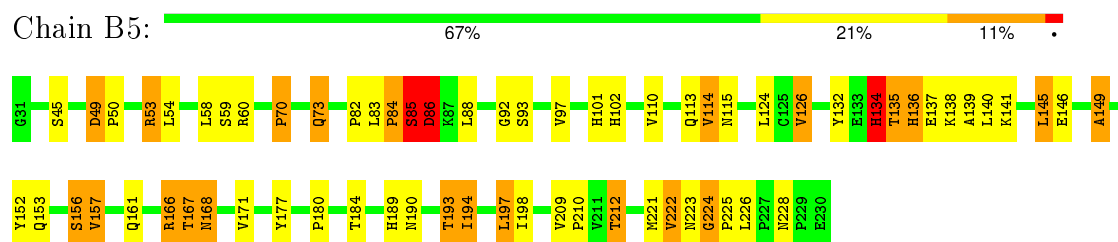
Chain B3: 65% 23% 11%



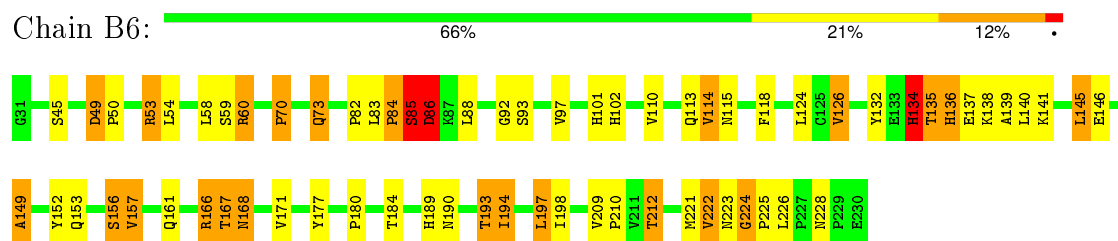
- Molecule 2: P1



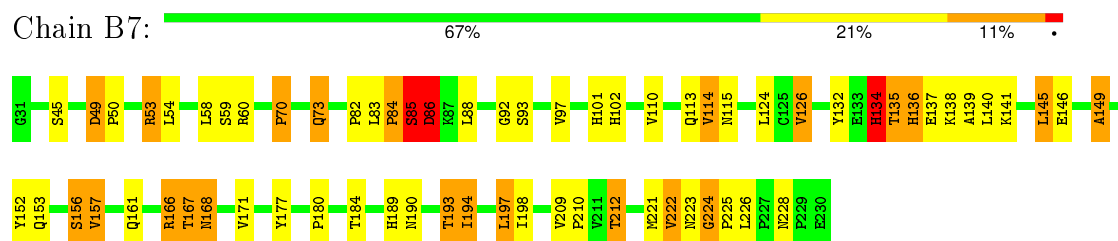
- Molecule 2: P1



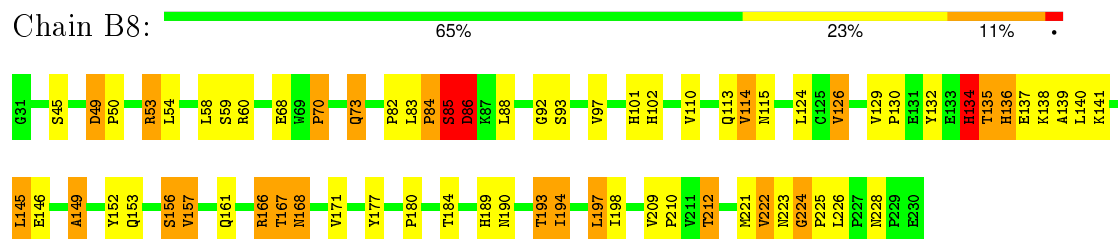
- Molecule 2: P1



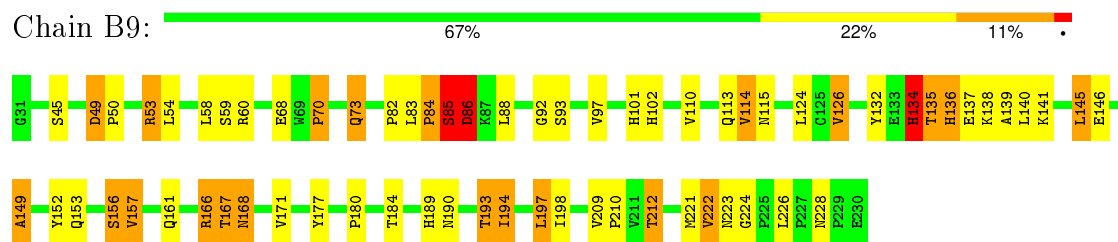
- Molecule 2: P1



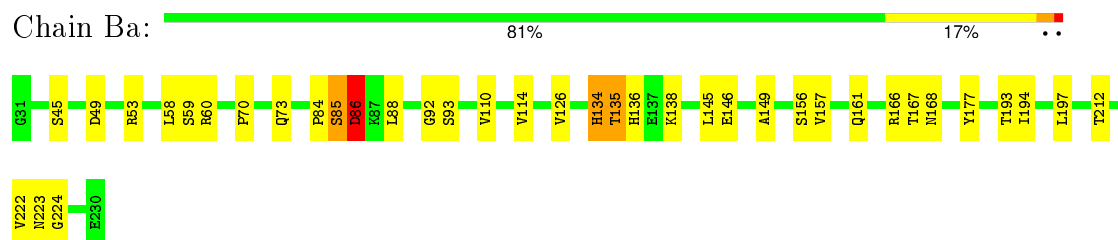
- Molecule 2: P1



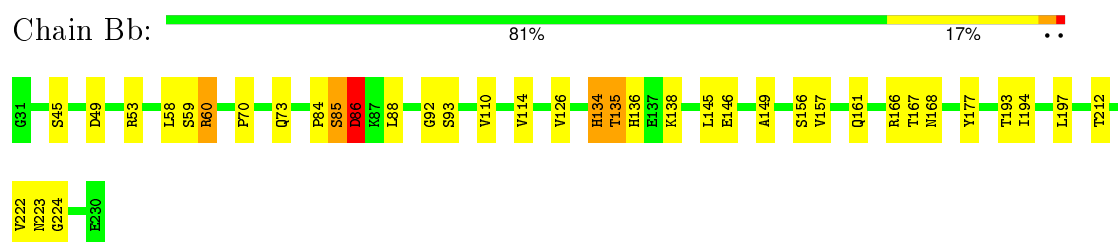
- Molecule 2: P1



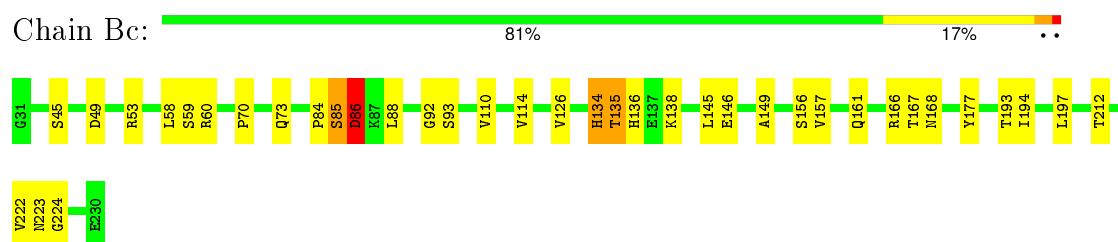
• Molecule 2: P1



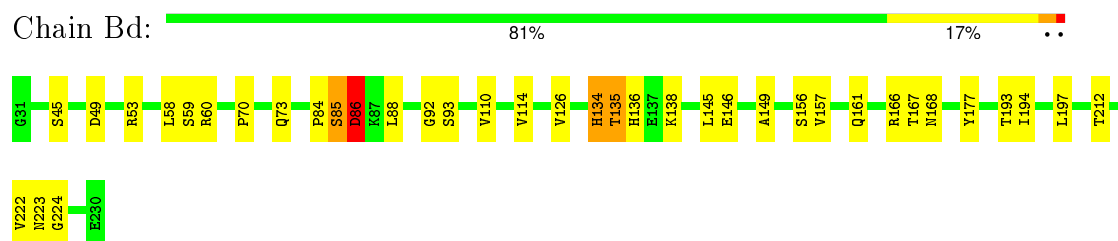
• Molecule 2: P1



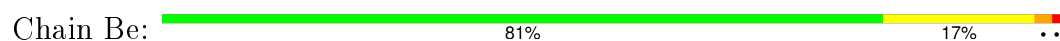
• Molecule 2: P1

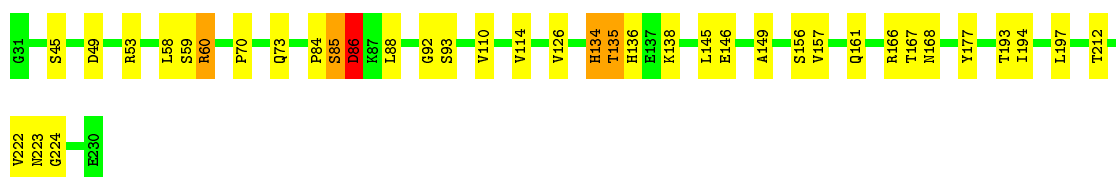


• Molecule 2: P1



• Molecule 2: P1





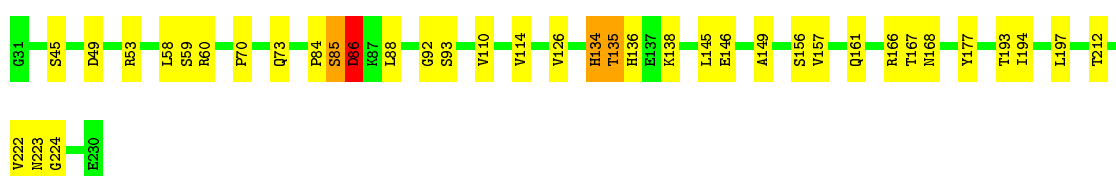
- Molecule 2: P1

Chain Bf: 81% 17% ..



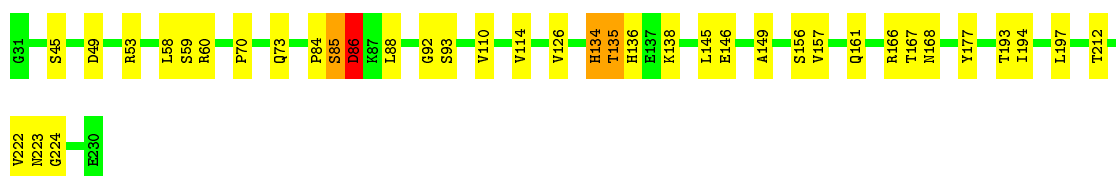
- Molecule 2: P1

Chain Bg: 81% 17% ..



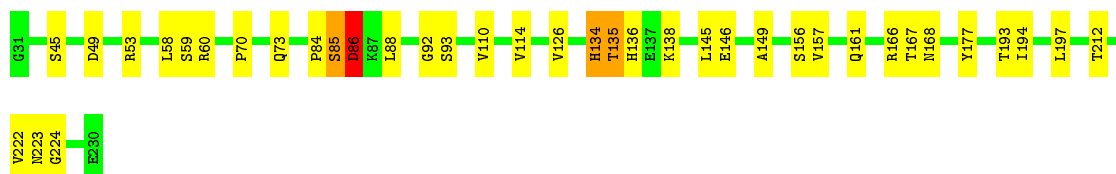
- Molecule 2: P1

Chain Bh: 81% 17% ..



- Molecule 2: P1

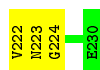
Chain Bi: 81% 17% ..



- Molecule 2: P1

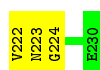
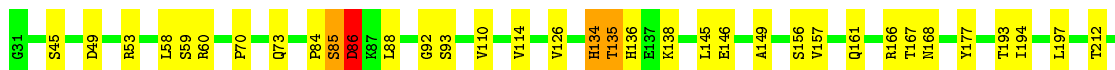
Chain Bj: 81% 17% ..





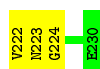
● Molecule 2: P1

Chain Bk: 81% 17% ..



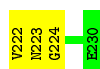
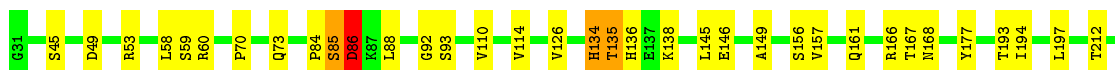
● Molecule 2: P1

Chain Bl: 81% 17% ..



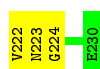
● Molecule 2: P1

Chain Bm: 81% 17% ..



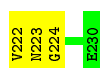
● Molecule 2: P1

Chain Bn: 81% 17% ..

