



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 05:11 PM EDT

PDB ID : 6YFB  
Title : Virus-like particle of bacteriophage AVE016  
Authors : Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.  
Deposited on : 2020-03-26  
Resolution : 3.59 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

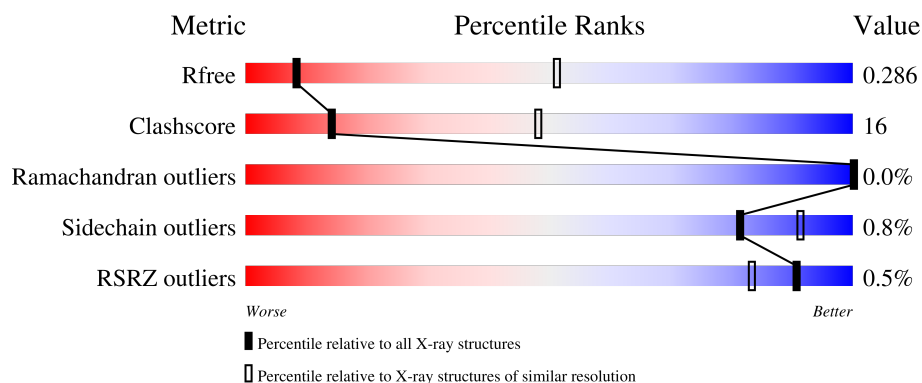
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.59 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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

Mol	Chain	Length	Quality of chain
1	AA	166	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>34%</div> <div>.</div> </div> </div>
1	AB	166	<div> <div></div> <div>67%</div> <div>33%</div> <div>.</div> </div>
1	AC	166	<div> <div></div> <div>72%</div> <div>28%</div> <div>.</div> </div>
1	AD	166	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>30%</div> <div>.</div> </div> </div>
1	AE	166	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>28%</div> <div>.</div> </div> </div>


























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Mol	Chain	Length	Quality of chain
1	AF	166	 72% 28%
1	AG	166	 69% 30%
1	AH	166	 69% 30%
1	AI	166	 69% 31%
1	AJ	166	 64% 35%
1	AK	166	 69% 30%
1	AL	166	 69% 29%
1	AM	166	 62% 37%
1	AN	166	 63% 37%
1	AO	166	 66% 33%
1	AP	166	 66% 34%
1	AQ	166	 68% 32%
1	AR	166	 73% 27%
1	AS	166	 64% 36%
1	AT	166	 67% 33%
1	AU	166	 61% 37%
1	AV	166	 63% 36%
1	AW	166	 66% 33%
1	AX	166	 71% 28%
1	AY	166	 71% 28%
1	AZ	166	 71% 28%
1	BA	166	 71% 28%
1	BB	166	 69% 31%
1	BC	166	 70% 28%
1	BD	166	 73% 27%














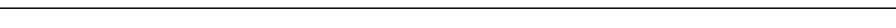











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Mol	Chain	Length	Quality of chain
1	BE	166	 68% 31% .
1	BF	166	 70% 29% .
1	BG	166	 71% 28% .
1	BH	166	 63% 36% .
1	BI	166	 65% 35% .
1	BJ	166	 66% 33% .
1	BK	166	 66% 34% .
1	BL	166	 69% 31% .
1	BM	166	 71% 29% .
1	BN	166	 65% 35% .
1	BO	166	 66% 33% .
1	BP	166	 62% 36% .
1	BQ	166	 64% 34% .
1	BR	166	 68% 31% .
1	BS	166	 71% 28% .
1	BT	166	 69% 30% .
1	BU	166	 69% 30% .
1	BV	166	 68% 31% .
1	BW	166	 70% 29% .
1	BX	166	 70% 28% .
1	BY	166	 72% 27% .
1	BZ	166	 67% 32% .
1	CA	166	 69% 30% .
1	CB	166	 69% 30% .
1	CC	166	 63% 36% .



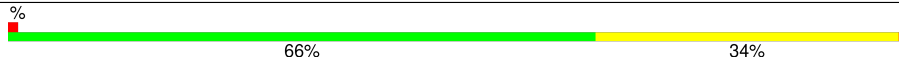
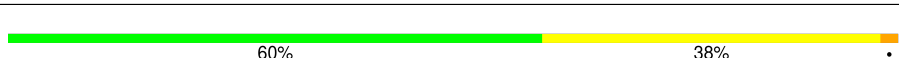
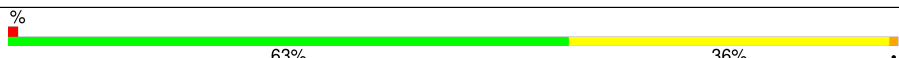
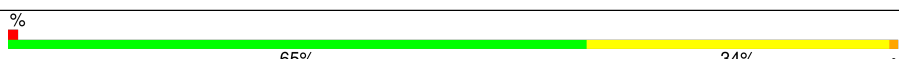
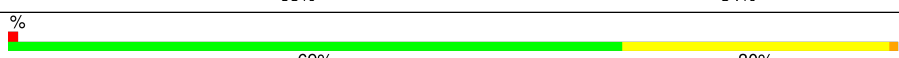
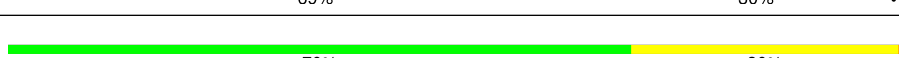
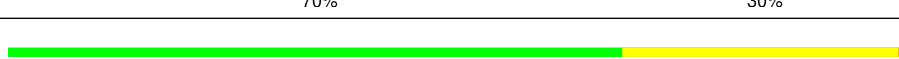

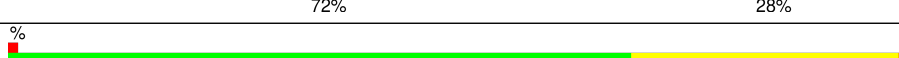







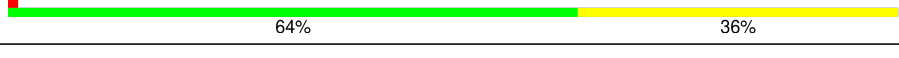
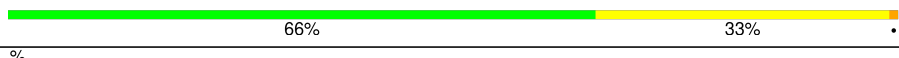

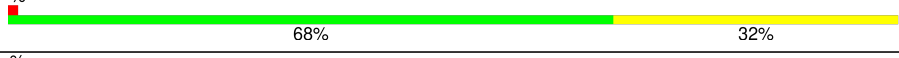



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Mol	Chain	Length	Quality of chain
1	CD	166	 63% 37%
1	CE	166	 64% 35% .
1	CF	166	 66% 34%
1	CG	166	 67% 33%
1	CH	166	 71% 29%
1	CI	166	 64% 36%
1	CJ	166	 65% 34% .
1	CK	166	 61% 38% .
1	CL	166	 63% 36% .
1	CM	166	 67% 33% .
1	CN	166	 70% 30% .
1	CO	166	 70% 29% .
1	CP	166	 72% 28% .
1	CQ	166	 70% 29% .
1	CR	166	 67% 32% .
1	CS	166	 69% 30% .
1	CT	166	 73% 26% .
1	CU	166	 67% 32% .
1	CV	166	 70% 29% .
1	CW	166	 70% 28% .
1	CX	166	 66% 33% .
1	CY	166	 64% 36%
1	CZ	166	 66% 33% .
1	DA	166	 66% 34%
1	DB	166	 69% 31%


























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Mol	Chain	Length	Quality of chain	
1	DC	166		
1	DD	166		
1	DE	166		
1	DF	166		
1	DG	166		
1	DH	166		
1	DI	166		
1	DJ	166		
1	DK	166		
1	DL	166		
1	DM	166		
1	DN	166		
1	DO	166		
1	DP	166		
1	DQ	166		
1	DR	166		
1	DS	166		
1	DT	166		
1	DU	166		
1	DV	166		
1	DW	166		
1	DX	166		
1	DY	166		
1	DZ	166		
1	EA	166		














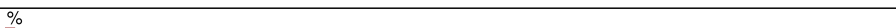











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Mol	Chain	Length	Quality of chain
1	EB	166	 62% 37% .
1	EC	166	 68% 31% .
1	ED	166	 70% 30% .
1	EE	166	 71% 28% .
1	EF	166	 70% 30% .
1	EG	166	 70% 29% .
1	EH	166	 68% 31% .
1	EI	166	 70% 28% .
1	EJ	166	 72% 27% .
1	EK	166	 68% 31% .
1	EL	166	 69% 30% .
1	EM	166	 72% 27% .
1	EN	166	 61% 37% .
1	EO	166	 66% 34% .
1	EP	166	 67% 32% .
1	EQ	166	 66% 34% .
1	ER	166	 68% 32% .
1	ES	166	 70% 30% .
1	ET	166	 64% 36% .
1	EU	166	 64% 35% .
1	EV	166	 60% 38% .
1	EW	166	 63% 36% .
1	EX	166	 66% 33% .
1	EY	166	 70% 30% .
1	EZ	166	 71% 28% .

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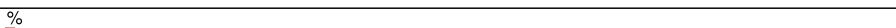











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Mol	Chain	Length	Quality of chain
1	FA	166	 70% 29% .
1	FB	166	 70% 29% .
1	FC	166	 72% 27% .
1	FD	166	 70% 29% .
1	FE	166	 72% 28% .
1	FF	166	 67% 33% .
1	FG	166	 70% 28% .
1	FH	166	 70% 29% .
1	FI	166	 63% 36% .
1	FJ	166	 64% 36% .
1	FK	166	 66% 33% .
1	FL	166	 66% 34% .
1	FM	166	 67% 33% .
1	FN	166	 70% 30% .
1	FO	166	 64% 36% .
1	FP	166	 68% 31% .
1	FQ	166	 61% 37% .
1	FR	166	 63% 36% .
1	FS	166	 67% 32% .
1	FT	166	 72% 28% .
1	FU	166	 70% 29% .
1	FV	166	 72% 28% .
1	FW	166	 70% 29% .
1	FX	166	 70% 30% .
1	FY	166	 69% 30% .

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Mol	Chain	Length	Quality of chain
1	FZ	166	 70% 29% .
1	GA	166	 67% 31% .
1	GB	166	 70% 28% .
1	GC	166	 72% 27% .
1	GD	166	 64% 35% .
1	GE	166	 64% 36% .
1	GF	166	 66% 33% .
1	GG	166	 67% 33% .
1	GH	166	 69% 31% .
1	GI	166	 72% 28% .
1	GJ	166	 64% 36% .
1	GK	166	 69% 30% .
1	GL	166	 62% 36% .
1	GM	166	 64% 34% .
1	GN	166	 67% 32% .
1	GO	166	 72% 28% .
1	GP	166	 70% 29% .
1	GQ	166	 72% 27% .
1	GR	166	 70% 30% .
1	GS	166	 68% 31% .
1	GT	166	 70% 29% .
1	GU	166	 71% 28% .
1	GV	166	 66% 34% .
1	GW	166	 70% 29% .
1	GX	166	 70% 28% .

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Mol	Chain	Length	Quality of chain
1	GY	166	
1	GZ	166	
1	HA	166	
1	HB	166	
1	HC	166	
1	HD	166	
1	HE	166	
1	HF	166	
1	HG	166	
1	HH	166	
1	HI	166	
1	HJ	166	
1	HK	166	
1	HL	166	
1	HM	166	
1	HN	166	
1	HO	166	
1	HP	166	
1	HQ	166	
1	HR	166	
1	HS	166	
1	HT	166	
1	HU	166	
1	HV	166	
1	HW	166	

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Mol	Chain	Length	Quality of chain
1	HX	166	<div><div></div><div>%</div><div><div></div><div>69%</div><div>31%</div></div></div>
1	HY	166	<div><div></div><div>2%</div><div><div></div><div>72%</div><div>28%</div></div></div>
1	HZ	166	<div><div></div><div>2%</div><div><div></div><div>66%</div><div>34%</div></div></div>
1	IA	166	<div><div></div><div>%</div><div><div></div><div>67%</div><div>32%</div><div></div><div>.</div></div></div>
1	IB	166	<div><div></div><div></div><div><div></div><div>65%</div><div>33%</div><div></div><div>.</div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 275100 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AB	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AC	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AD	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AE	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AF	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AG	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AH	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AI	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AJ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AK	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AL	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AM	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AN	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AO	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AP	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AQ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AR	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AS	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AT	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AU	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AV	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AW	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AX	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AY	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	AZ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BA	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BB	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BC	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BD	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BE	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BF	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BG	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BH	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BI	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BJ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BK	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BL	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BM	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BN	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BO	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BP	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BQ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BR	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BS	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BT	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BU	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BV	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BW	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BX	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BY	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	BZ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CA	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CB	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CC	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CD	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CE	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CF	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CG	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CH	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CI	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CJ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CK	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CL	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CM	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CN	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CO	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CP	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CQ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CR	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CS	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CT	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CU	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CV	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CW	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CX	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CY	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	CZ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DA	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	DB	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DC	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DD	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DE	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DF	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DG	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DH	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DI	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DJ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DK	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DL	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DM	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DN	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DO	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DP	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DQ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DR	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DS	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DT	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DU	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DV	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	DW	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DX	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DY	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	DZ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EA	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EB	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EC	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	ED	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EE	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EF	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EG	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EH	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EI	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EJ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EK	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EL	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EM	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EN	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EO	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EP	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EQ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	ER	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	ES	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	ET	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EU	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EV	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EW	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EX	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EY	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	EZ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FA	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FB	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FC	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FD	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FE	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FF	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FG	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FH	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FI	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FJ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FK	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FL	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	FM	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FN	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FO	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FP	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FQ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FR	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FS	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FT	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FU	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FV	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FW	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FX	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FY	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	FZ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GA	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GB	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GC	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GD	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GE	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GF	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GG	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	GH	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GI	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GJ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GK	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GL	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GM	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GN	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GO	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GP	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GQ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GR	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GS	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GT	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GU	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GV	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GW	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GX	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GY	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	GZ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HA	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HB	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	HC	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HD	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HE	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HF	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HG	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HH	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HI	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HJ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HK	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HL	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HM	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HN	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HO	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HP	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HQ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HR	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HS	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HT	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HU	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HV	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HW	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			