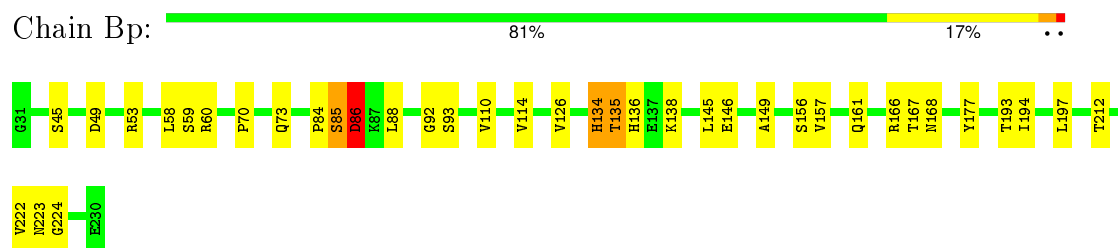


● Molecule 2: P1

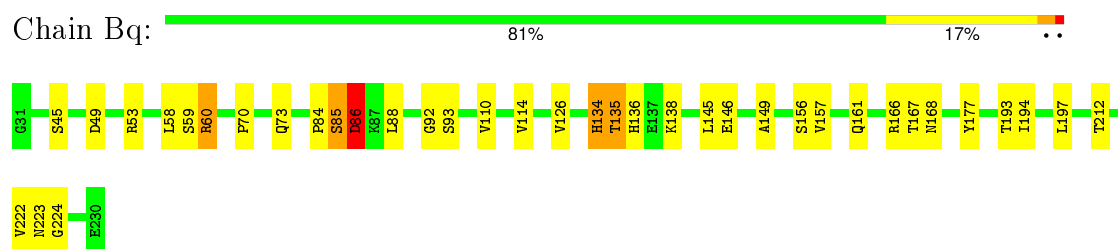
Chain Bo: 81% 17% ..



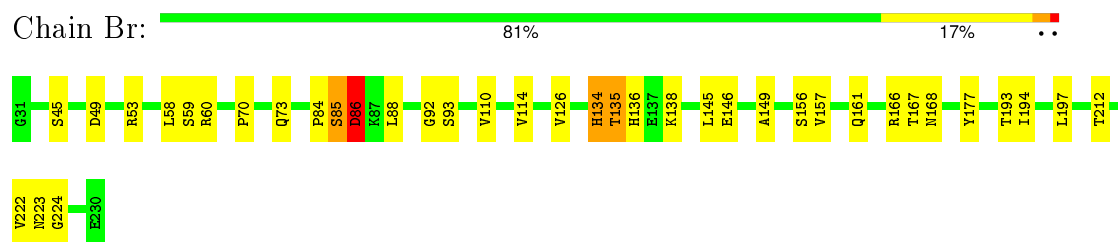
● Molecule 2: P1



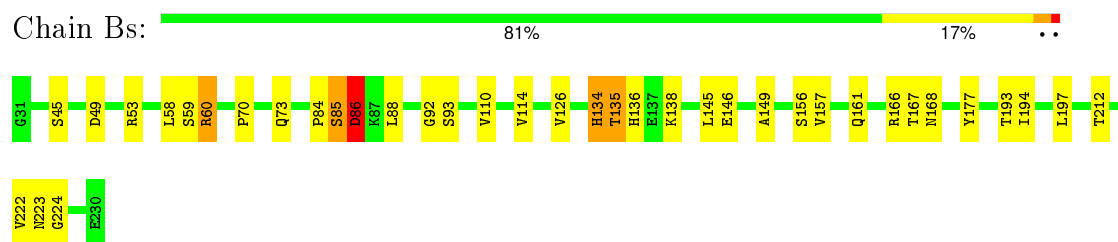
● Molecule 2: P1



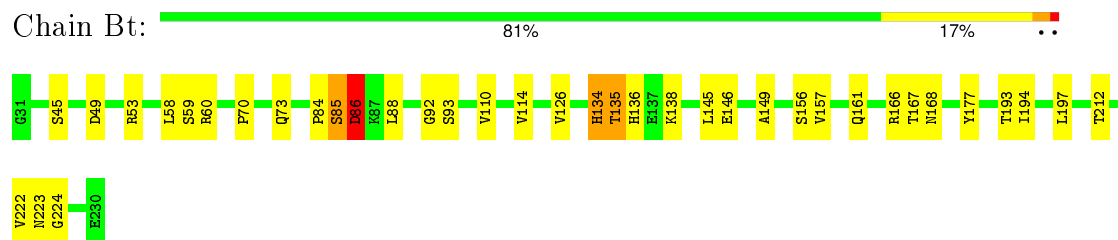
● Molecule 2: P1



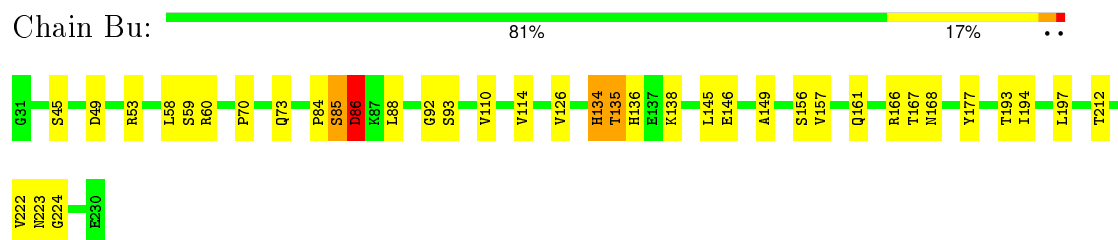
● Molecule 2: P1



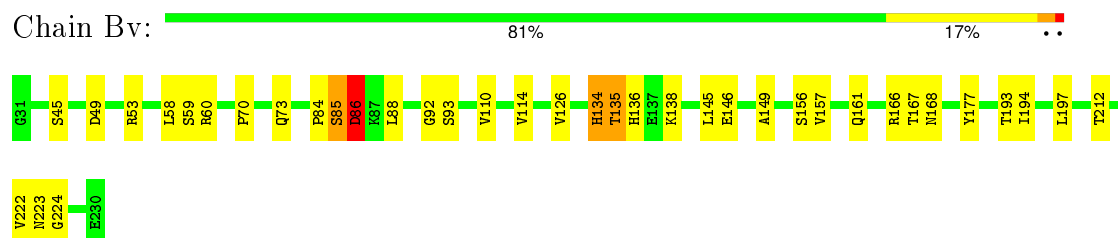
● Molecule 2: P1



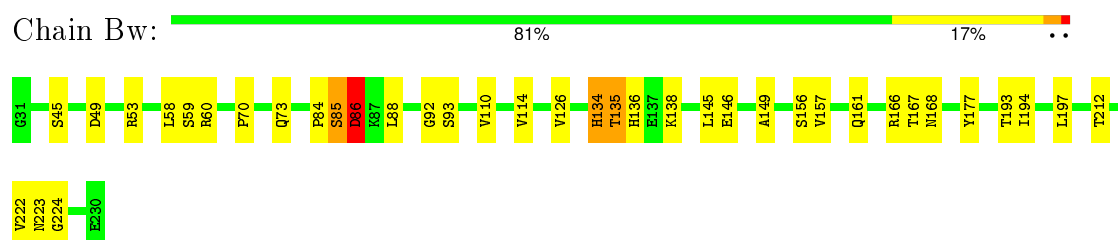
● Molecule 2: P1



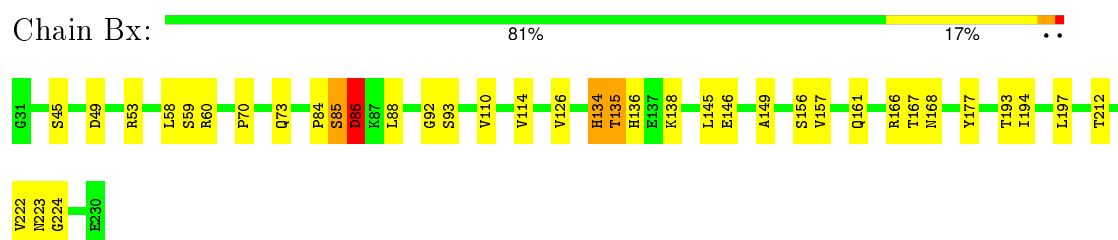
- Molecule 2: P1



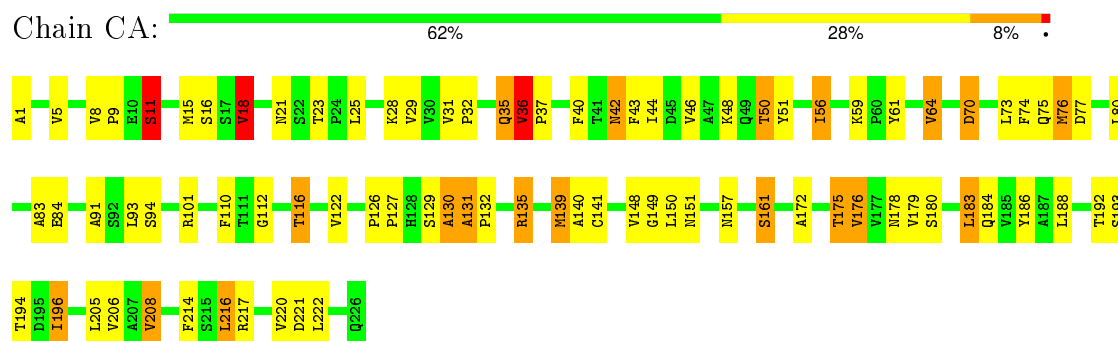
- Molecule 2: P1



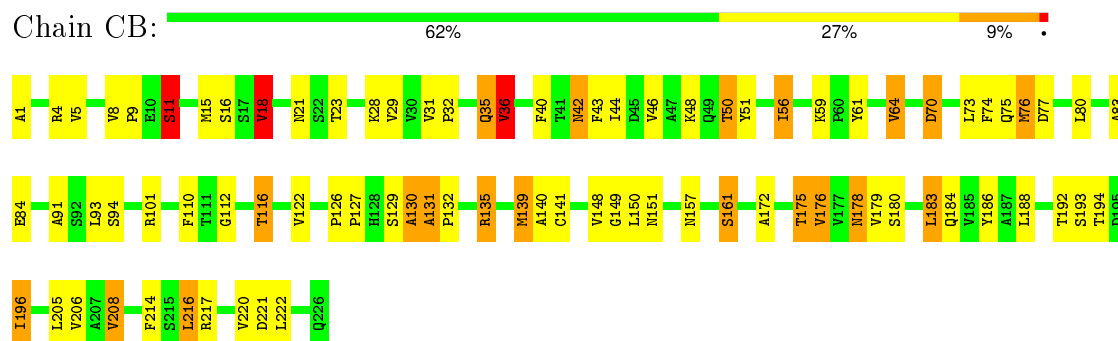
- Molecule 2: P1



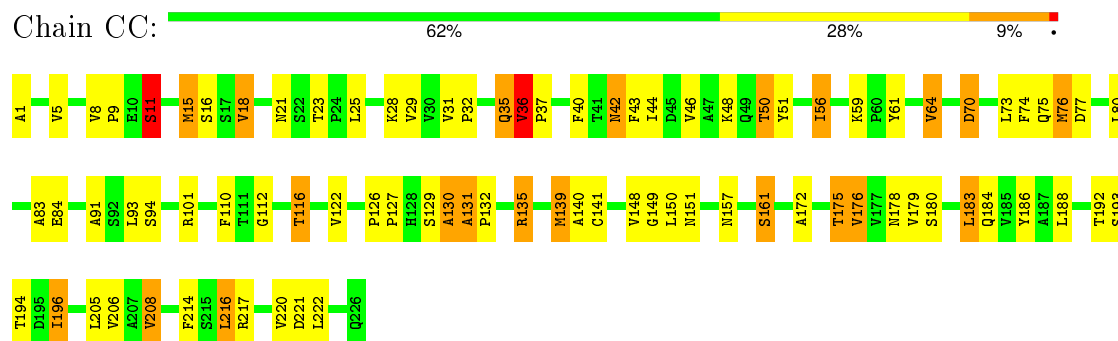
- Molecule 3: P1



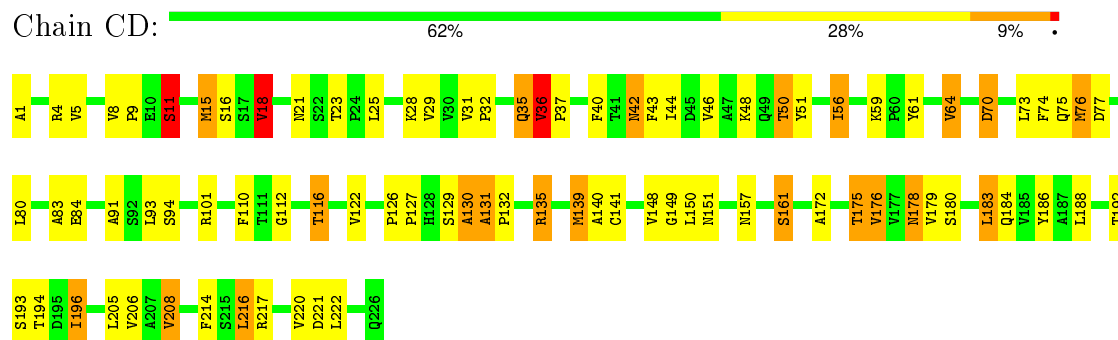
- Molecule 3: P1



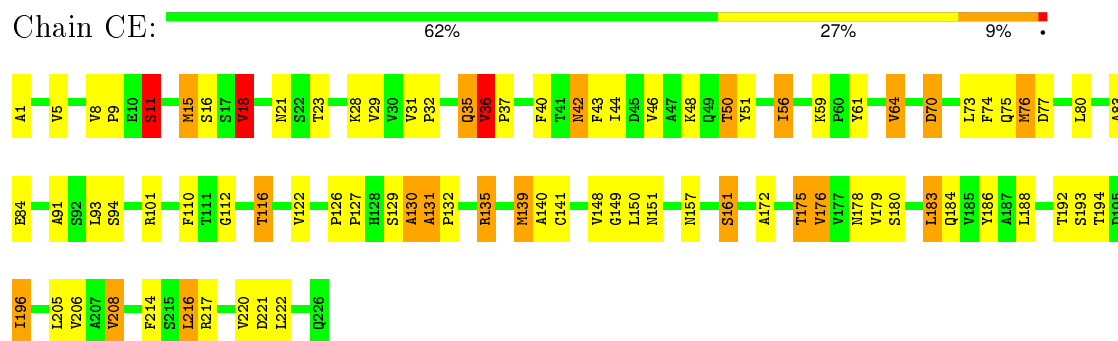
- Molecule 3: P1



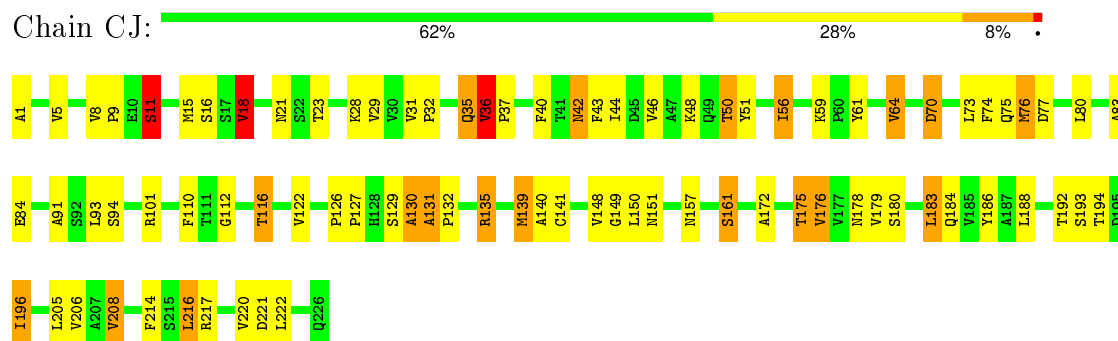
- Molecule 3: P1



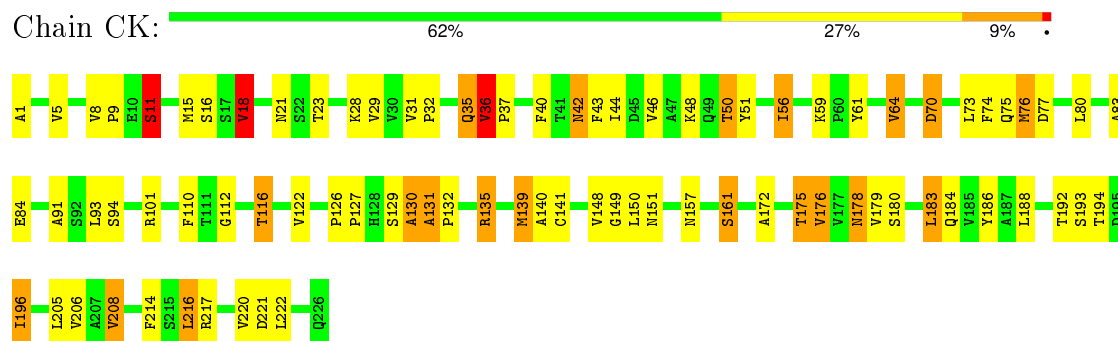
- Molecule 3: P1



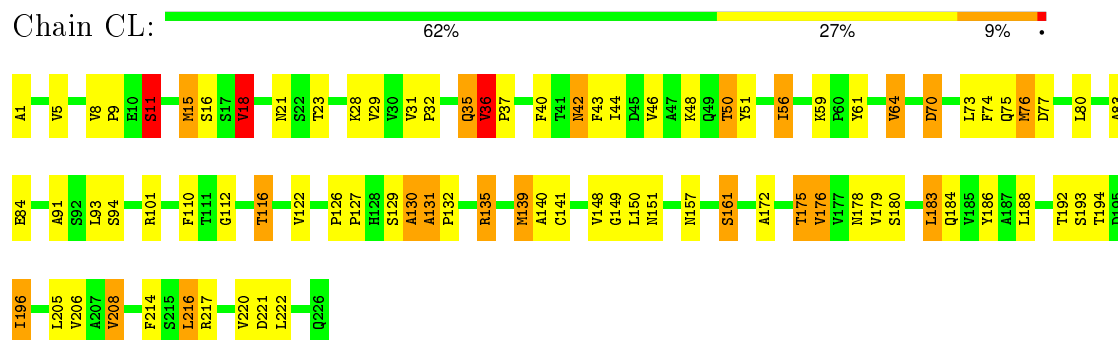
- Molecule 3: P1



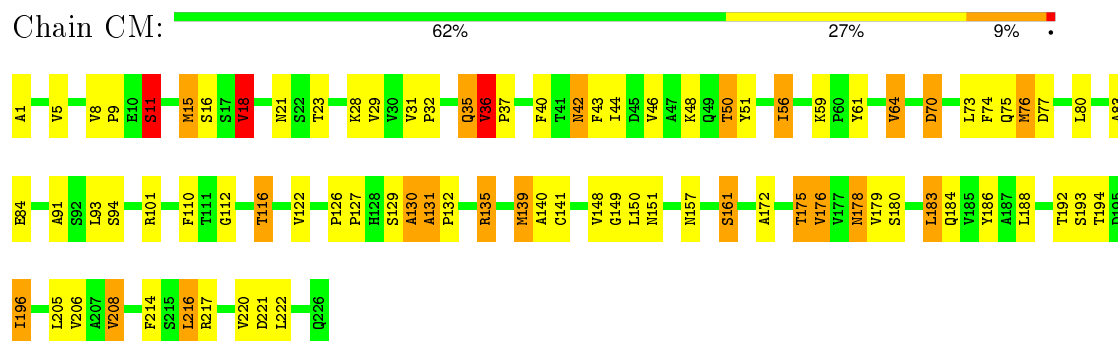
- Molecule 3: P1



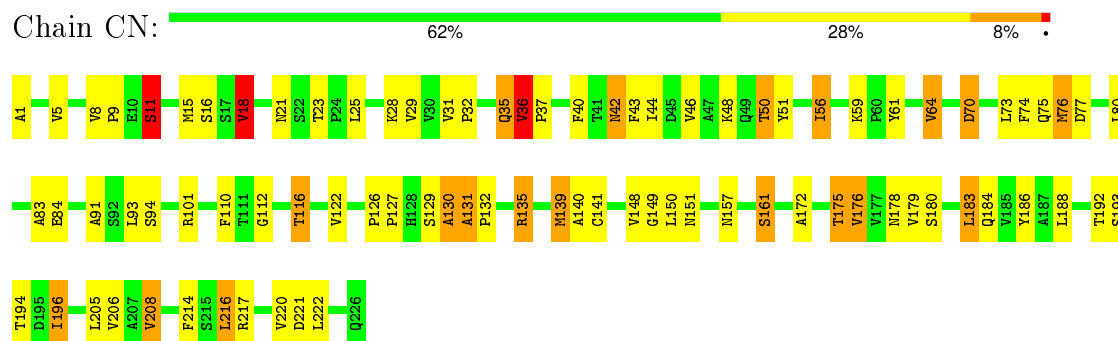
- Molecule 3: P1