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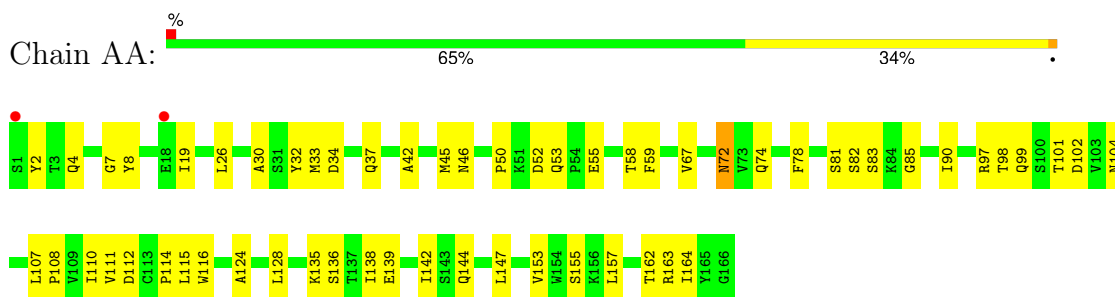
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	HX	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HY	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	HZ	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
1	IA	166	Total	C	N	O	S	0	0	0
			1310	828	215	262	5			
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			1310	828	215	262	5			

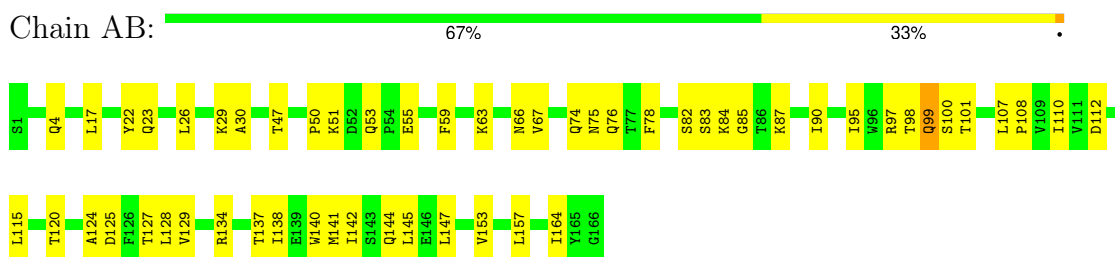
### 3 Residue-property plots

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

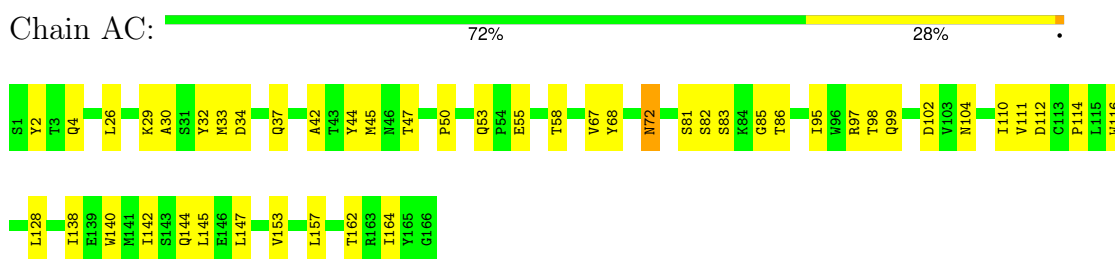
- Molecule 1: coat protein



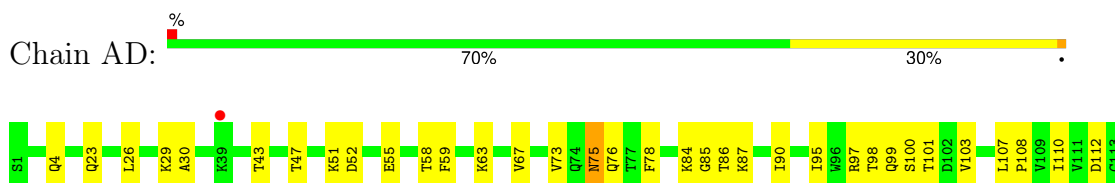
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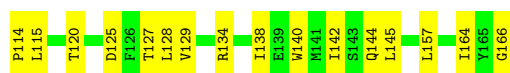


- Molecule 1: coat protein

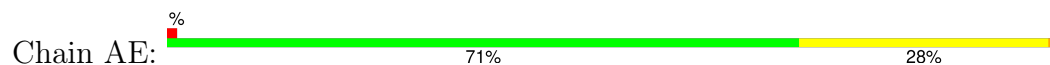


- Molecule 1: coat protein





- Molecule 1: coat protein



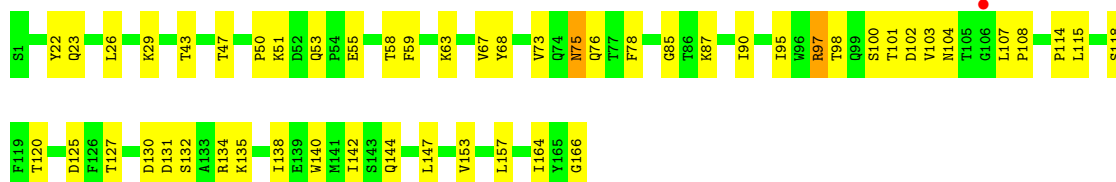
- Molecule 1: coat protein



- Molecule 1: coat protein



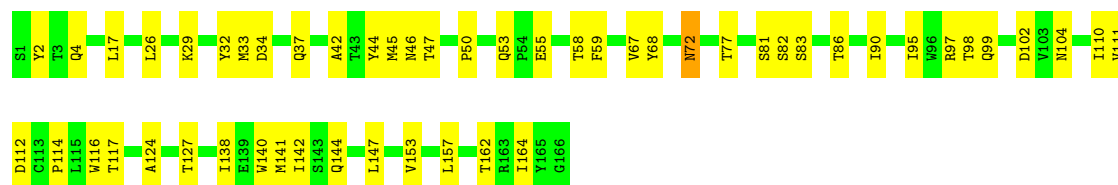
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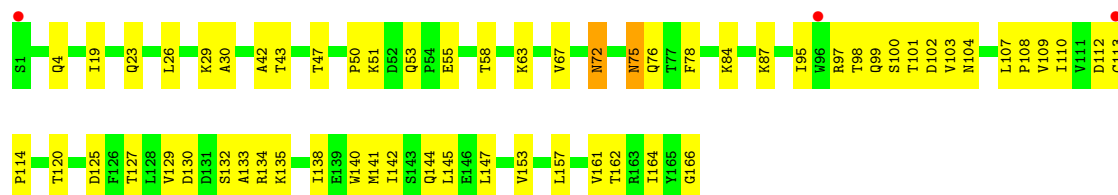
- Molecule 1: coat protein