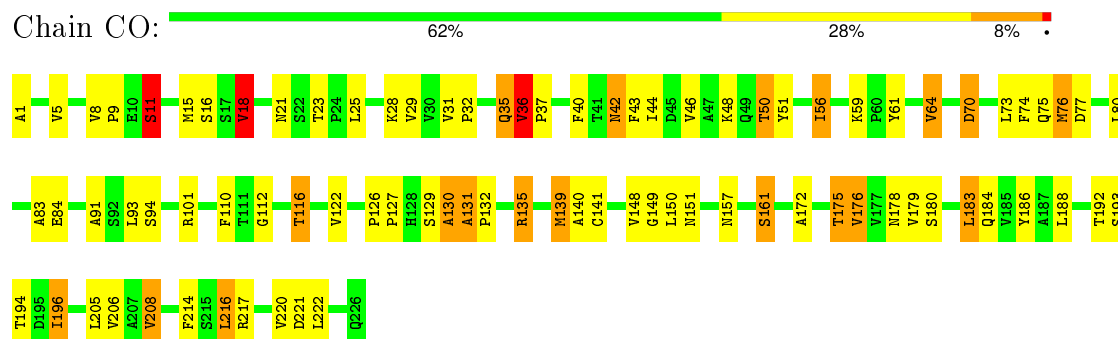
- Molecule 3: P1



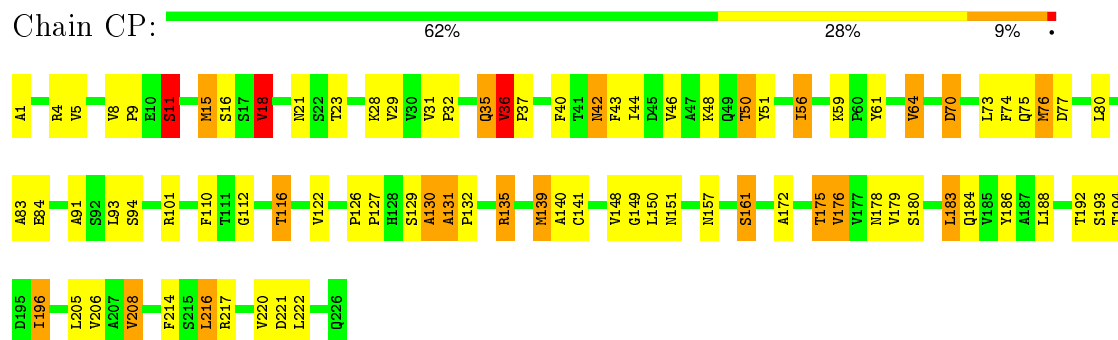
- Molecule 3: P1



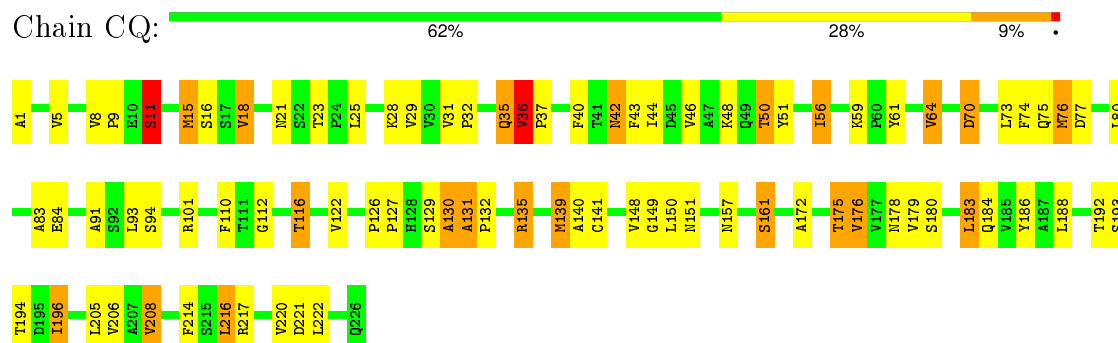
- Molecule 3: P1



- Molecule 3: P1

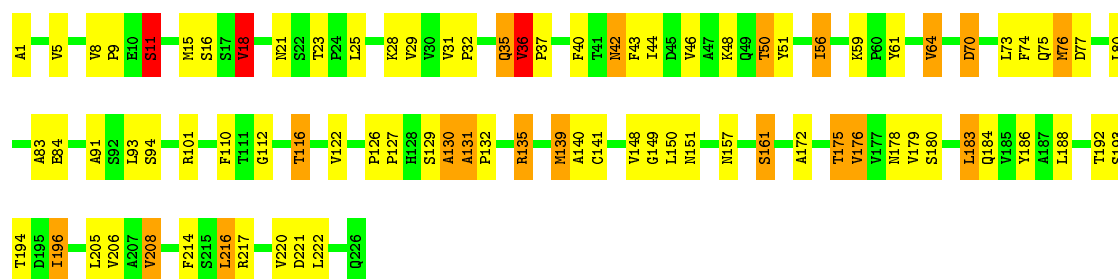


- Molecule 3: P1



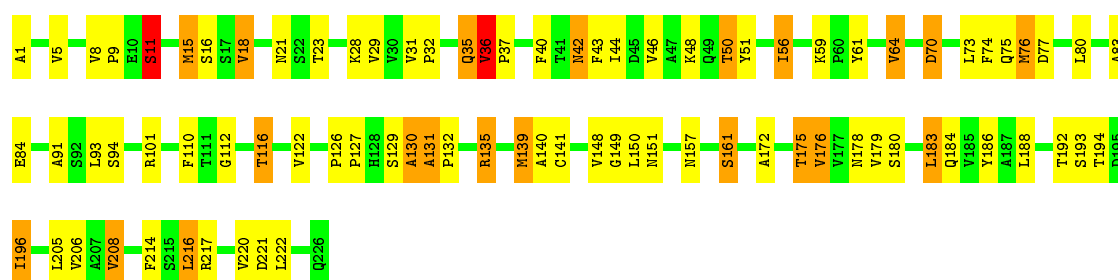
- Molecule 3: P1

Chain CR:  62% 28% 8%



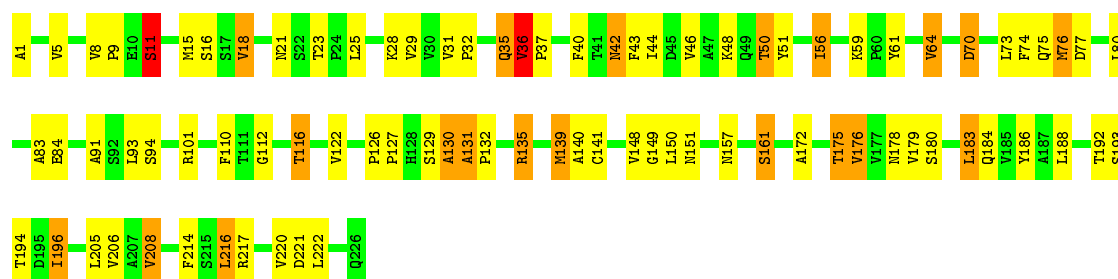
• Molecule 3: P1

Chain CS:  62% 27% 9%



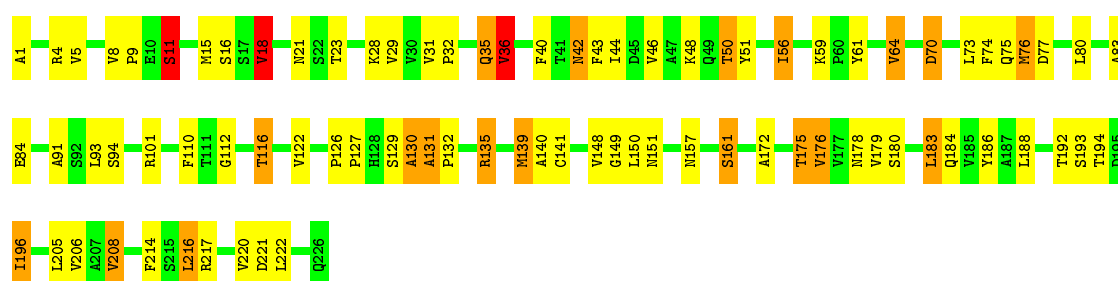
• Molecule 3: P1

Chain CT:  62% 28% 9%

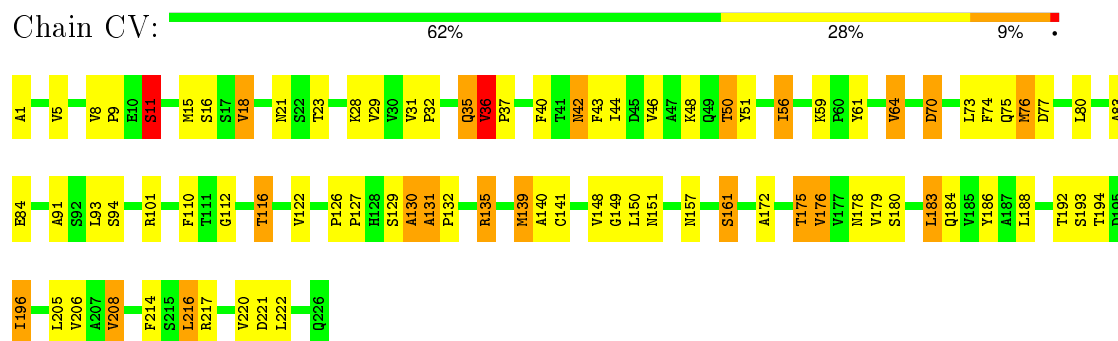


• Molecule 3: P1

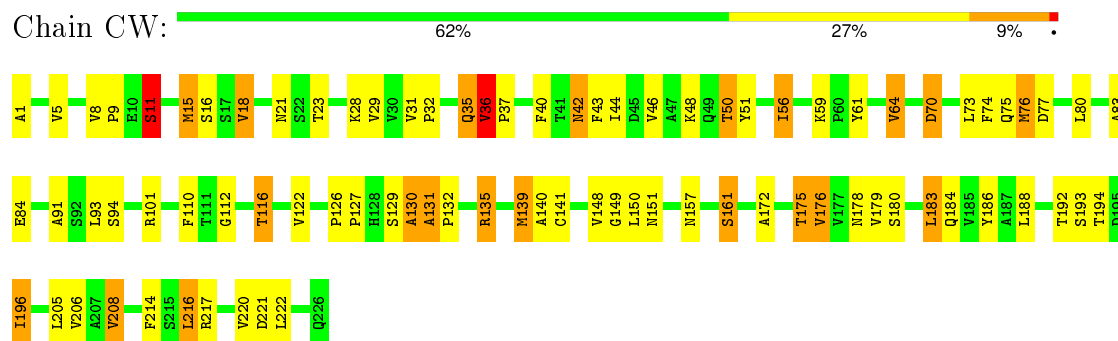
Chain CU:  62% 28% 8%



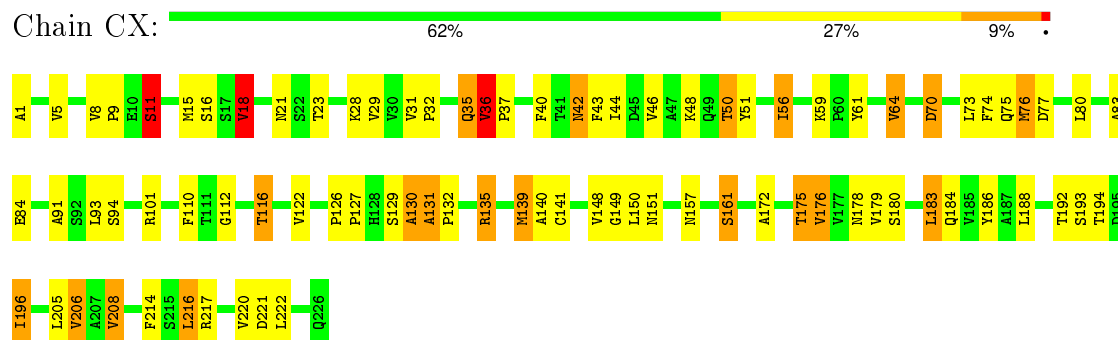
• Molecule 3: P1



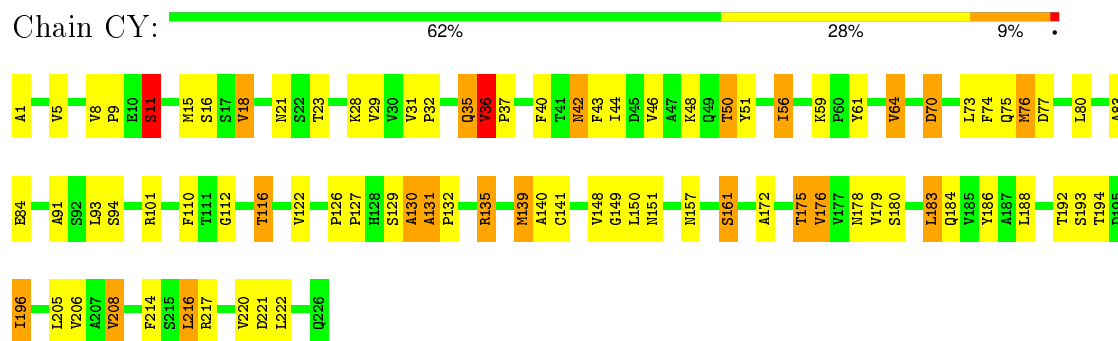
- Molecule 3: P1



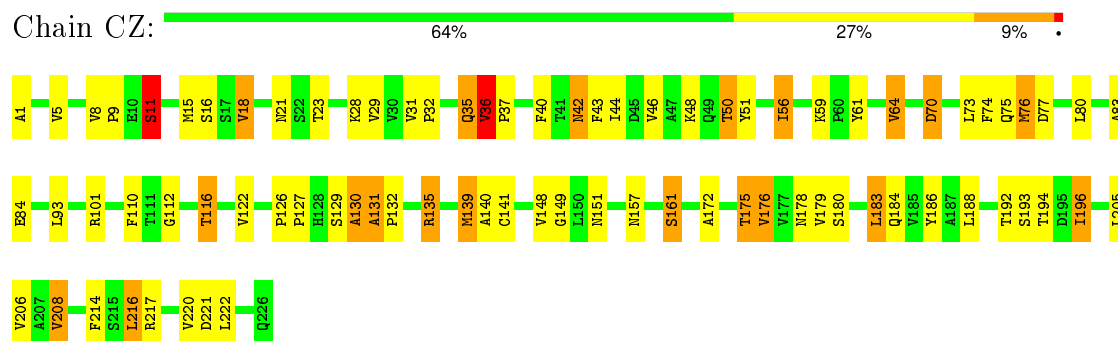
- Molecule 3: P1



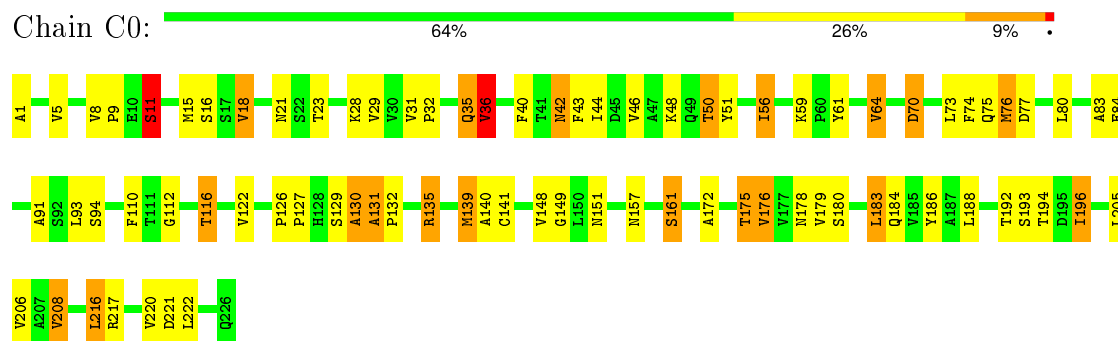
- Molecule 3: P1



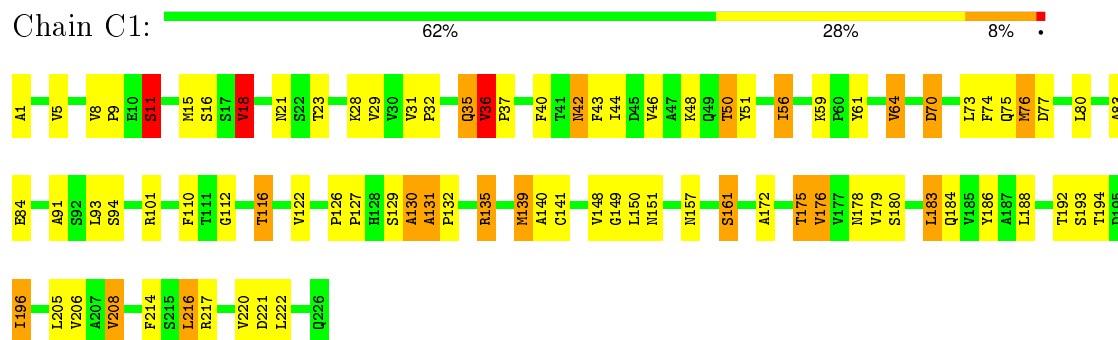
- Molecule 3: P1



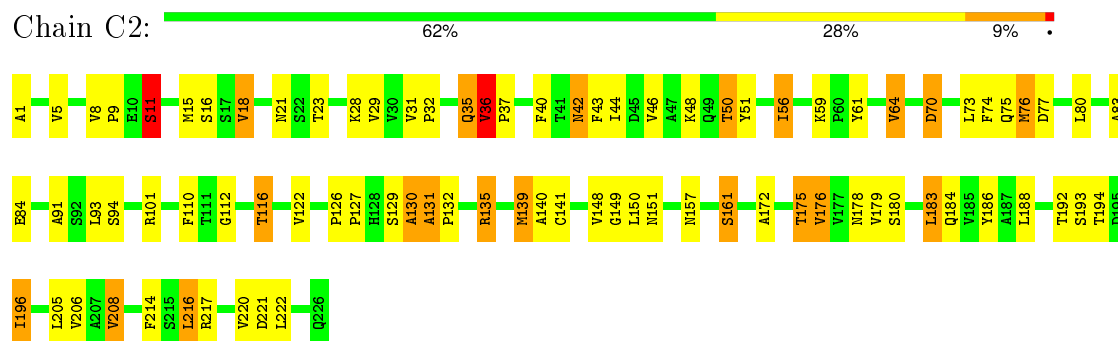
- Molecule 3: P1



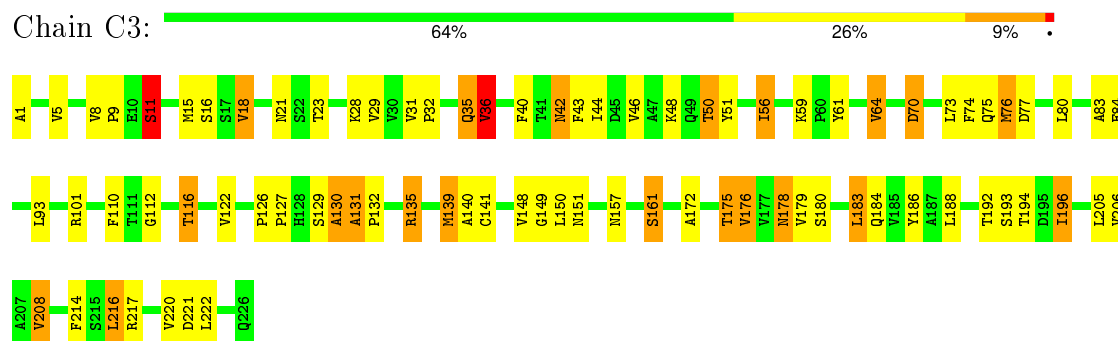