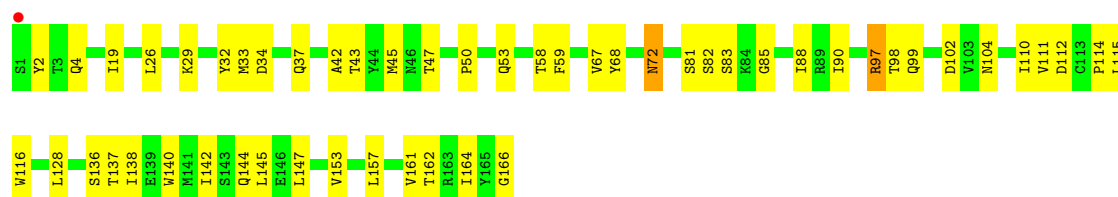




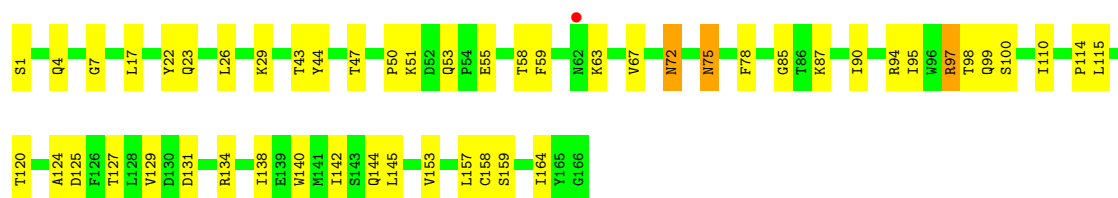
- Molecule 1: coat protein



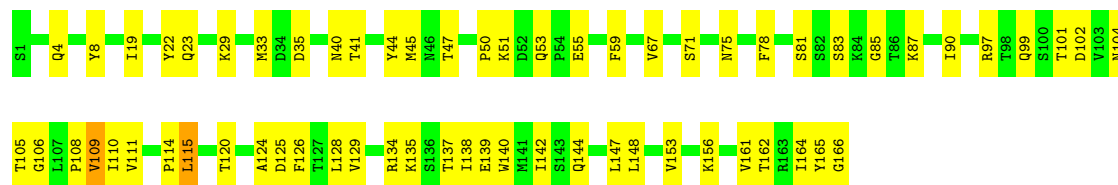
- Molecule 1: coat protein



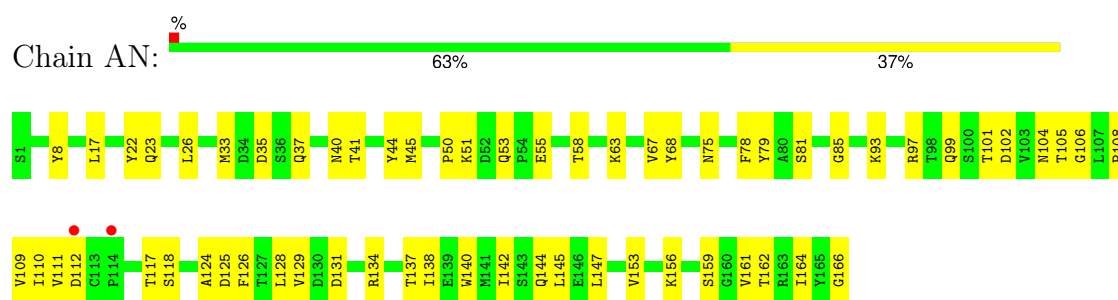
- Molecule 1: coat protein



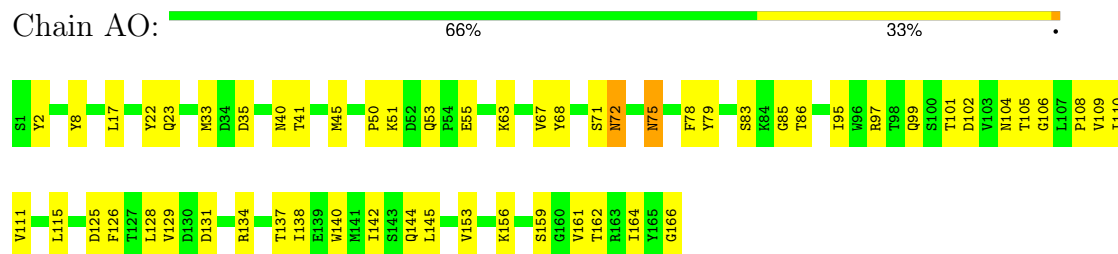
- Molecule 1: coat protein



- Molecule 1: coat protein



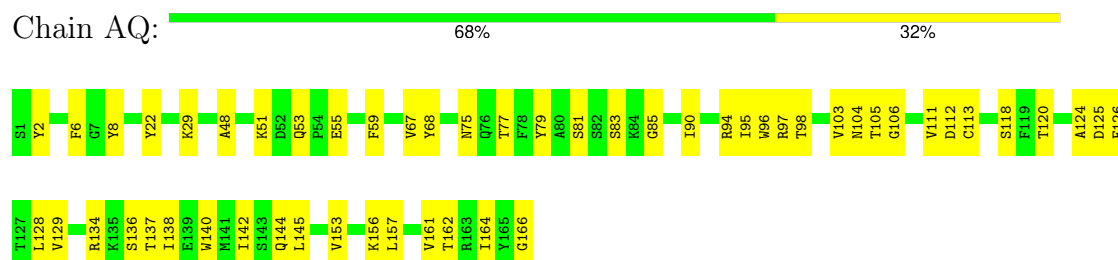
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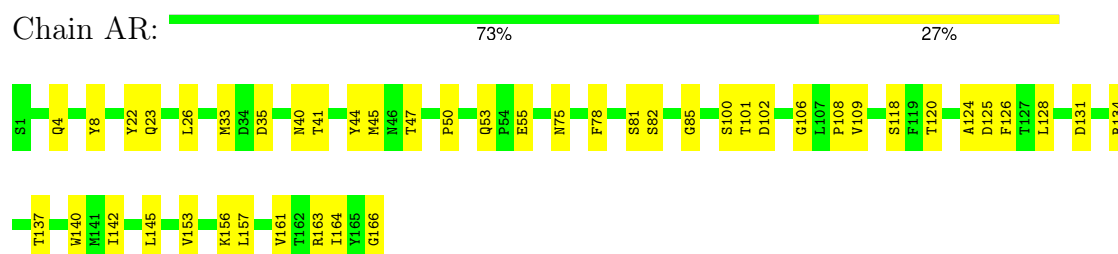
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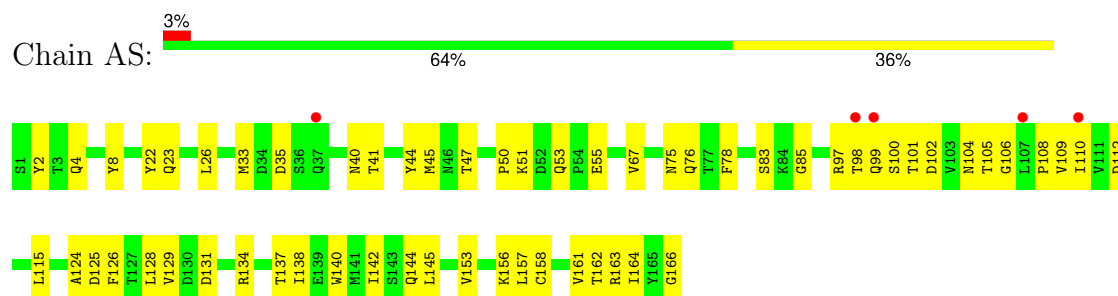
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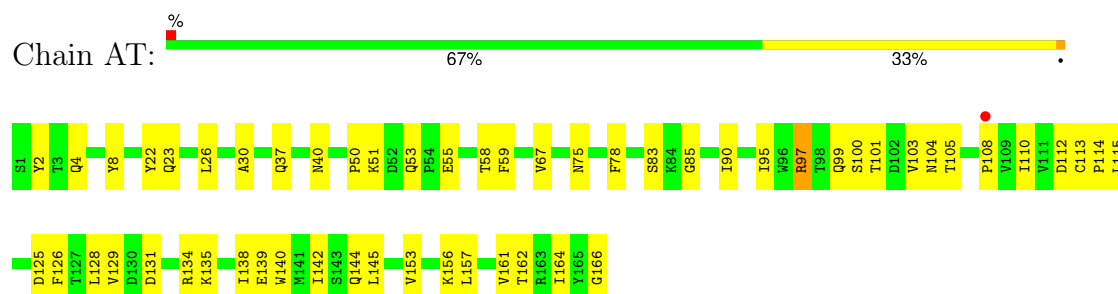
- Molecule 1: coat protein



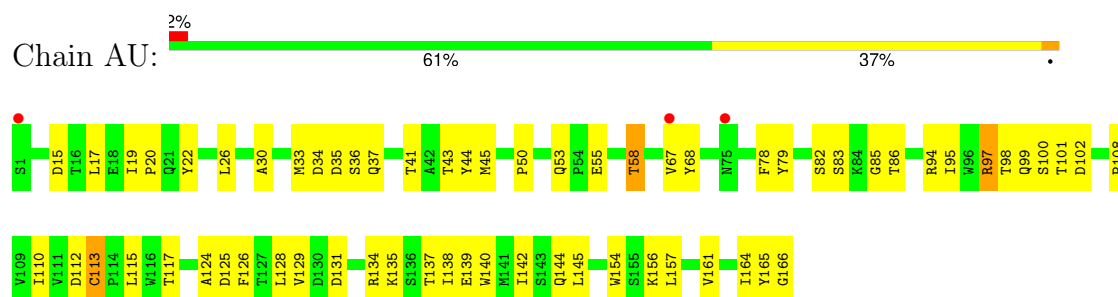
- Molecule 1: coat protein



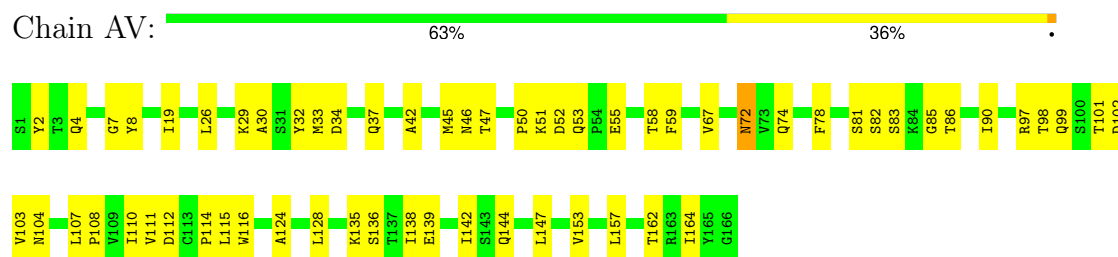
- Molecule 1: coat protein



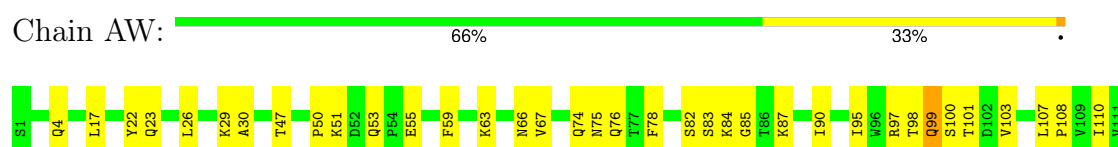
- Molecule 1: coat protein



- Molecule 1: coat protein



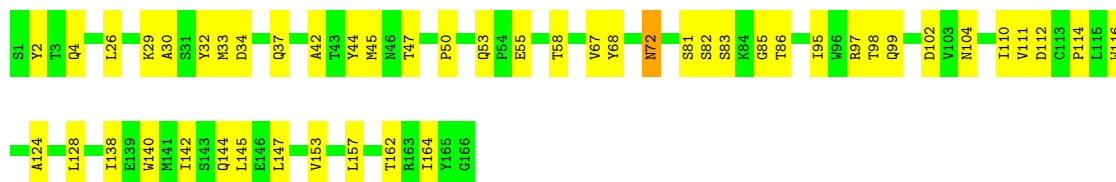
- Molecule 1: coat protein





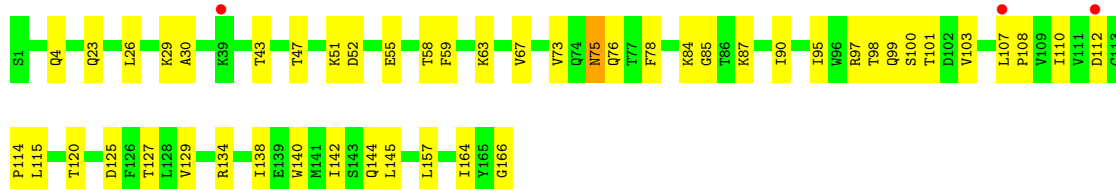
- Molecule 1: coat protein

Chain AX: 71% 28% .



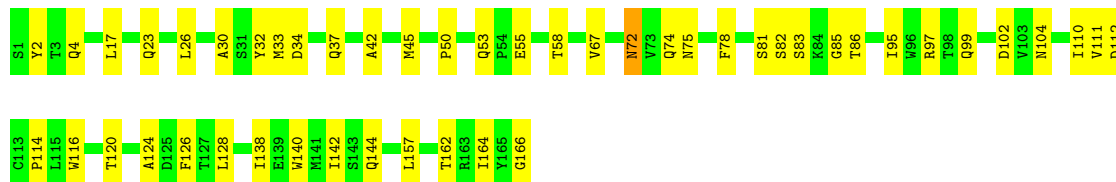
- Molecule 1: coat protein

Chain AY: 71% 28% .



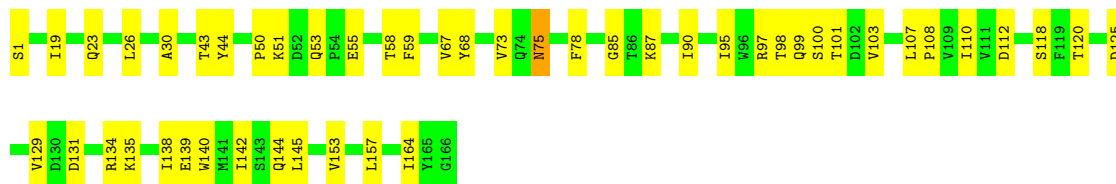
- Molecule 1: coat protein

Chain AZ: 71% 28% .



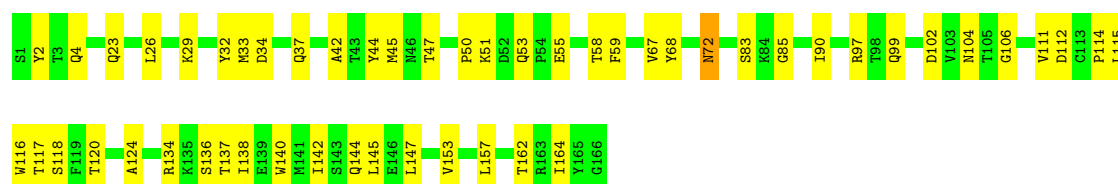
- Molecule 1: coat protein

Chain BA: 71% 28% .



- Molecule 1: coat protein

Chain BB: 69% 31% .



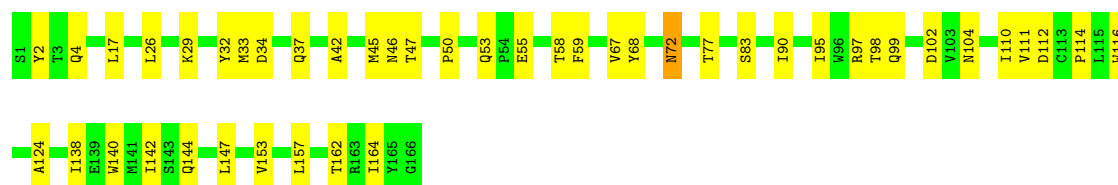
- Molecule 1: coat protein

Chain BC: 70% 28% .



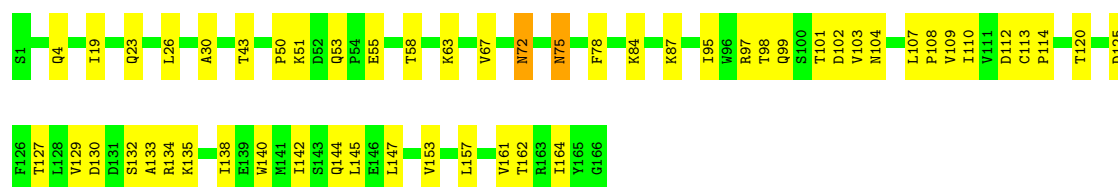
- Molecule 1: coat protein

Chain BD: 73% 27% .



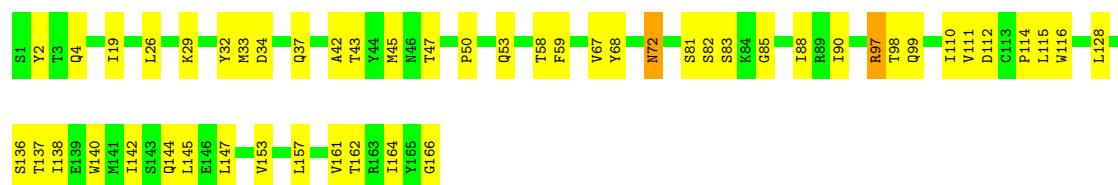
- Molecule 1: coat protein

Chain BE: 68% 31% .



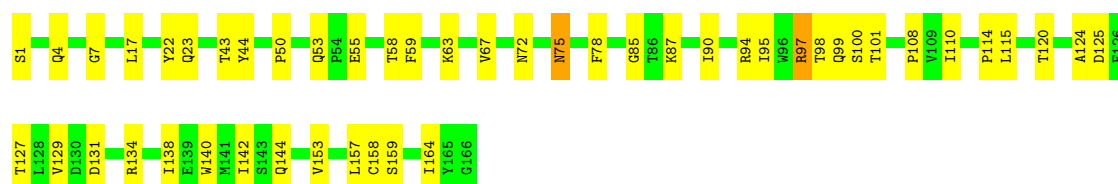
- Molecule 1: coat protein

Chain BF: 70% 29% .

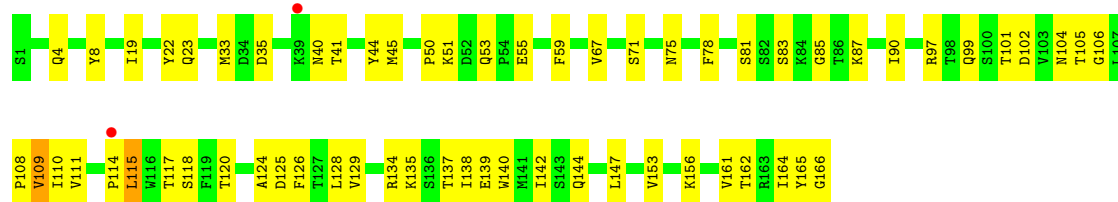


- Molecule 1: coat protein

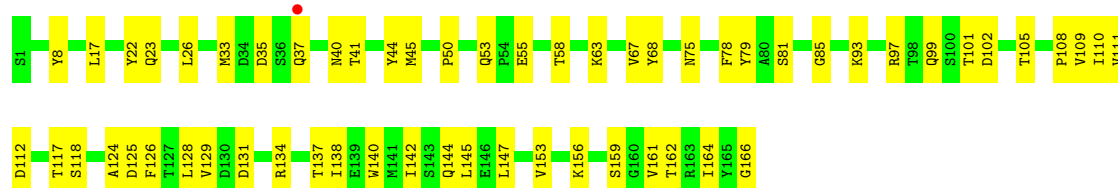
Chain BG: 71% 28% .



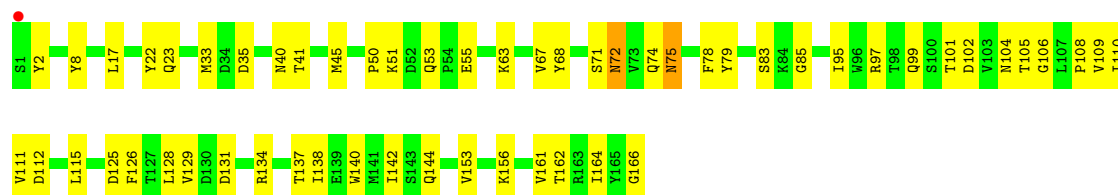
- Molecule 1: coat protein



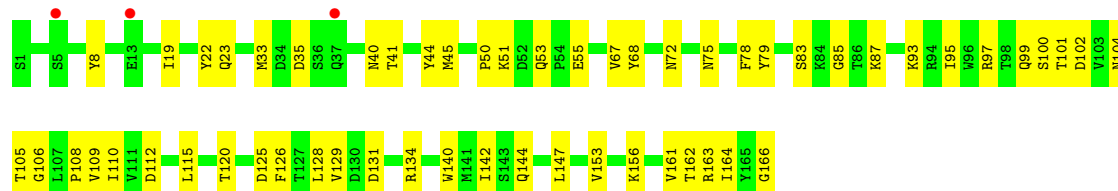
- Molecule 1: coat protein



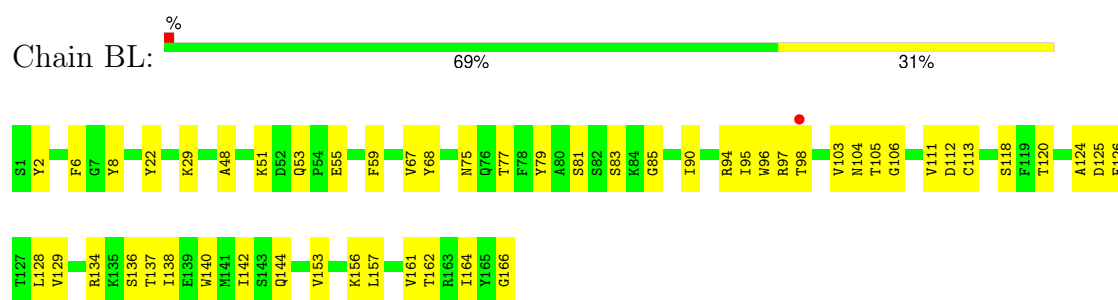
- Molecule 1: coat protein



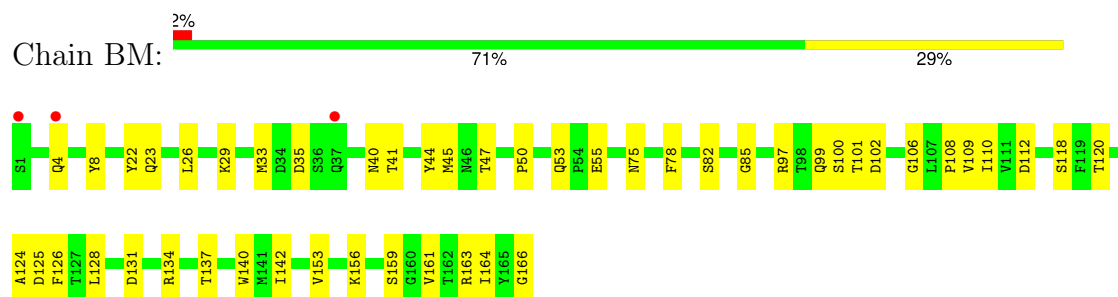
- Molecule 1: coat protein



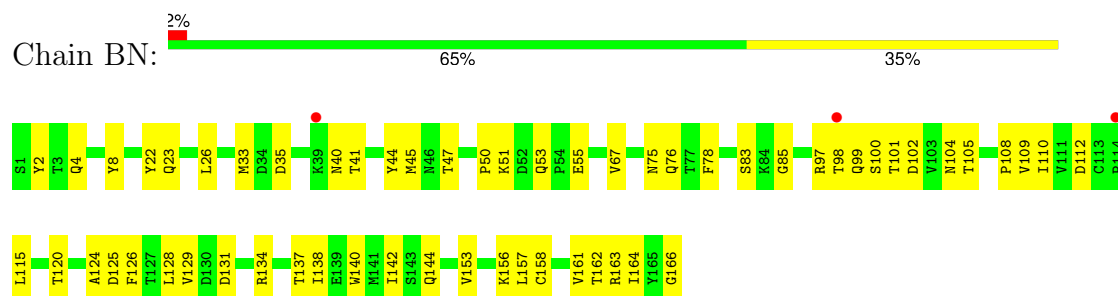
- Molecule 1: coat protein



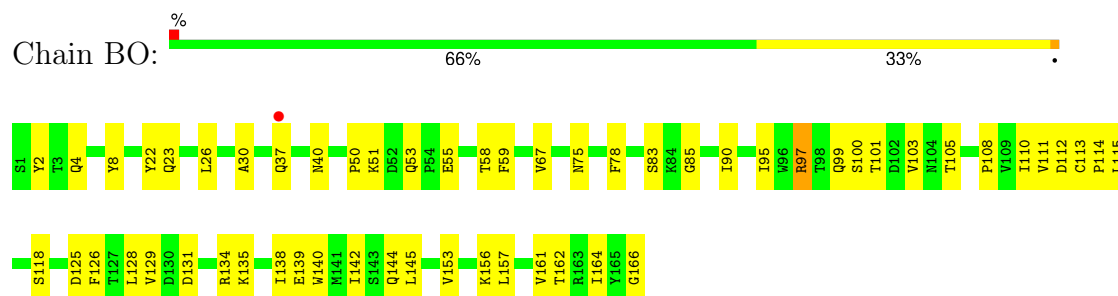
- Molecule 1: coat protein



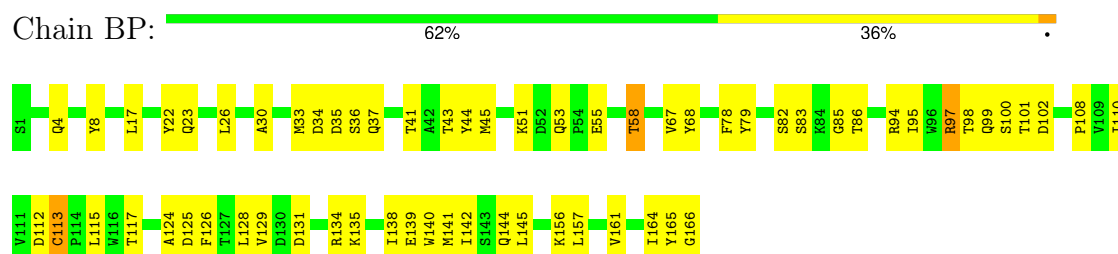
- Molecule 1: coat protein



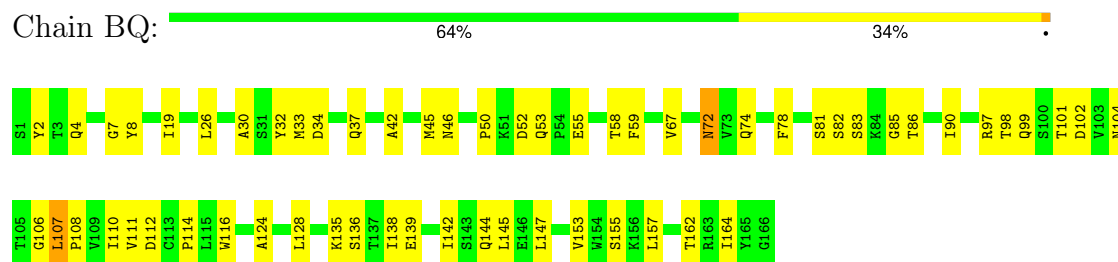
- Molecule 1: coat protein



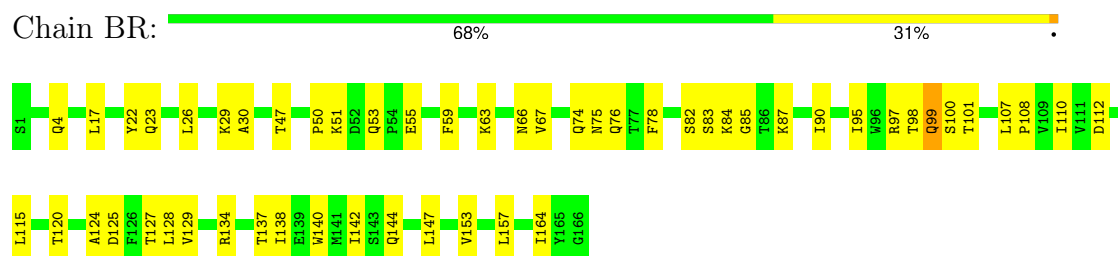
- Molecule 1: coat protein



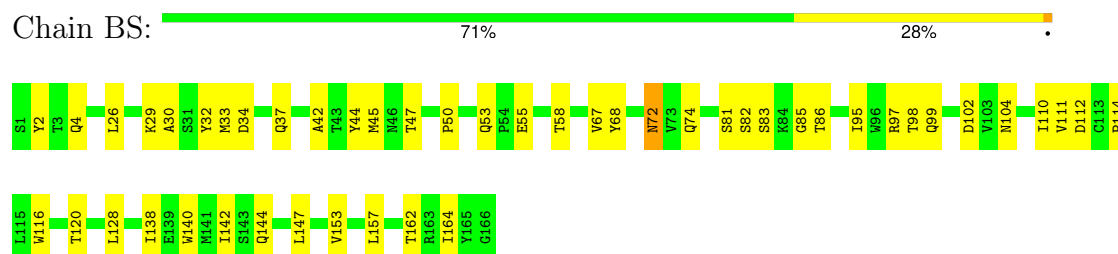
- Molecule 1: coat protein



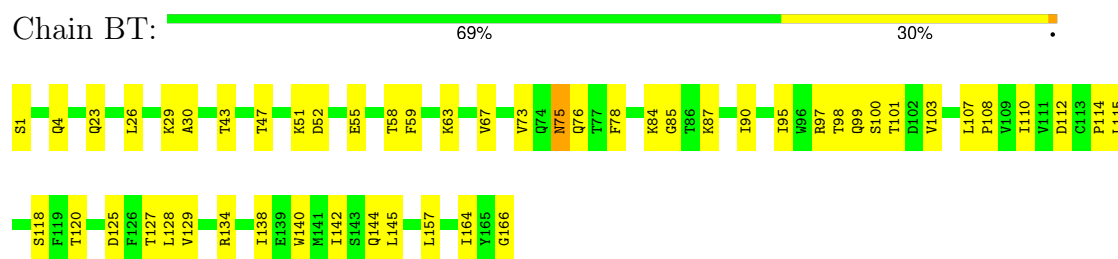
- Molecule 1: coat protein



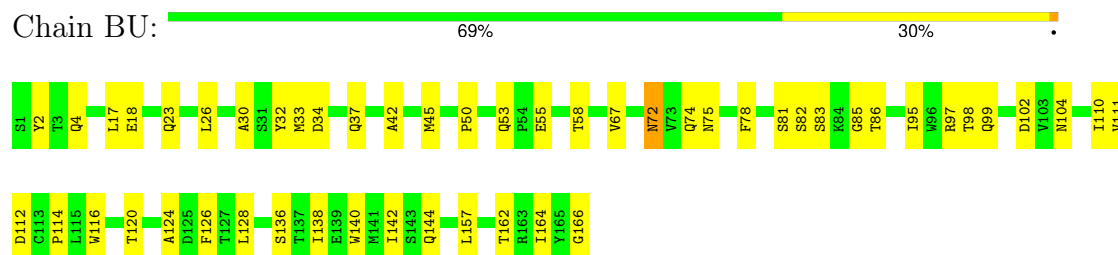
- Molecule 1: coat protein



- Molecule 1: coat protein

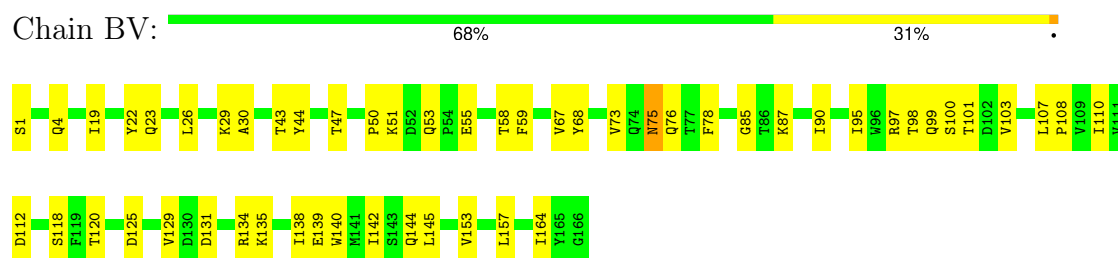


- Molecule 1: coat protein

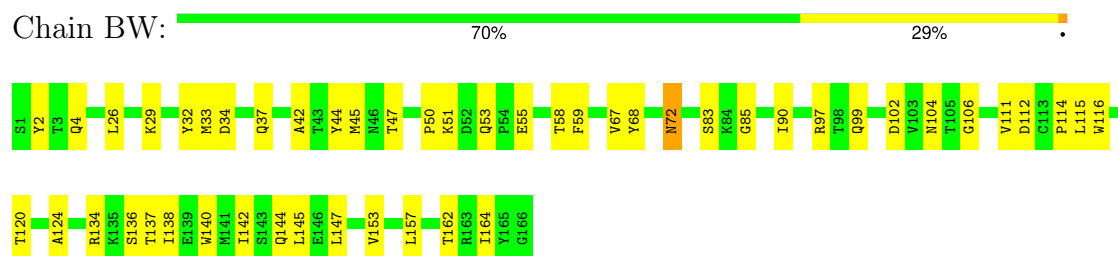




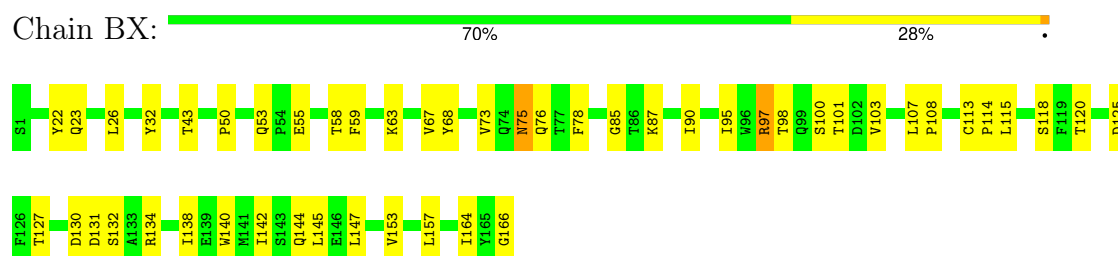
- Molecule 1: coat protein



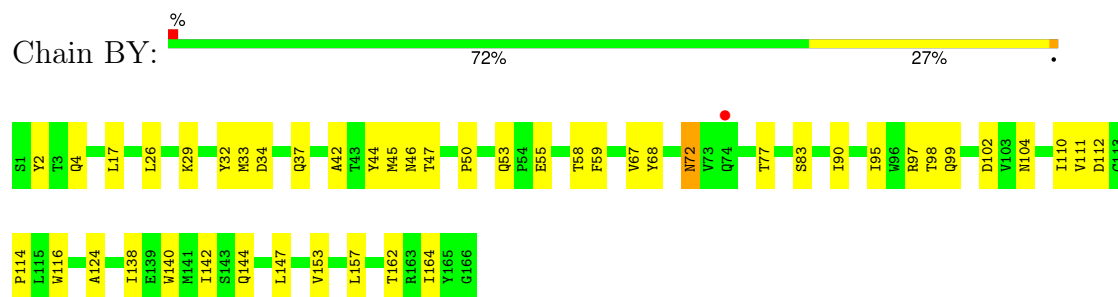
- Molecule 1: coat protein