- Molecule 3: P1



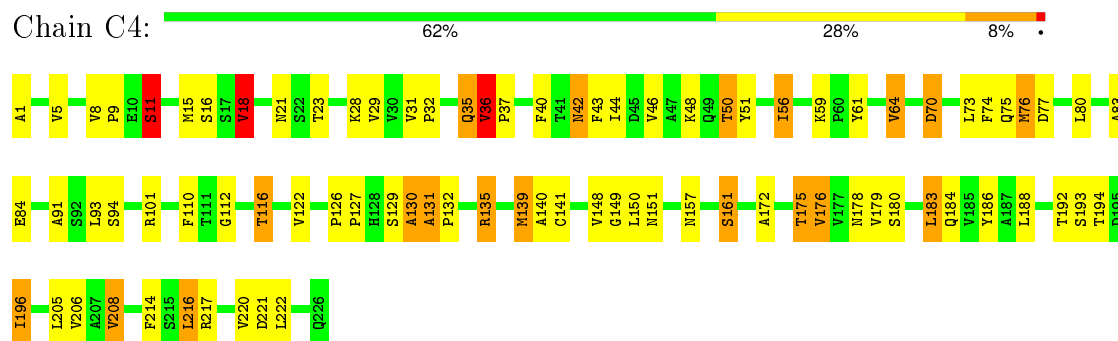
- Molecule 3: P1



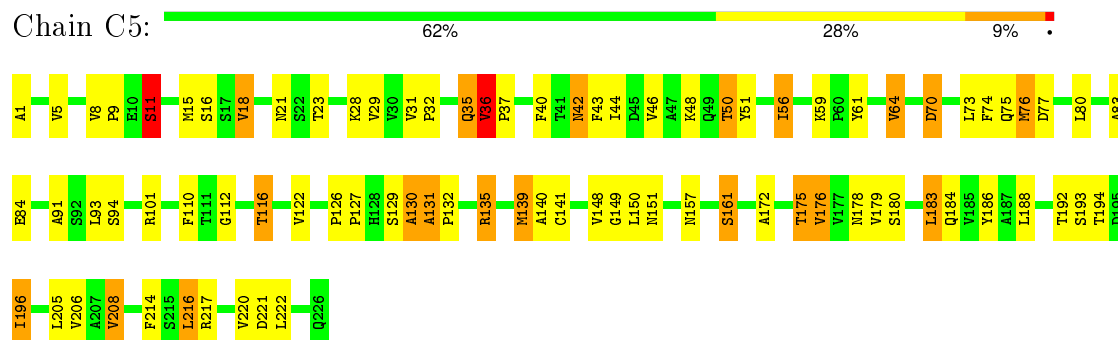
- Molecule 3: P1



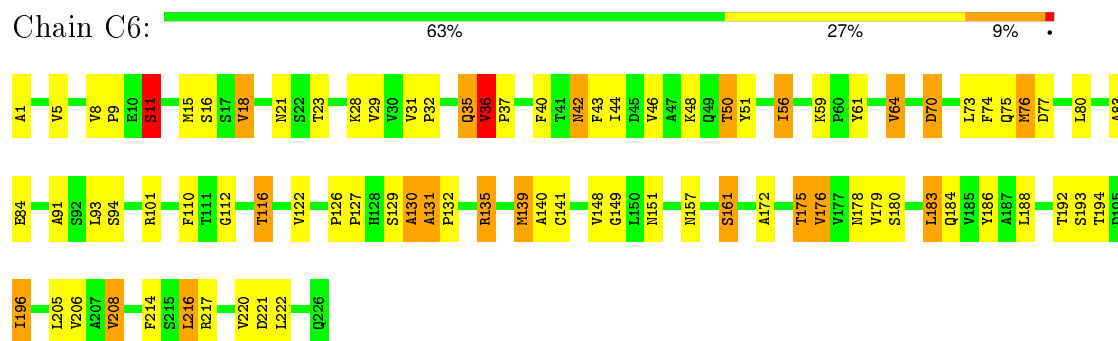
- Molecule 3: P1



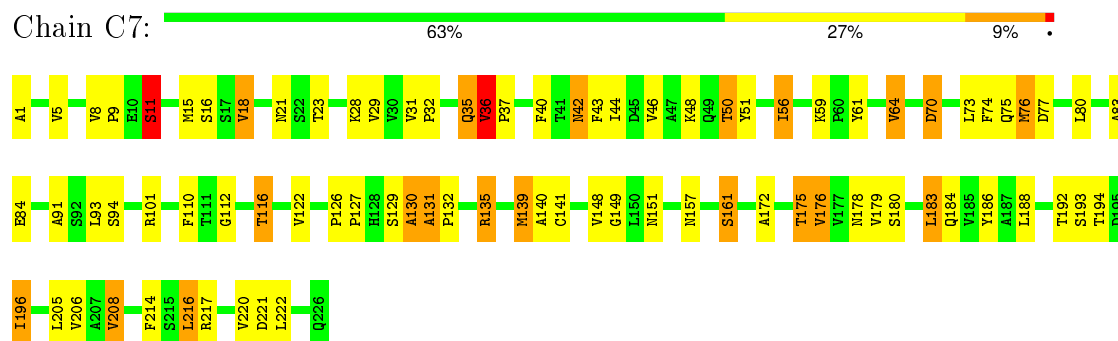
- Molecule 3: P1



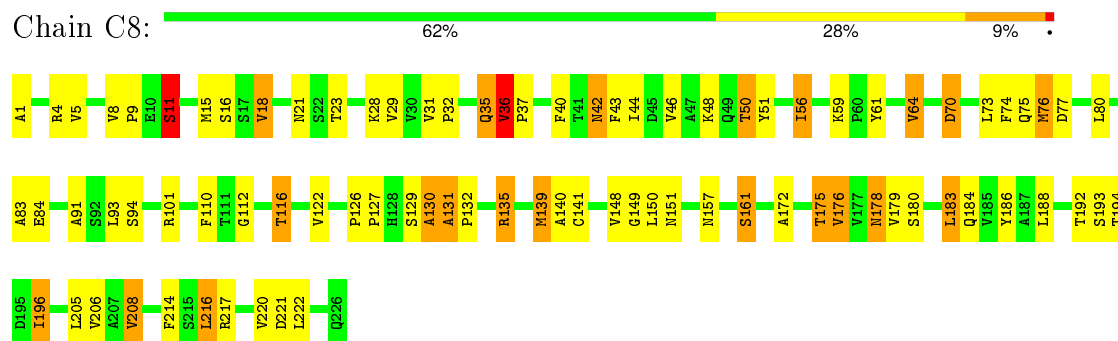
- Molecule 3: P1



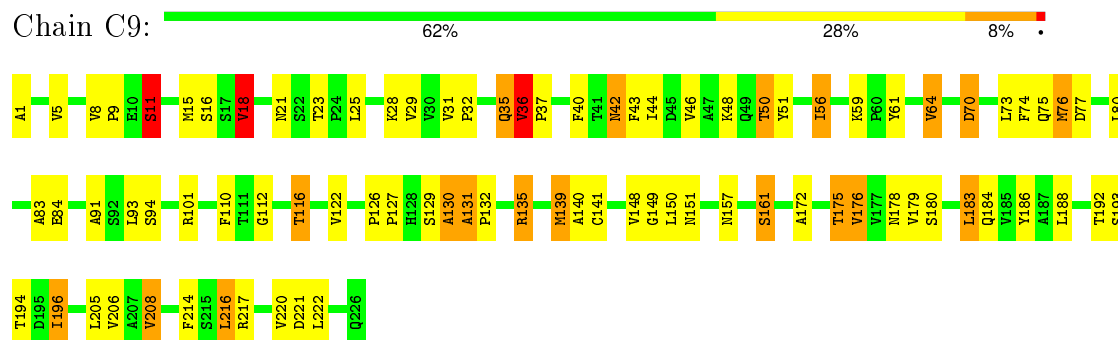
- Molecule 3: P1



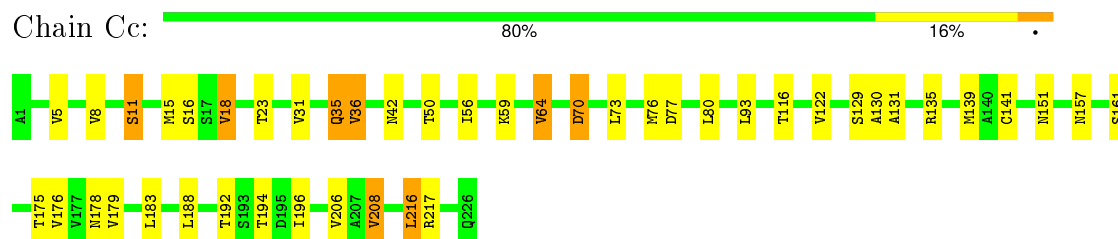
- Molecule 3: P1



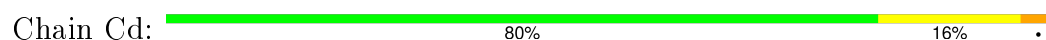
- Molecule 3: P1

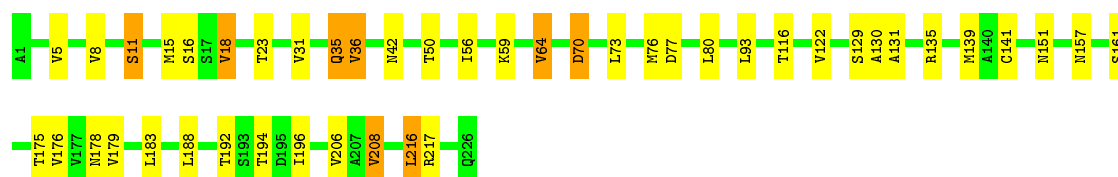


- Molecule 3: P1



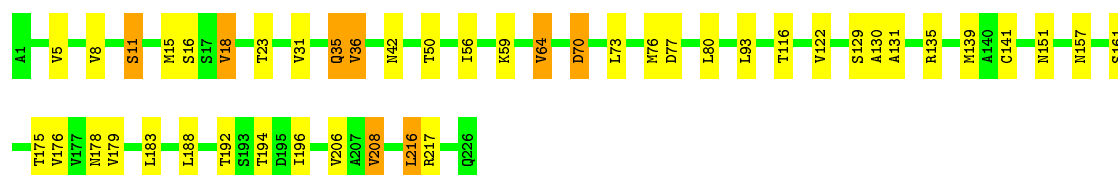
- Molecule 3: P1





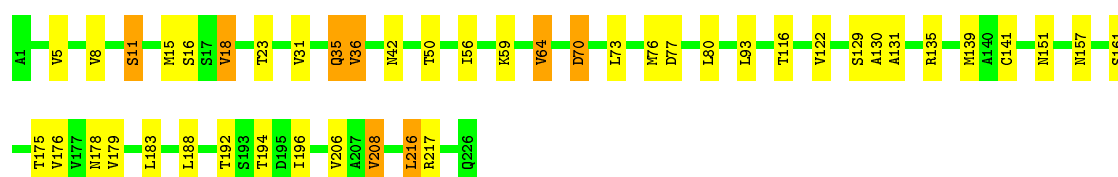
- Molecule 3: P1

Chain Ce: 80% 16%



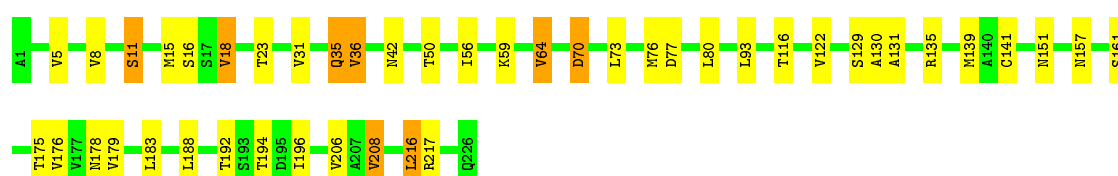
- Molecule 3: P1

Chain Cf: 80% 16%



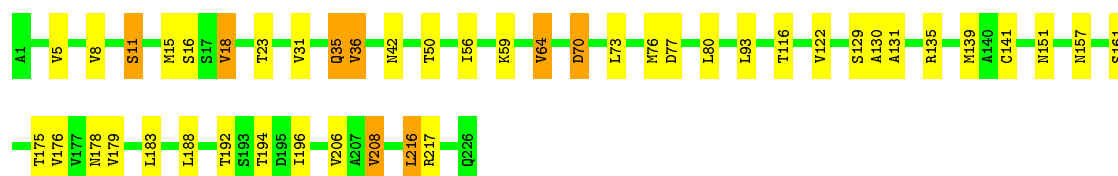
- Molecule 3: P1

Chain Cg: 80% 16%



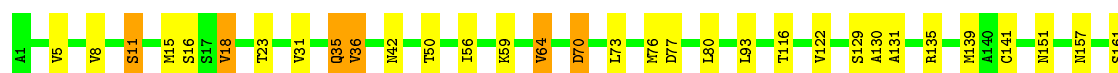
- Molecule 3: P1

Chain Ch: 80% 16%



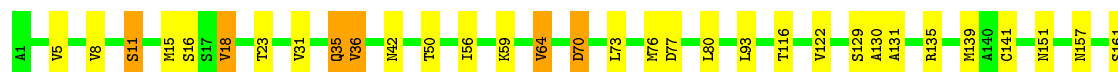
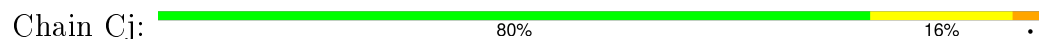
- Molecule 3: P1