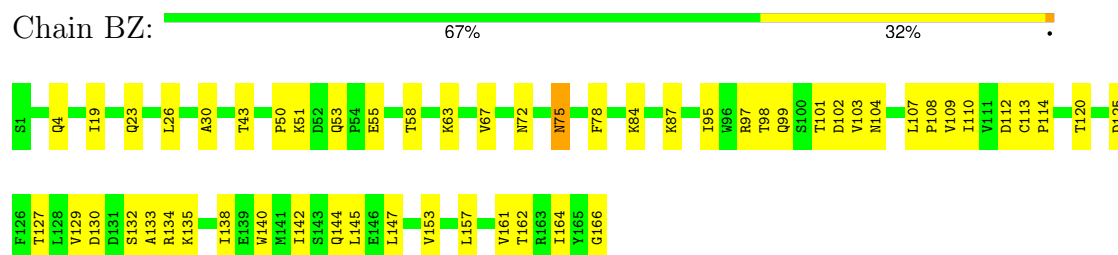
- Molecule 1: coat protein



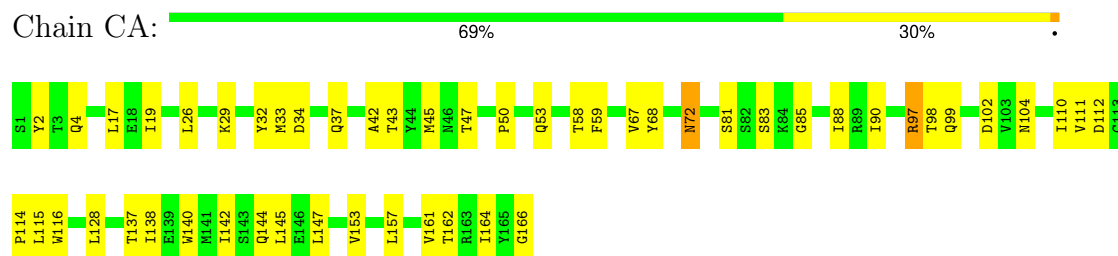
- Molecule 1: coat protein



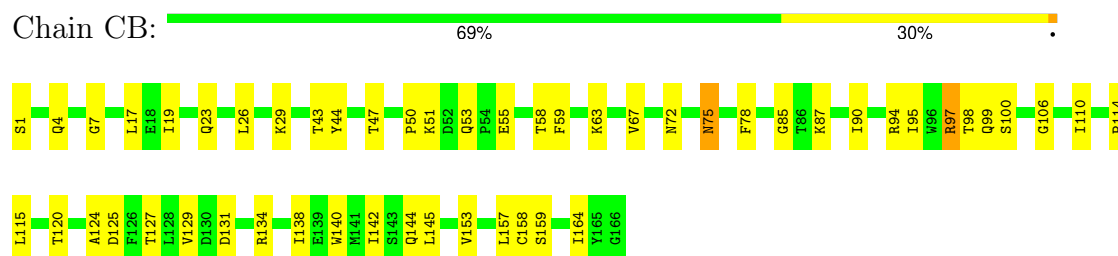
- Molecule 1: coat protein



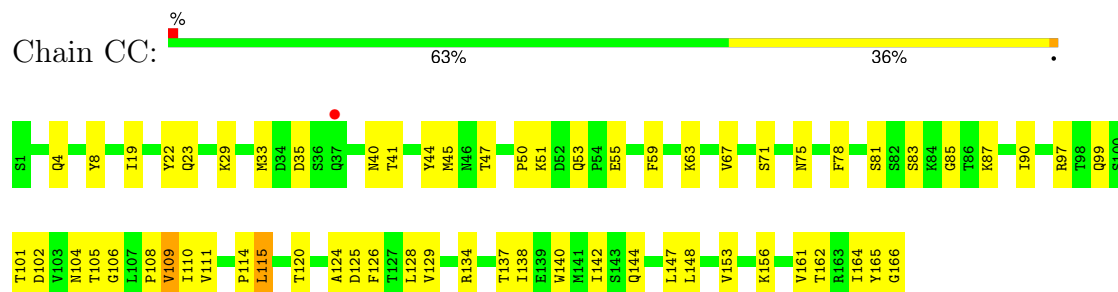
- Molecule 1: coat protein



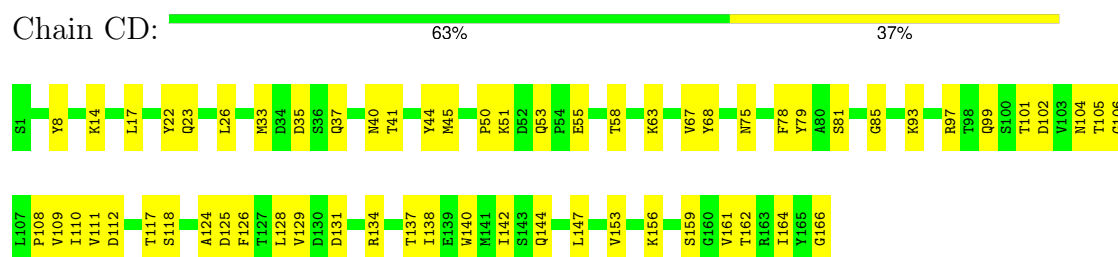
- Molecule 1: coat protein



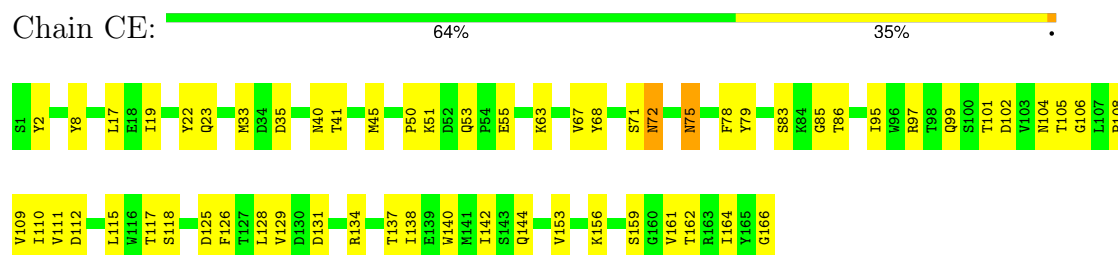
- Molecule 1: coat protein



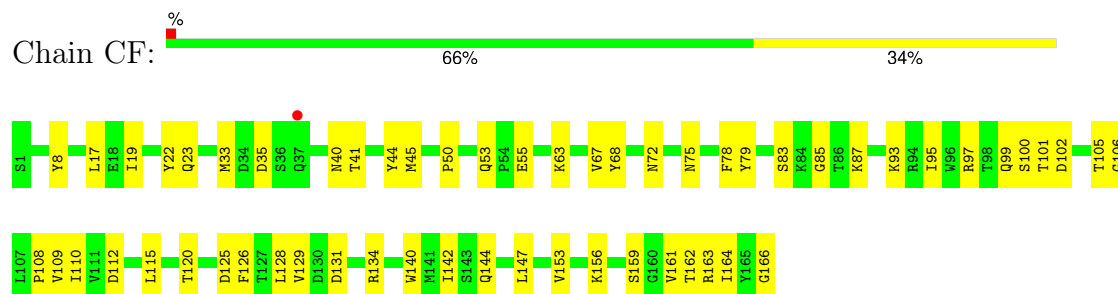
- Molecule 1: coat protein



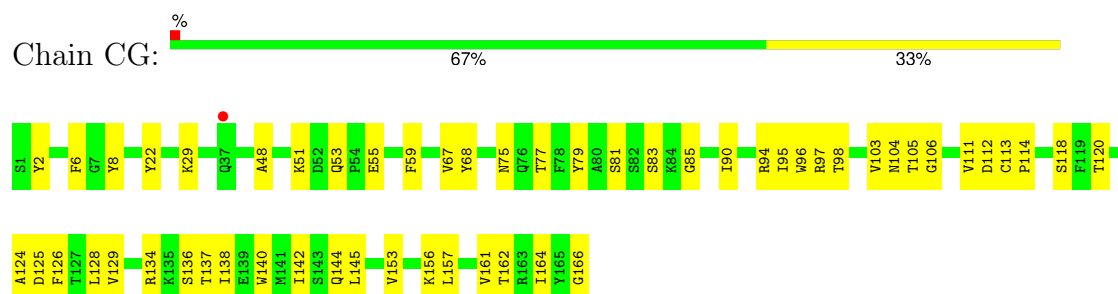
- Molecule 1: coat protein



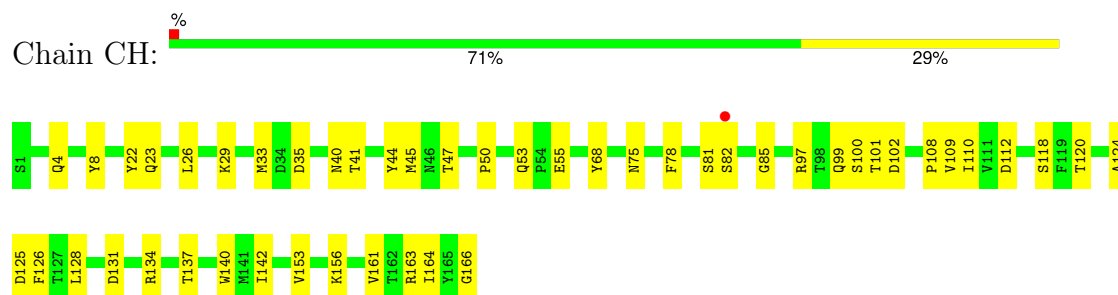
- Molecule 1: coat protein



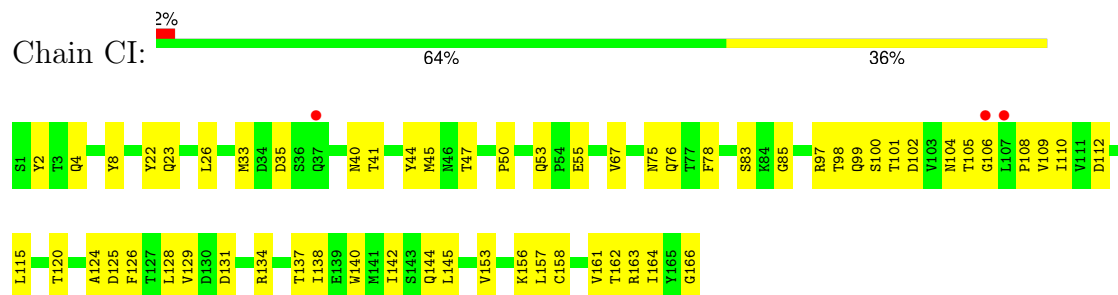
- Molecule 1: coat protein



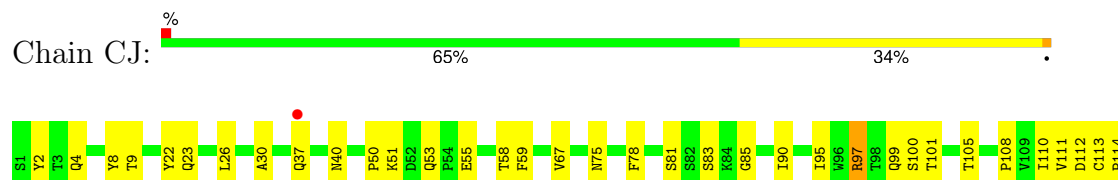
- Molecule 1: coat protein

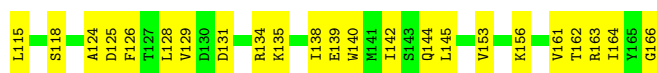


- Molecule 1: coat protein



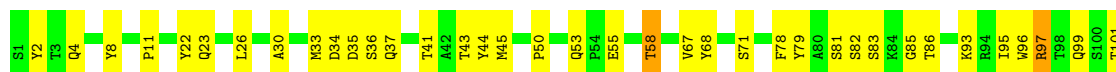
- Molecule 1: coat protein





- Molecule 1: coat protein

Chain CK: 61% 38%



- Molecule 1: coat protein

Chain CL: 2% 63% 36%



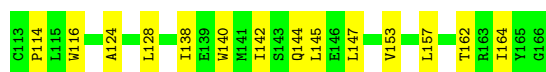
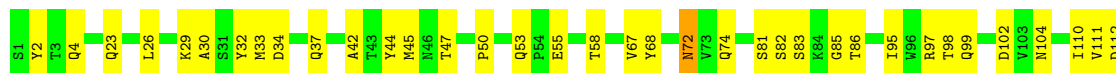
- Molecule 1: coat protein

Chain CM: 67% 33%



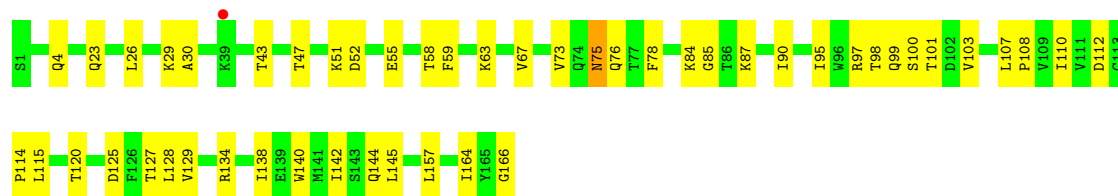
- Molecule 1: coat protein

Chain CN: 70% 30%



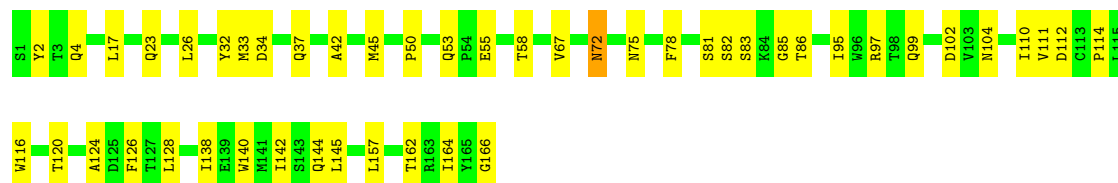
- Molecule 1: coat protein

Chain CO: 70% 29%



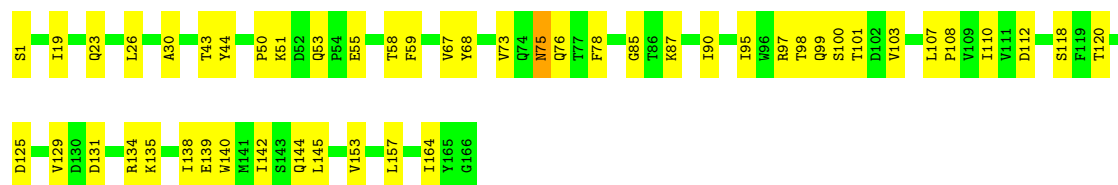
- Molecule 1: coat protein

Chain CP: 72% 28%



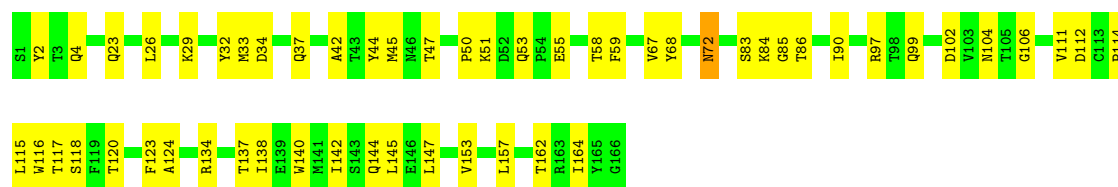
- Molecule 1: coat protein

Chain CQ: 70% 29%



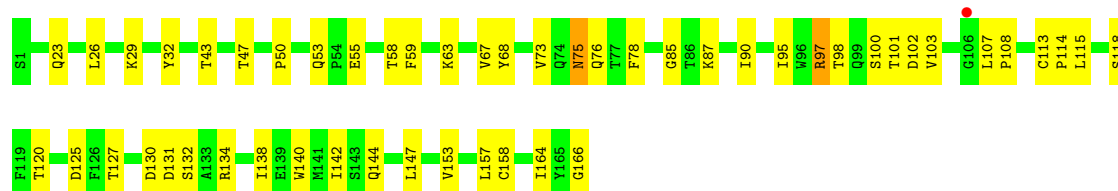
- Molecule 1: coat protein

Chain CR: 67% 32%

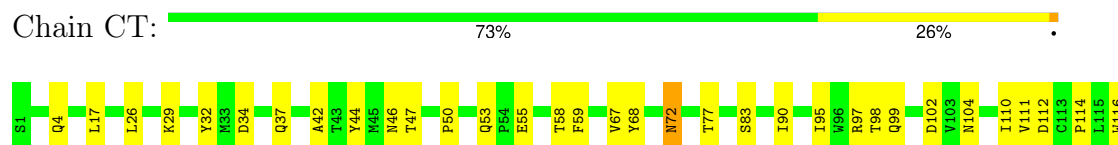


- Molecule 1: coat protein

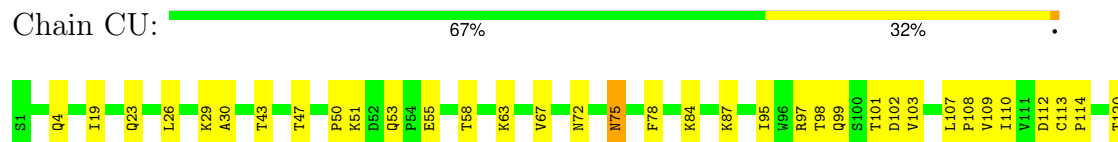
Chain CS: 69% 30%



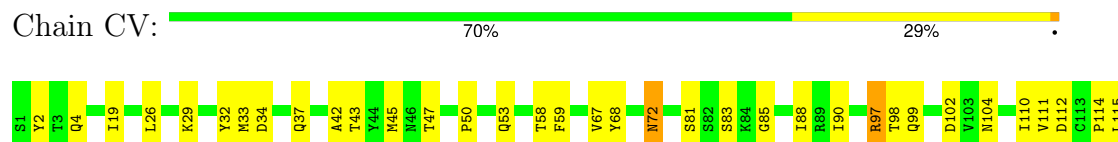
- Molecule 1: coat protein



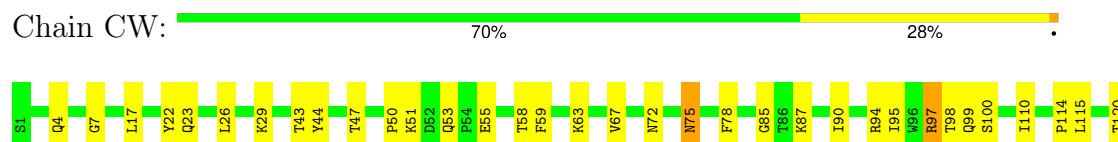
- Molecule 1: coat protein



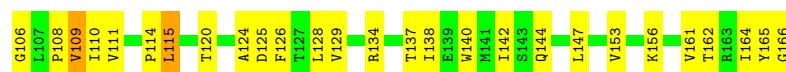
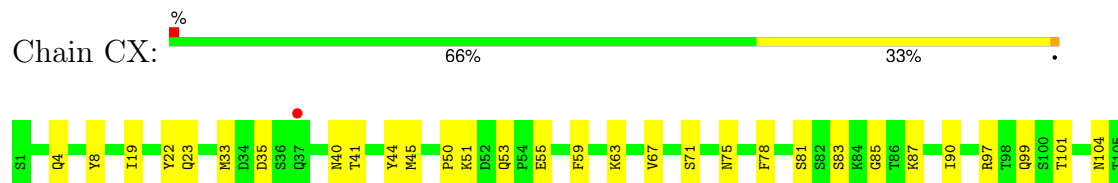
- Molecule 1: coat protein



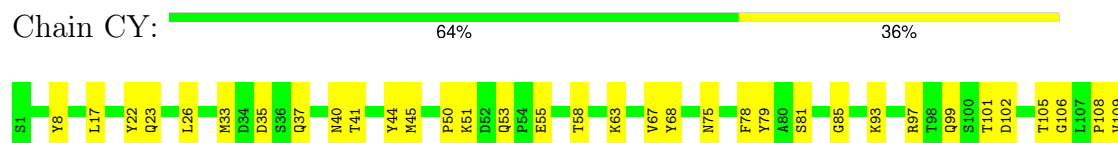
- Molecule 1: coat protein



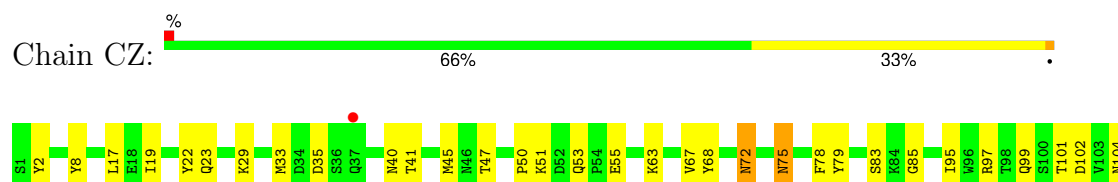
- Molecule 1: coat protein



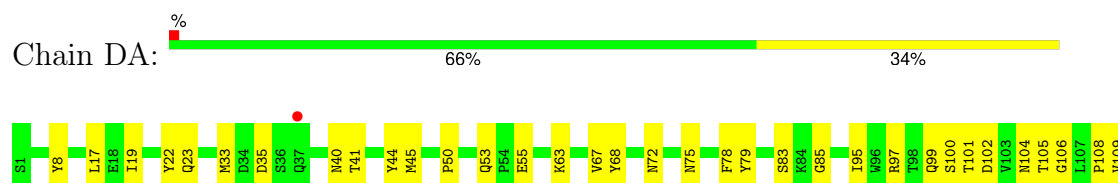
- Molecule 1: coat protein



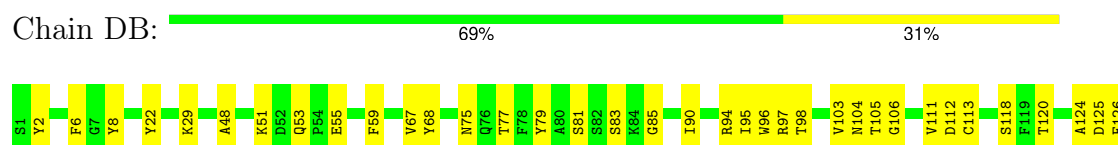
- Molecule 1: coat protein



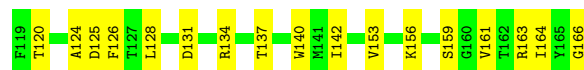
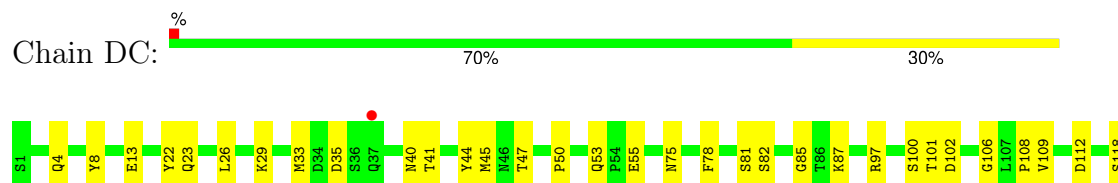
- Molecule 1: coat protein