Chain Ci: 80% 16%

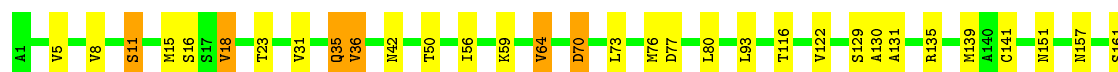
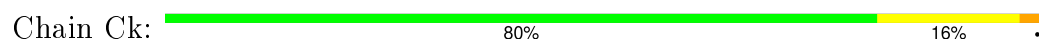




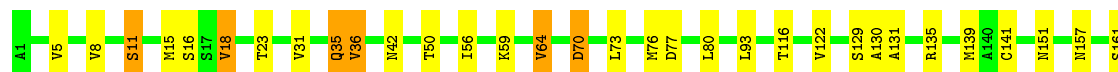
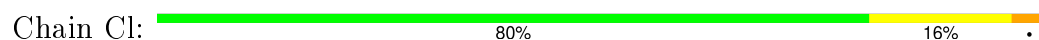
• Molecule 3: P1



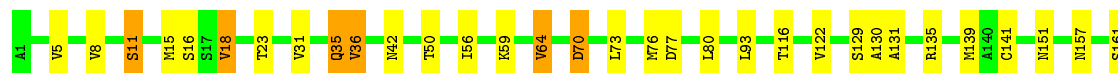
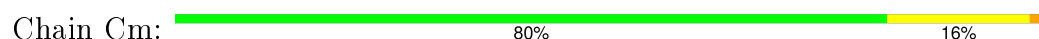
• Molecule 3: P1



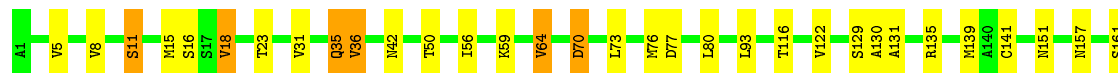
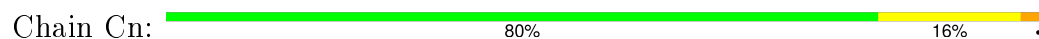
• Molecule 3: P1