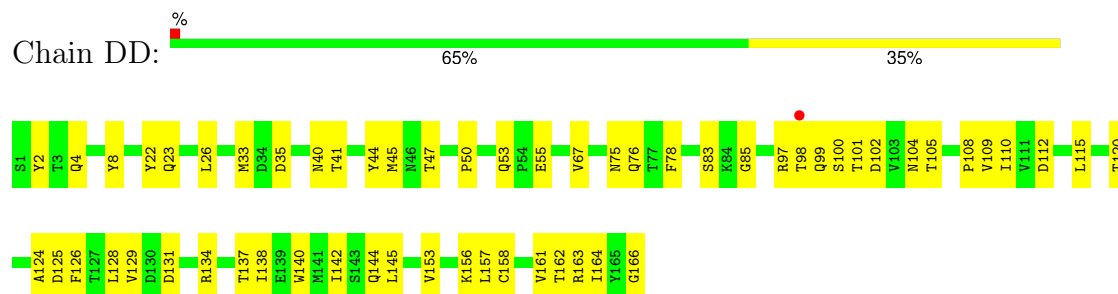
- Molecule 1: coat protein



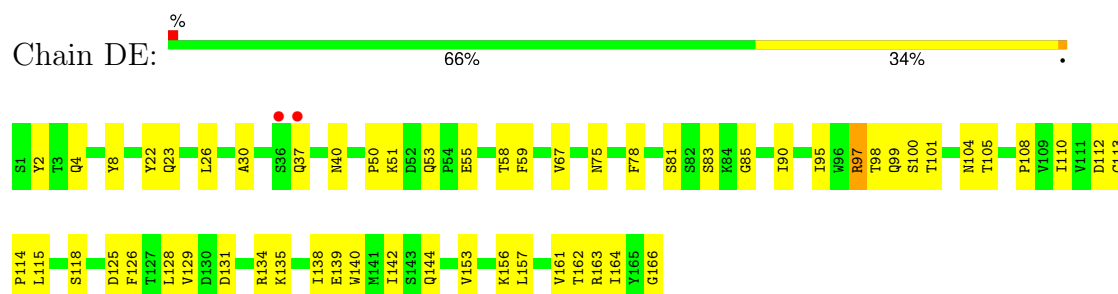
- Molecule 1: coat protein



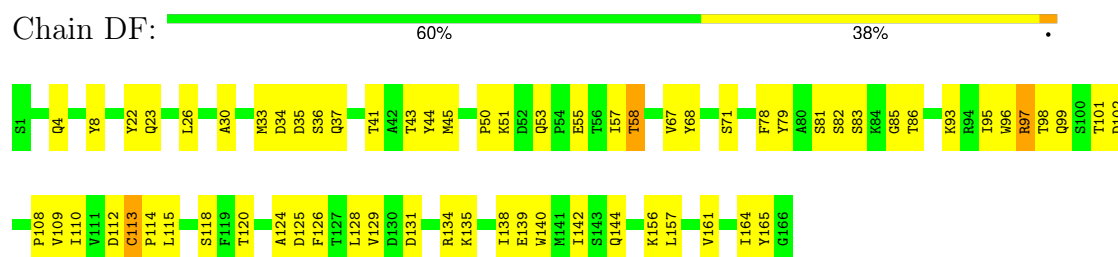
- Molecule 1: coat protein



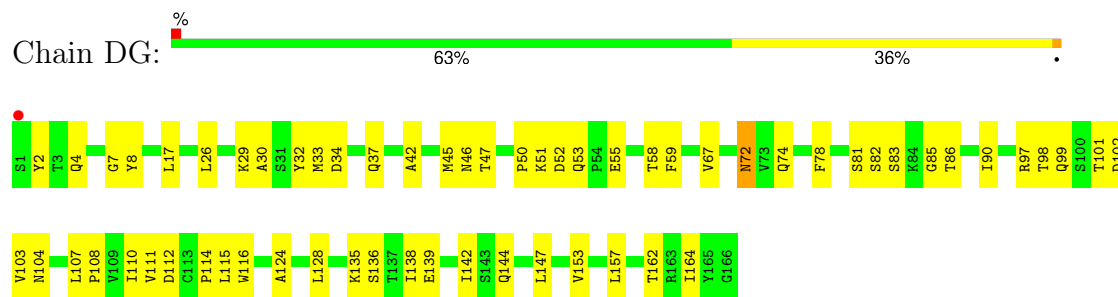
- Molecule 1: coat protein



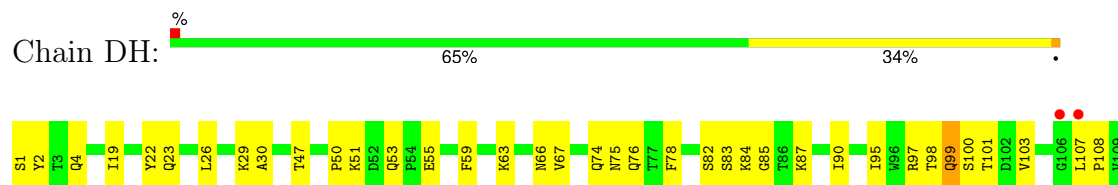
- Molecule 1: coat protein



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- Molecule 1: coat protein







- Molecule 1: coat protein



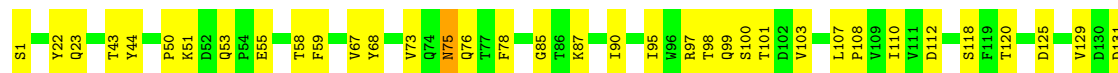
- Molecule 1: coat protein



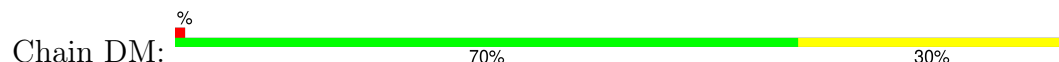
- Molecule 1: coat protein



- Molecule 1: coat protein

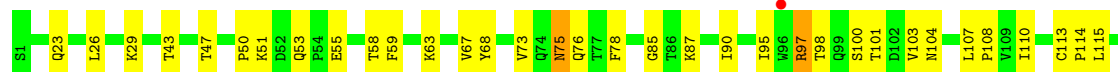


- Molecule 1: coat protein

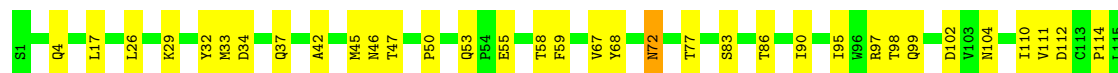




• Molecule 1: coat protein



• Molecule 1: coat protein



• Molecule 1: coat protein

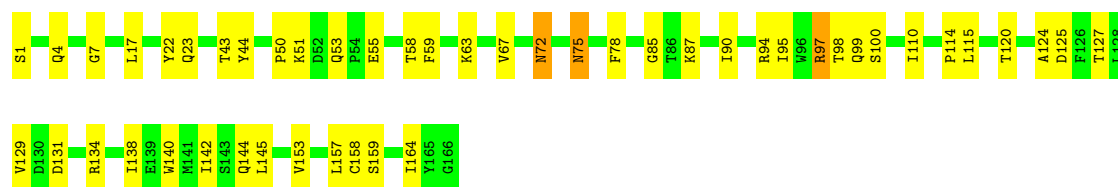


• Molecule 1: coat protein



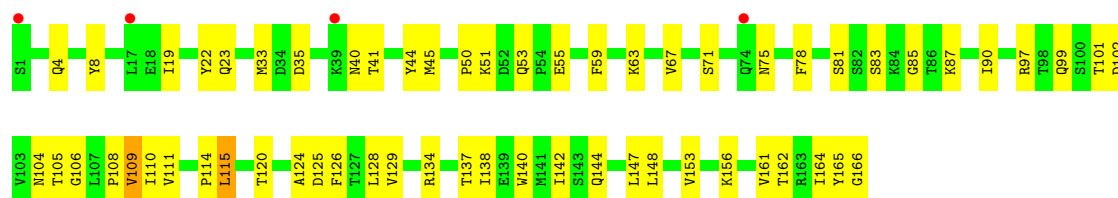
• Molecule 1: coat protein

Chain DR:  71% 27% .



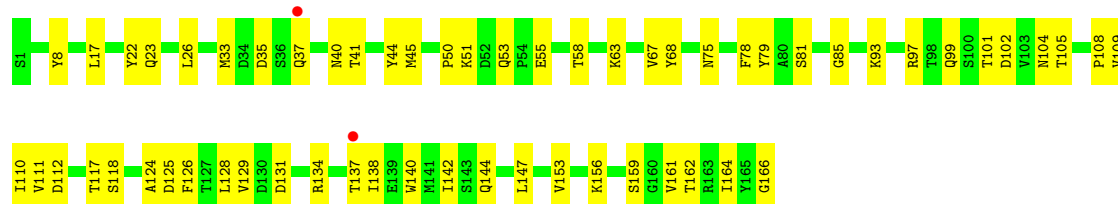
• Molecule 1: coat protein

Chain DS:  64% 35% .



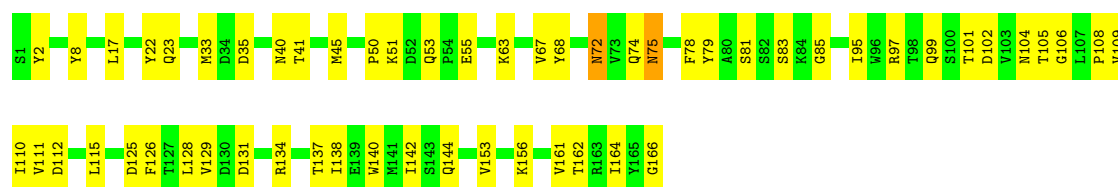
• Molecule 1: coat protein

Chain DT:  64% 36% .



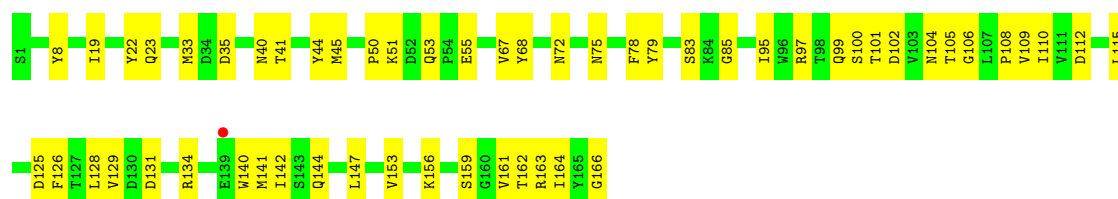
• Molecule 1: coat protein

Chain DU:  66% 33% .

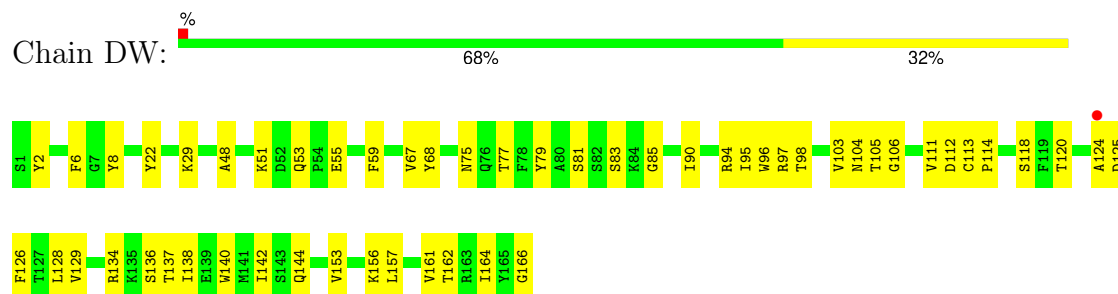


• Molecule 1: coat protein

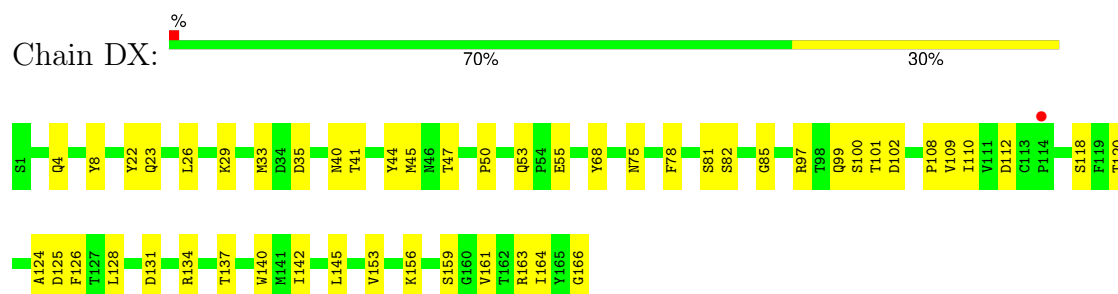
Chain DV:  67% 33% .



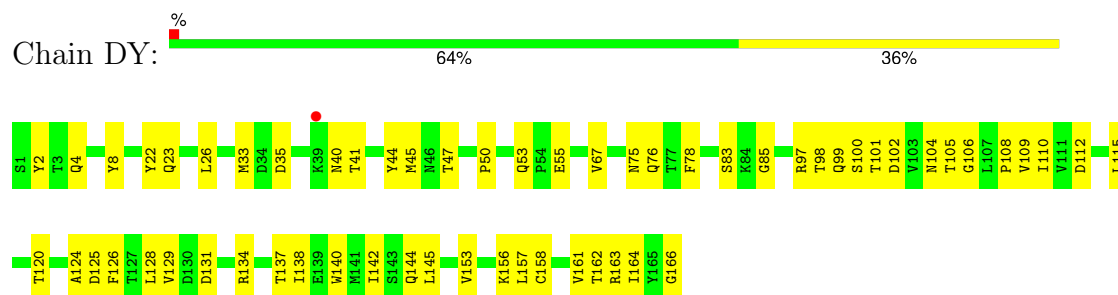
- Molecule 1: coat protein



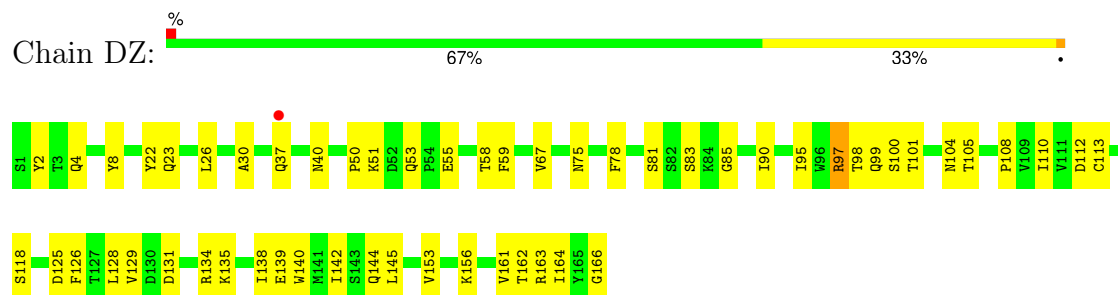
- Molecule 1: coat protein



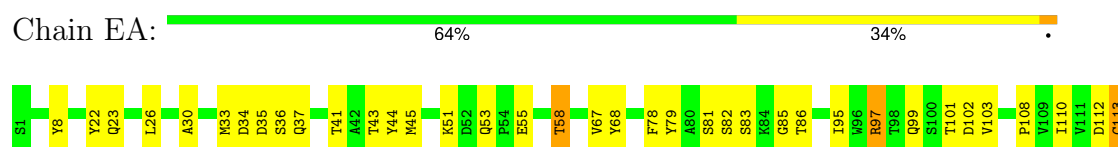
- Molecule 1: coat protein

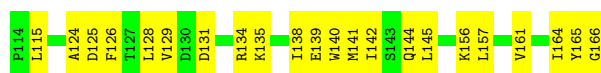


- Molecule 1: coat protein



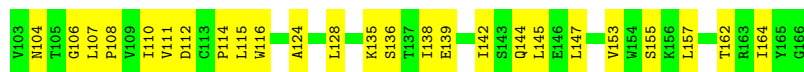
- Molecule 1: coat protein





- Molecule 1: coat protein

Chain EB: 62% 37% .