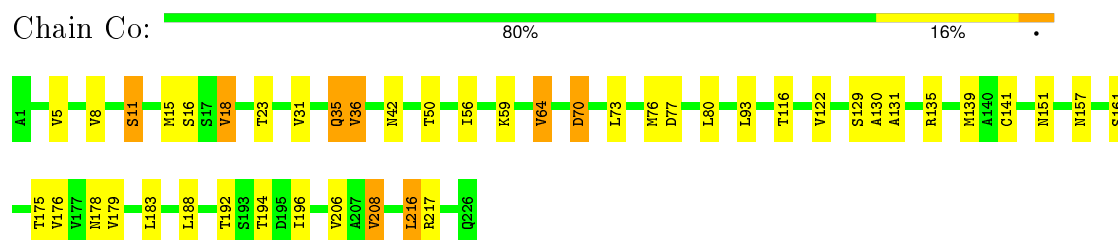
• Molecule 3: P1



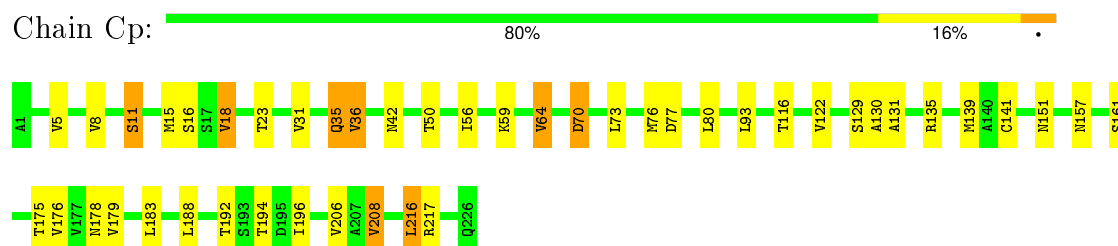
• Molecule 3: P1



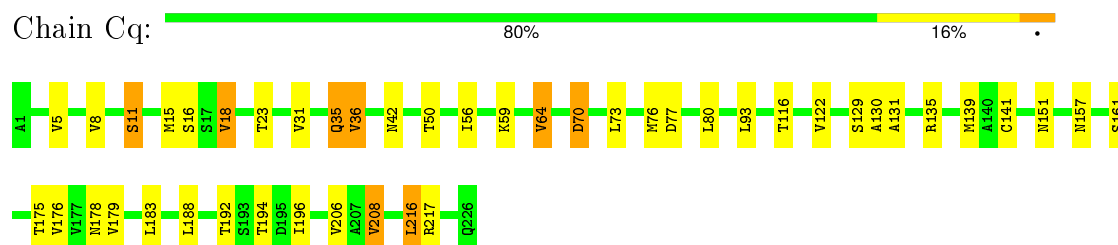
- Molecule 3: P1



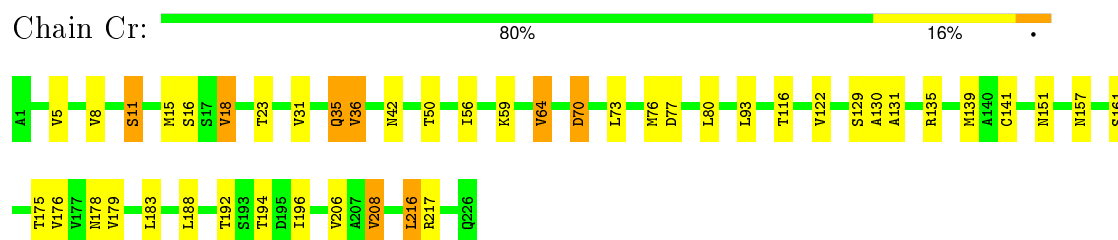
- Molecule 3: P1



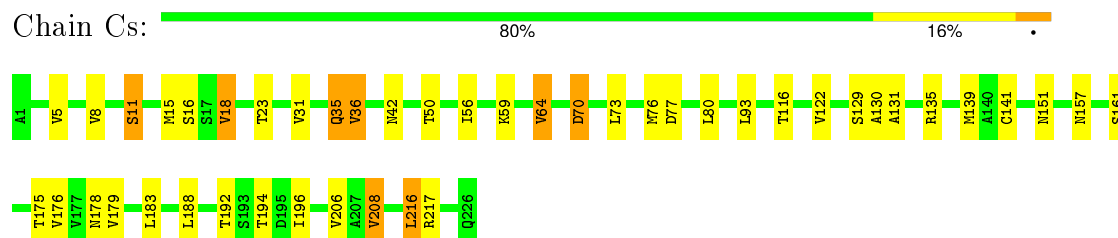
- Molecule 3: P1



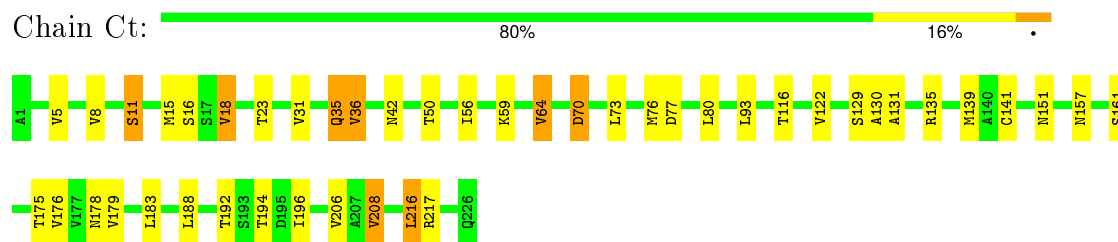
- Molecule 3: P1



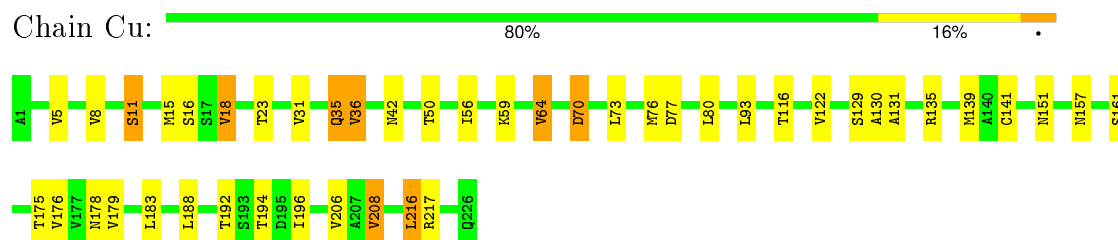
- Molecule 3: P1



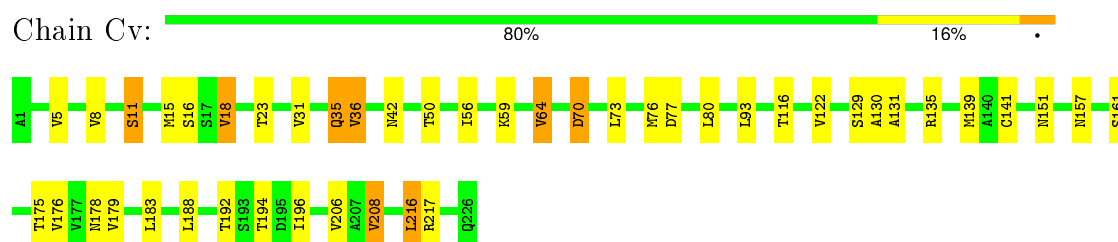
- Molecule 3: P1



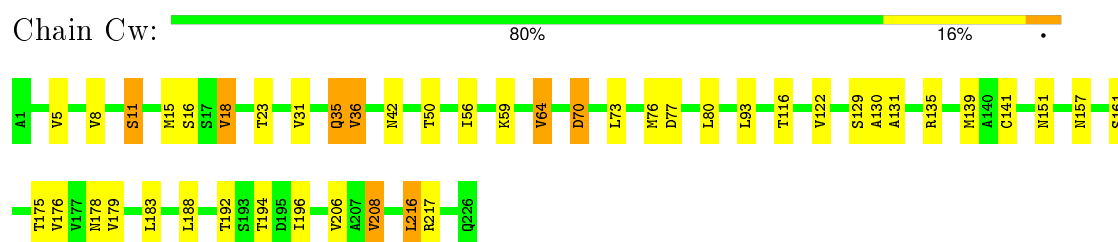
• Molecule 3: P1



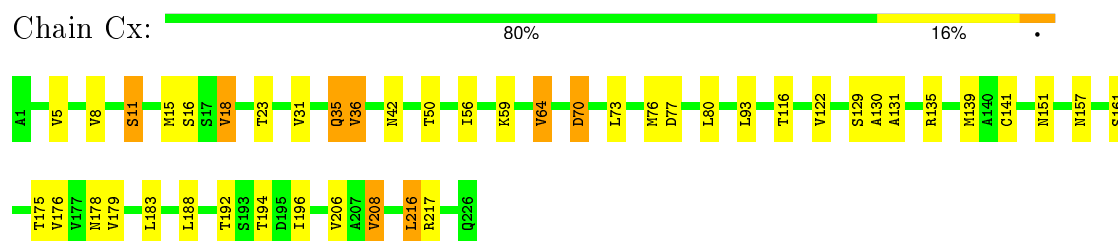
• Molecule 3: P1



• Molecule 3: P1

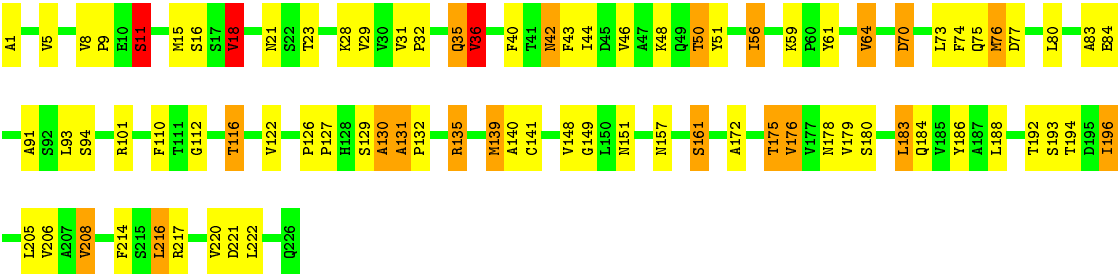


• Molecule 3: P1

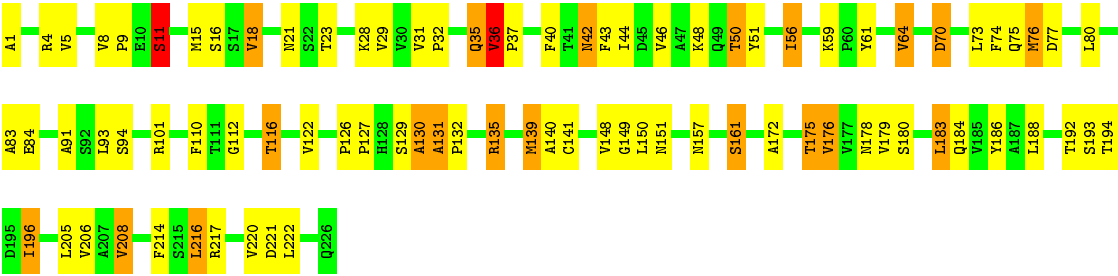


• Molecule 3: P1





● Molecule 3: P1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE FLIPPING, EACH PARTICLE	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN US4000SP	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A0	0.77	0/1992	1.12	17/2721 (0.6%)
1	A1	0.76	0/1992	1.12	17/2721 (0.6%)
1	A2	0.76	0/1992	1.13	17/2721 (0.6%)
1	A3	0.76	0/1992	1.12	17/2721 (0.6%)
1	A4	0.76	0/1992	1.12	17/2721 (0.6%)
1	A5	0.76	0/1992	1.13	17/2721 (0.6%)
1	A6	0.77	0/1992	1.12	17/2721 (0.6%)
1	A7	0.76	0/1992	1.12	18/2721 (0.7%)
1	A8	0.76	0/1992	1.13	17/2721 (0.6%)
1	A9	0.76	0/1992	1.12	17/2721 (0.6%)
1	AA	0.76	0/1992	1.12	17/2721 (0.6%)
1	AB	0.76	0/1992	1.12	17/2721 (0.6%)
1	AC	0.76	0/1992	1.12	17/2721 (0.6%)
1	AD	0.76	0/1992	1.12	17/2721 (0.6%)
1	AE	0.76	0/1992	1.12	18/2721 (0.7%)
1	AF	0.76	0/1992	1.12	18/2721 (0.7%)
1	AG	0.76	0/1992	1.12	17/2721 (0.6%)
1	AH	0.76	0/1992	1.12	17/2721 (0.6%)
1	AI	0.76	0/1992	1.12	17/2721 (0.6%)
1	AJ	0.76	0/1992	1.12	17/2721 (0.6%)
1	AK	0.76	0/1992	1.12	18/2721 (0.7%)
1	AL	0.76	0/1992	1.12	17/2721 (0.6%)
1	AM	0.76	0/1992	1.12	17/2721 (0.6%)
1	AN	0.77	0/1992	1.12	17/2721 (0.6%)
1	AO	0.76	0/1992	1.12	18/2721 (0.7%)
1	AP	0.76	0/1992	1.12	17/2721 (0.6%)
1	AQ	0.77	0/1992	1.12	17/2721 (0.6%)
1	AR	0.76	0/1992	1.12	17/2721 (0.6%)
1	AS	0.76	0/1992	1.12	18/2721 (0.7%)
1	AT	0.76	0/1992	1.12	17/2721 (0.6%)
1	AU	0.76	0/1992	1.12	17/2721 (0.6%)
1	AV	0.76	0/1992	1.12	17/2721 (0.6%)
1	AW	0.76	0/1992	1.12	17/2721 (0.6%)
1	AX	0.76	0/1992	1.12	18/2721 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	AY	0.76	0/1992	1.12	17/2721 (0.6%)
1	AZ	0.77	0/1992	1.12	17/2721 (0.6%)
1	Aa	0.76	0/1992	1.12	17/2721 (0.6%)
1	Ab	0.76	0/1992	1.12	17/2721 (0.6%)
1	Ac	0.77	0/1992	1.12	18/2721 (0.7%)
1	Ad	0.76	0/1992	1.12	17/2721 (0.6%)
1	Ae	0.76	0/1992	1.12	17/2721 (0.6%)
1	Af	0.76	0/1992	1.12	17/2721 (0.6%)
1	Ag	0.76	0/1992	1.12	17/2721 (0.6%)
1	Ah	0.76	0/1992	1.12	18/2721 (0.7%)
1	Ai	0.76	0/1992	1.12	18/2721 (0.7%)
1	Aj	0.76	0/1992	1.12	17/2721 (0.6%)
1	Ak	0.76	0/1992	1.12	17/2721 (0.6%)
1	Al	0.76	0/1992	1.12	17/2721 (0.6%)
1	Am	0.76	0/1992	1.12	17/2721 (0.6%)
1	An	0.76	0/1992	1.12	17/2721 (0.6%)
1	Ao	0.76	0/1992	1.12	17/2721 (0.6%)
1	DC	0.76	0/1992	1.12	17/2721 (0.6%)
1	DD	0.76	0/1992	1.12	17/2721 (0.6%)
1	DE	0.76	0/1992	1.12	17/2721 (0.6%)
1	DF	0.76	0/1992	1.12	17/2721 (0.6%)
1	DG	0.76	0/1992	1.12	17/2721 (0.6%)
1	DH	0.76	0/1992	1.12	17/2721 (0.6%)
1	DI	0.76	0/1992	1.12	17/2721 (0.6%)
1	DJ	0.76	0/1992	1.12	17/2721 (0.6%)
1	DK	0.76	0/1992	1.12	17/2721 (0.6%)
2	B0	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	B1	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	B2	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	B3	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	B4	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	B5	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	B6	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	B7	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	B8	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	B9	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BA	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BB	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BC	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BD	0.78	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BE	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BF	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BG	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
2	BH	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BI	0.78	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BJ	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BK	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BL	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BM	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BN	0.78	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BO	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BP	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BQ	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BR	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BS	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BT	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BU	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BV	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BW	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BX	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BY	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BZ	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Ba	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bb	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	Bc	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bd	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Be	0.78	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	Bf	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bg	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bh	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bi	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bj	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	Bk	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bl	0.77	1/1607 (0.1%)	0.99	8/2208 (0.4%)
2	Bm	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bn	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bo	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bp	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bq	0.77	1/1607 (0.1%)	0.99	8/2208 (0.4%)
2	Br	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bs	0.78	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	Bt	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bu	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bv	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bw	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bx	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
3	C0	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	C1	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	C2	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	C3	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	C4	0.82	1/1768 (0.1%)	1.04	6/2420 (0.2%)
3	C5	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	C6	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	C7	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	C8	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	C9	0.82	1/1768 (0.1%)	1.04	6/2420 (0.2%)
3	CA	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CB	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CC	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CD	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CE	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CF	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CG	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CH	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CI	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CJ	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CK	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CL	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CM	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CN	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CO	0.82	1/1768 (0.1%)	1.04	6/2420 (0.2%)
3	CP	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CQ	0.82	1/1768 (0.1%)	1.04	6/2420 (0.2%)
3	CR	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CS	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CT	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CU	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CV	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CW	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CX	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CY	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CZ	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cc	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cd	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Ce	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cf	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cg	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Ch	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Ci	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
3	Cj	0.82	1/1768 (0.1%)	1.04	6/2420 (0.2%)
3	Ck	0.82	1/1768 (0.1%)	1.03	7/2420 (0.3%)
3	Cl	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cm	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cn	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Co	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cp	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cq	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cr	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cs	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Ct	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cu	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cv	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cw	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cx	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	DA	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	DB	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
All	All	0.79	120/322020 (0.0%)	1.06	1771/440940 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A0	0	1
1	A1	0	1
1	A2	0	1
1	A3	0	1
1	A4	0	1
1	A5	0	1
1	A6	0	1
1	A7	0	1
1	A8	0	1
1	A9	0	1
1	AA	0	1
1	AB	0	1
1	AC	0	1
1	AD	0	1
1	AE	0	1
1	AF	0	1
1	AG	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	AH	0	1
1	AI	0	1
1	AJ	0	1
1	AK	0	1
1	AL	0	1
1	AM	0	1
1	AN	0	1
1	AO	0	1
1	AP	0	1
1	AQ	0	1
1	AR	0	1
1	AS	0	1
1	AT	0	1
1	AU	0	1
1	AV	0	1
1	AW	0	1
1	AX	0	1
1	AY	0	1
1	AZ	0	1
1	Aa	0	1
1	Ab	0	1
1	Ac	0	1
1	Ad	0	1
1	Ae	0	1
1	Af	0	1
1	Ag	0	1
1	Ah	0	1
1	Ai	0	1
1	Aj	0	1
1	Ak	0	1
1	Al	0	1
1	Am	0	1
1	An	0	1
1	Ao	0	1
1	DC	0	1
1	DD	0	1
1	DE	0	1
1	DF	0	1
1	DG	0	1
1	DH	0	1
1	DI	0	1
1	DJ	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	DK	0	1
2	B0	0	2
2	B1	0	2
2	B2	0	2
2	B3	0	2
2	B4	0	2
2	B5	0	2
2	B6	0	2
2	B7	0	2
2	B8	0	2
2	B9	0	2
2	BA	0	2
2	BB	0	2
2	BC	0	2
2	BD	0	2
2	BE	0	2
2	BF	0	2
2	BG	0	2
2	BH	0	2
2	BI	0	2
2	BJ	0	2
2	BK	0	2
2	BL	0	2
2	BM	0	2
2	BN	0	2
2	BO	0	2
2	BP	0	2
2	BQ	0	2
2	BR	0	2
2	BS	0	2
2	BT	0	2
2	BU	0	2
2	BV	0	2
2	BW	0	2
2	BX	0	2
2	BY	0	2
2	BZ	0	2
2	Ba	0	2
2	Bb	0	2
2	Bc	0	2
2	Bd	0	2
2	Be	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	Bf	0	2
2	Bg	0	2
2	Bh	0	2
2	Bi	0	2
2	Bj	0	2
2	Bk	0	2
2	Bl	0	2
2	Bm	0	2
2	Bn	0	2
2	Bo	0	2
2	Bp	0	2
2	Bq	0	2
2	Br	0	2
2	Bs	0	2
2	Bt	0	2
2	Bu	0	2
2	Bv	0	2
2	Bw	0	2
2	Bx	0	2
All	All	0	180

The worst 5 of 120 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B2	222	VAL	CB-CG1	-5.18	1.42	1.52
3	Cc	141	CYS	CB-SG	-5.17	1.73	1.81
3	Cg	141	CYS	CB-SG	-5.16	1.73	1.81
3	C1	141	CYS	CB-SG	-5.15	1.73	1.81
3	Cq	141	CYS	CB-SG	-5.15	1.73	1.81

The worst 5 of 1771 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DE	5	GLY	N-CA-C	10.76	140.00	113.10
1	Ah	5	GLY	N-CA-C	10.76	140.00	113.10
1	A1	5	GLY	N-CA-C	10.76	139.99	113.10
1	A2	5	GLY	N-CA-C	10.75	139.97	113.10
1	AM	5	GLY	N-CA-C	10.75	139.97	113.10

There are no chirality outliers.

5 of 180 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	208	TYR	Sidechain
1	AB	208	TYR	Sidechain
1	AC	208	TYR	Sidechain
1	AD	208	TYR	Sidechain
1	AE	208	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	1928	0	1864	92	0
1	A1	1928	0	1864	93	0
1	A2	1928	0	1864	94	0
1	A3	1928	0	1864	92	0
1	A4	1928	0	1864	92	0
1	A5	1928	0	1864	90	0
1	A6	1928	0	1864	92	0
1	A7	1928	0	1864	93	0
1	A8	1928	0	1864	91	0
1	A9	1928	0	1864	93	0
1	AA	1928	0	1864	119	0
1	AB	1928	0	1864	122	0
1	AC	1928	0	1864	133	0
1	AD	1928	0	1864	136	0
1	AE	1928	0	1864	133	0
1	AF	1928	0	1864	120	0
1	AG	1928	0	1864	123	0
1	AH	1928	0	1864	135	0
1	AI	1928	0	1864	131	0
1	AJ	1928	0	1864	129	0
1	AK	1928	0	1864	132	0
1	AL	1928	0	1864	133	0
1	AM	1928	0	1864	127	0
1	AN	1928	0	1864	130	0
1	AO	1928	0	1864	123	0
1	AP	1928	0	1864	94	0
1	AQ	1928	0	1864	90	0
1	AR	1928	0	1864	93	0
1	AS	1928	0	1864	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AT	1928	0	1864	92	0
1	AU	1928	0	1864	92	0
1	AV	1928	0	1864	91	0
1	AW	1928	0	1864	94	0
1	AX	1928	0	1864	92	0
1	AY	1928	0	1864	92	0
1	AZ	1928	0	1864	90	0
1	Aa	1928	0	1864	0	0
1	Ab	1928	0	1864	0	0
1	Ac	1928	0	1864	0	0
1	Ad	1928	0	1864	0	0
1	Ae	1928	0	1864	0	0
1	Af	1928	0	1864	0	0
1	Ag	1928	0	1864	0	0
1	Ah	1928	0	1864	0	0
1	Ai	1928	0	1864	0	0
1	Aj	1928	0	1864	0	0
1	Ak	1928	0	1864	0	0
1	Al	1928	0	1864	0	0
1	Am	1928	0	1864	0	0
1	An	1928	0	1864	0	0
1	Ao	1928	0	1864	0	0
1	DC	1928	0	1864	90	0
1	DD	1928	0	1864	93	0
1	DE	1928	0	1864	90	0
1	DF	1928	0	1864	90	0
1	DG	1928	0	1864	91	0
1	DH	1928	0	1864	92	0
1	DI	1928	0	1864	92	0
1	DJ	1928	0	1864	91	0
1	DK	1928	0	1864	92	0
2	B0	1553	0	1523	59	0
2	B1	1553	0	1523	57	0
2	B2	1553	0	1523	57	0
2	B3	1553	0	1523	58	0
2	B4	1553	0	1523	58	0
2	B5	1553	0	1523	58	0
2	B6	1553	0	1523	57	0
2	B7	1553	0	1523	57	0
2	B8	1553	0	1523	58	0
2	B9	1553	0	1523	55	0
2	BA	1553	0	1523	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BB	1553	0	1523	67	0
2	BC	1553	0	1523	69	0
2	BD	1553	0	1523	67	0
2	BE	1553	0	1523	70	0
2	BF	1553	0	1523	66	0
2	BG	1553	0	1523	70	0
2	BH	1553	0	1523	68	0
2	BI	1553	0	1523	70	0
2	BJ	1553	0	1523	74	0
2	BK	1553	0	1523	71	0
2	BL	1553	0	1523	75	0
2	BM	1553	0	1523	76	0
2	BN	1553	0	1523	76	0
2	BO	1553	0	1523	66	0
2	BP	1553	0	1523	74	0
2	BQ	1553	0	1523	76	0
2	BR	1553	0	1523	76	0
2	BS	1553	0	1523	75	0
2	BT	1553	0	1523	74	0
2	BU	1553	0	1523	72	0
2	BV	1553	0	1523	74	0
2	BW	1553	0	1523	74	0
2	BX	1553	0	1523	75	0
2	BY	1553	0	1523	56	0
2	BZ	1553	0	1523	57	0
2	Ba	1553	0	1523	0	0
2	Bb	1553	0	1523	0	0
2	Bc	1553	0	1523	0	0
2	Bd	1553	0	1523	0	0
2	Be	1553	0	1523	0	0
2	Bf	1553	0	1523	0	0
2	Bg	1553	0	1523	0	0
2	Bh	1553	0	1523	0	0
2	Bi	1553	0	1523	0	0
2	Bj	1553	0	1523	0	0
2	Bk	1553	0	1523	0	0
2	Bl	1553	0	1523	0	0
2	Bm	1553	0	1523	0	0
2	Bn	1553	0	1523	0	0
2	Bo	1553	0	1523	0	0
2	Bp	1553	0	1523	0	0
2	Bq	1553	0	1523	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Br	1553	0	1523	0	0
2	Bs	1553	0	1523	0	0
2	Bt	1553	0	1523	0	0
2	Bu	1553	0	1523	0	0
2	Bv	1553	0	1523	0	0
2	Bw	1553	0	1523	0	0
2	Bx	1553	0	1523	0	0
3	C0	1718	0	1677	54	0
3	C1	1718	0	1677	56	0
3	C2	1718	0	1677	56	0
3	C3	1718	0	1677	54	0
3	C4	1718	0	1677	56	0
3	C5	1718	0	1677	59	0
3	C6	1718	0	1677	56	0
3	C7	1718	0	1677	54	0
3	C8	1718	0	1677	59	0
3	C9	1718	0	1677	57	0
3	CA	1718	0	1677	57	0
3	CB	1718	0	1677	58	0
3	CC	1718	0	1677	86	0
3	CD	1718	0	1677	85	0
3	CE	1718	0	1677	88	0
3	CF	1718	0	1677	86	0
3	CG	1718	0	1677	87	0
3	CH	1718	0	1677	85	0
3	CI	1718	0	1677	82	0
3	CJ	1718	0	1677	86	0
3	CK	1718	0	1677	75	0
3	CL	1718	0	1677	76	0
3	CM	1718	0	1677	78	0
3	CN	1718	0	1677	72	0
3	CO	1718	0	1677	75	0
3	CP	1718	0	1677	71	0
3	CQ	1718	0	1677	85	0
3	CR	1718	0	1677	86	0
3	CS	1718	0	1677	85	0
3	CT	1718	0	1677	88	0
3	CU	1718	0	1677	85	0
3	CV	1718	0	1677	85	0
3	CW	1718	0	1677	81	0
3	CX	1718	0	1677	82	0
3	CY	1718	0	1677	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CZ	1718	0	1677	52	0
3	Cc	1718	0	1677	0	0
3	Cd	1718	0	1677	0	0
3	Ce	1718	0	1677	0	0
3	Cf	1718	0	1677	0	0
3	Cg	1718	0	1677	0	0
3	Ch	1718	0	1677	0	0
3	Ci	1718	0	1677	0	0
3	Cj	1718	0	1677	0	0
3	Ck	1718	0	1677	0	0
3	Cl	1718	0	1677	0	0
3	Cm	1718	0	1677	0	0
3	Cn	1718	0	1677	0	0
3	Co	1718	0	1677	0	0
3	Cp	1718	0	1677	0	0
3	Cq	1718	0	1677	0	0
3	Cr	1718	0	1677	0	0
3	Cs	1718	0	1677	0	0
3	Ct	1718	0	1677	0	0
3	Cu	1718	0	1677	0	0
3	Cv	1718	0	1677	0	0
3	Cw	1718	0	1677	0	0
3	Cx	1718	0	1677	0	0
3	DA	1718	0	1677	55	0
3	DB	1718	0	1677	59	0
All	All	311940	0	303840	7281	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 7281 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AN:115:THR:HG21	1:AN:131:GLN:HB3	1.44	1.00
1:AF:115:THR:HG21	1:AF:131:GLN:HB3	1.44	1.00
1:AP:115:THR:HG21	1:AP:131:GLN:HB3	1.44	1.00
1:AV:115:THR:HG21	1:AV:131:GLN:HB3	1.44	1.00
1:AA:115:THR:HG21	1:AA:131:GLN:HB3	1.44	1.00

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	A1	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	A2	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	A3	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	A4	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	A5	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	A6	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	A7	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	A8	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	A9	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AA	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AB	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AC	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AD	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AE	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AF	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AG	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AH	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AI	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AJ	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AK	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AL	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AM	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AN	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AO	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AP	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AQ	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AR	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AS	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AT	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AU	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AV	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AW	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AX	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AY	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	AZ	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	Aa	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	Ab	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	Ac	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	Ad	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	Ae	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	Af	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	Ag	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	Ah	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	Ai	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	Aj	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	Ak	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	Al	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	Am	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	An	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	Ao	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	DC	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	DD	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	DE	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	DF	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	DG	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DH	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	DI	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	DJ	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
1	DK	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	2	28
2	B0	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	B1	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	B2	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	B3	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	B4	198/200 (99%)	184 (93%)	6 (3%)	8 (4%)	4	35
2	B5	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	B6	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	B7	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	B8	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	B9	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BA	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BB	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BC	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BD	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BE	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BF	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BG	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BH	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BI	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BJ	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BK	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BL	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BM	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BN	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BO	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BP	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BQ	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BR	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BS	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BT	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BU	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BV	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BW	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BX	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BY	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	BZ	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Ba	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Bb	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Bc	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Bd	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Be	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Bf	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Bg	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Bh	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Bi	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Bj	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Bk	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Bl	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Bm	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Bn	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Bo	198/200 (99%)	184 (93%)	6 (3%)	8 (4%)	4	35
2	Bp	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Bq	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Br	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Bs	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Bt	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Bu	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Bv	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Bw	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
2	Bx	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	4	35
3	C0	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	C1	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	C2	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	C3	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	C4	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	C5	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	C6	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	C7	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	C8	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	C9	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CA	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CB	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CC	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CD	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CE	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CF	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CG	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CH	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CI	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CJ	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CK	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CL	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CM	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CN	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CO	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CP	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CQ	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CR	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CS	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CT	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CU	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CV	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CW	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CX	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CY	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	CZ	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Cc	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Cd	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Ce	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Cf	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Cg	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Ch	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Ci	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Cj	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Ck	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Cl	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Cm	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Cn	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Co	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Cp	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Cq	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Cr	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Cs	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Ct	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Cu	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Cv	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Cw	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	Cx	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	DA	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45
3	DB	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	6	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	39960/40320 (99%)	35582 (89%)	2698 (7%)	1680 (4%)	6	34

5 of 1680 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	THR
1	AA	5	GLY
1	AA	41	GLU
1	AA	202	HIS
1	AA	244	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	A1	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	A2	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	A3	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	A4	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	A5	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	A6	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	A7	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	A8	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	A9	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AA	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AB	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AC	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AD	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AE	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AF	208/208 (100%)	184 (88%)	24 (12%)	7	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AG	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AH	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AI	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AJ	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AK	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AL	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AM	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AN	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AO	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AP	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AQ	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AR	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AS	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AT	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AU	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AV	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AW	208/208 (100%)	183 (88%)	25 (12%)	6	31
1	AX	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AY	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	AZ	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	Aa	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	Ab	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	Ac	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	Ad	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	Ae	208/208 (100%)	183 (88%)	25 (12%)	6	31
1	Af	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	Ag	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	Ah	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	Ai	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	Aj	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	Ak	208/208 (100%)	184 (88%)	24 (12%)	7	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Al	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	Am	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	An	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	Ao	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	DC	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	DD	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	DE	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	DF	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	DG	208/208 (100%)	183 (88%)	25 (12%)	6	31
1	DH	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	DI	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	DJ	208/208 (100%)	184 (88%)	24 (12%)	7	32
1	DK	208/208 (100%)	184 (88%)	24 (12%)	7	32
2	B0	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	B1	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	B2	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	B3	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	B4	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	B5	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	B6	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	B7	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	B8	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	B9	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BA	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BB	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BC	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BD	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BE	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BF	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BG	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BH	176/176 (100%)	150 (85%)	26 (15%)	4	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BI	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BJ	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BK	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BL	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BM	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BN	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BO	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BP	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BQ	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BR	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BS	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BT	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BU	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BV	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BW	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BX	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BY	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	BZ	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Ba	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bb	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bc	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bd	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Be	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bf	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bg	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bh	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bi	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bj	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bk	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bl	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bm	176/176 (100%)	150 (85%)	26 (15%)	4	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Bn	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bo	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bp	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bq	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Br	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bs	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bt	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bu	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bv	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bw	176/176 (100%)	150 (85%)	26 (15%)	4	24
2	Bx	176/176 (100%)	150 (85%)	26 (15%)	4	24
3	C0	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	C1	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	C2	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	C3	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	C4	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	C5	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	C6	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	C7	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	C8	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	C9	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CA	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CB	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CC	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CD	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CE	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CF	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CG	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CH	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CI	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CJ	190/190 (100%)	150 (79%)	40 (21%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	CK	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CL	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CM	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CN	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CO	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CP	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CQ	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CR	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CS	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CT	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CU	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CV	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CW	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CX	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CY	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	CZ	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Cc	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Cd	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Ce	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Cf	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Cg	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Ch	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Ci	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Cj	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Ck	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Cl	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Cm	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Cn	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Co	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Cp	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Cq	190/190 (100%)	150 (79%)	40 (21%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Cr	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Cs	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Ct	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Cu	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Cv	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Cw	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	Cx	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	DA	190/190 (100%)	150 (79%)	40 (21%)	1	9
3	DB	190/190 (100%)	150 (79%)	40 (21%)	1	9
All	All	34440/34440 (100%)	29037 (84%)	5403 (16%)	7	21

5 of 5403 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Bk	193	THR
3	CF	216	LEU
3	Cv	35	GLN
2	Bn	146	GLU
2	Bw	110	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1200 such sidechains are listed below:

Mol	Chain	Res	Type
2	B3	134	HIS
2	Bj	136	HIS
3	Ct	184	GLN
2	B5	134	HIS
2	Bb	190	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.