- Molecule 1: coat protein

Chain EC: 68% 31% .



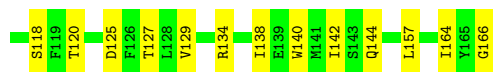
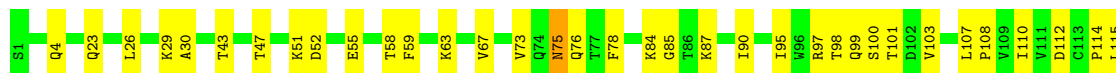
- Molecule 1: coat protein

Chain ED: 70% 30% .



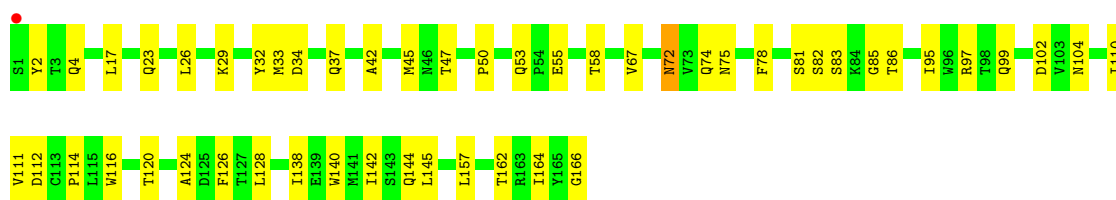
- Molecule 1: coat protein

Chain EE: 71% 28% .



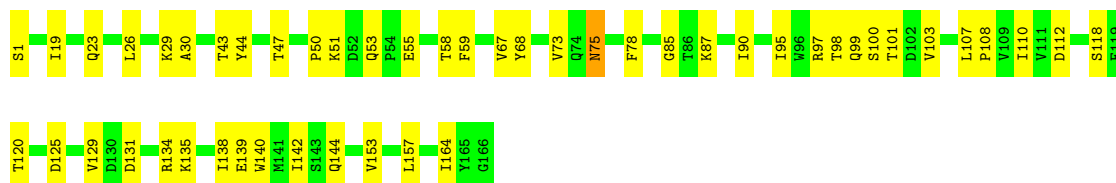
- Molecule 1: coat protein

Chain EF: 70% 30% .



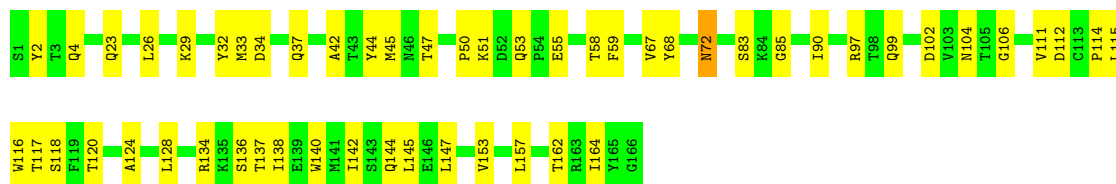
- Molecule 1: coat protein

Chain EG: 70% 29%



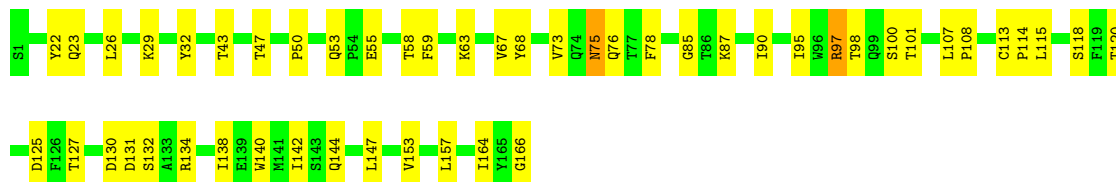
- Molecule 1: coat protein

Chain EH: 68% 31%



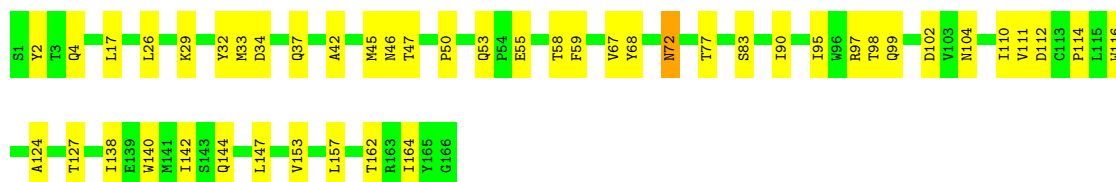
- Molecule 1: coat protein

Chain EI: 70% 28%

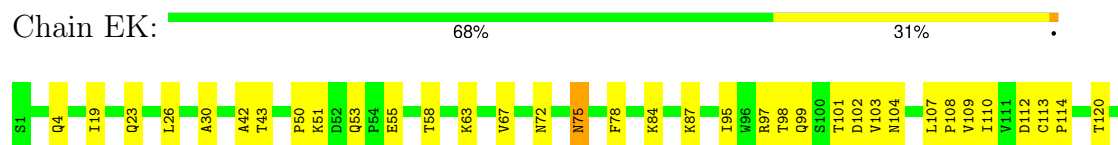


- Molecule 1: coat protein

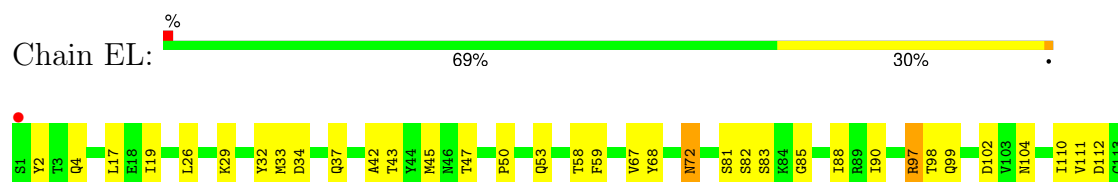
Chain EJ: 72% 27%



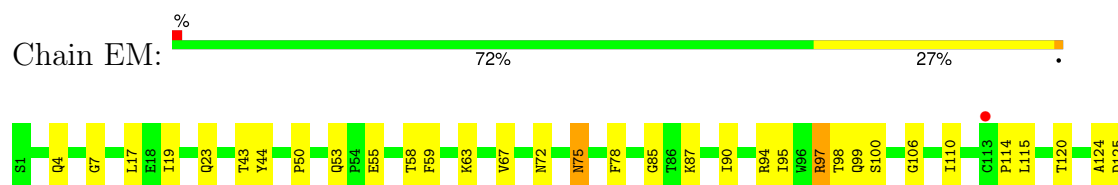
- Molecule 1: coat protein



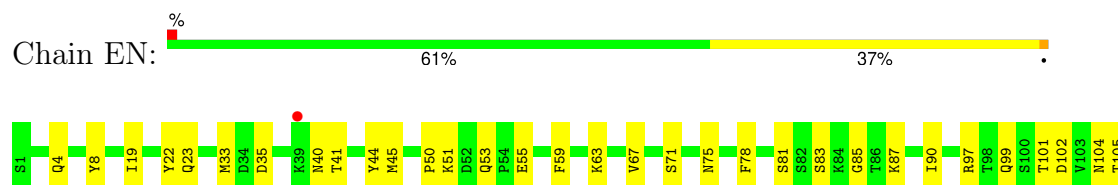
- Molecule 1: coat protein



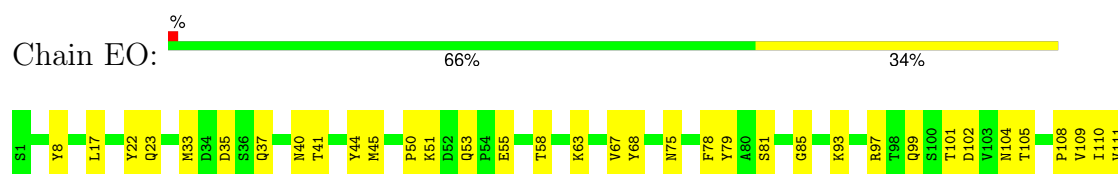
- Molecule 1: coat protein



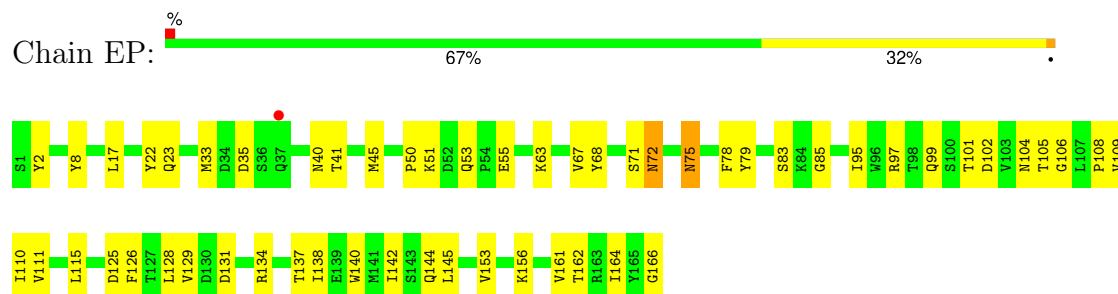
- Molecule 1: coat protein



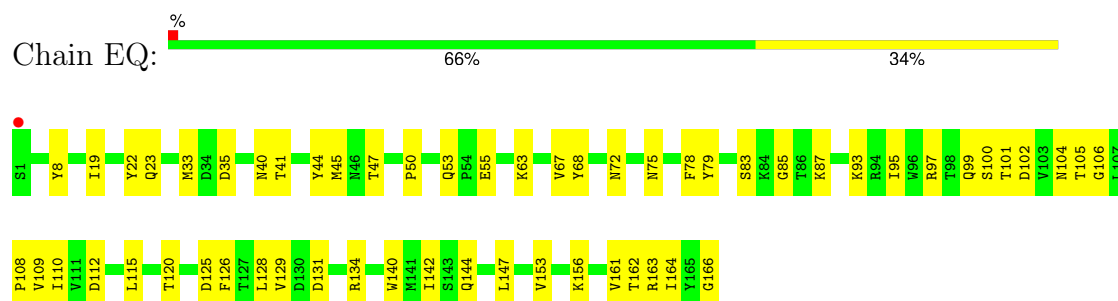
- Molecule 1: coat protein



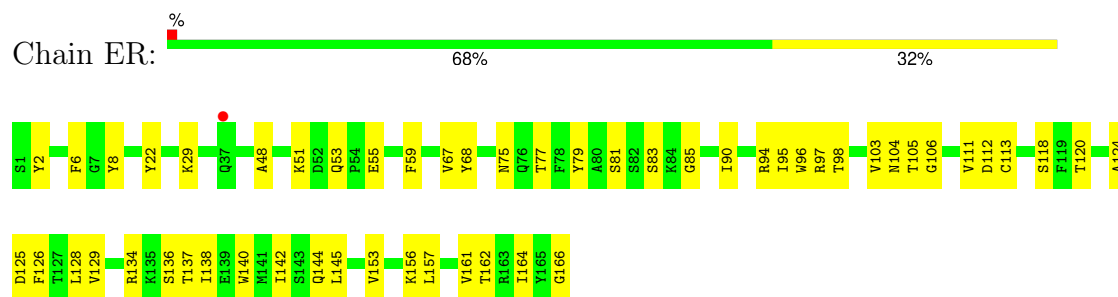
- Molecule 1: coat protein



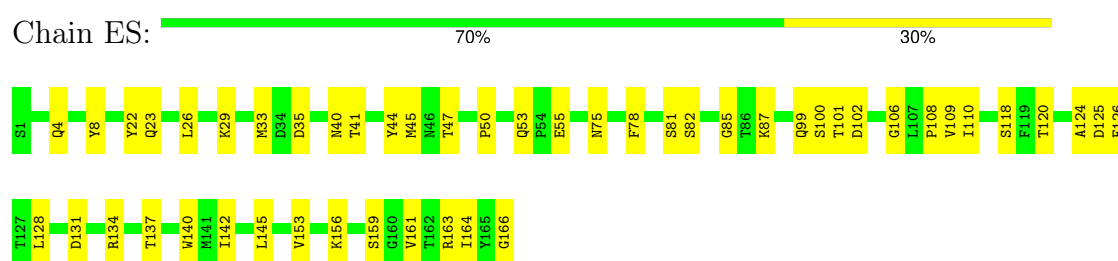
- Molecule 1: coat protein



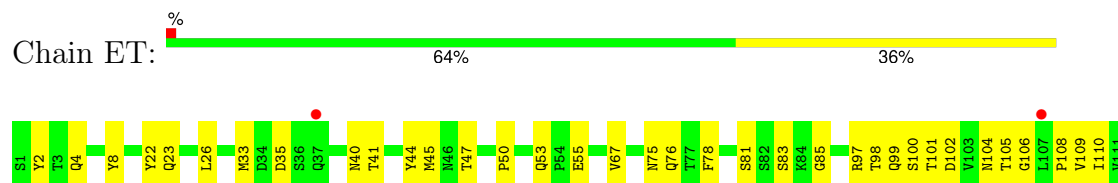
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein



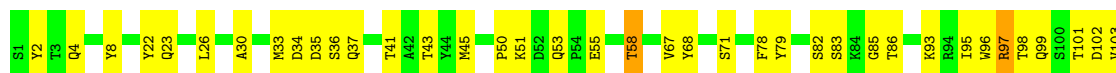




- Molecule 1: coat protein



- Molecule 1: coat protein



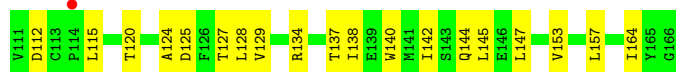
- Molecule 1: coat protein

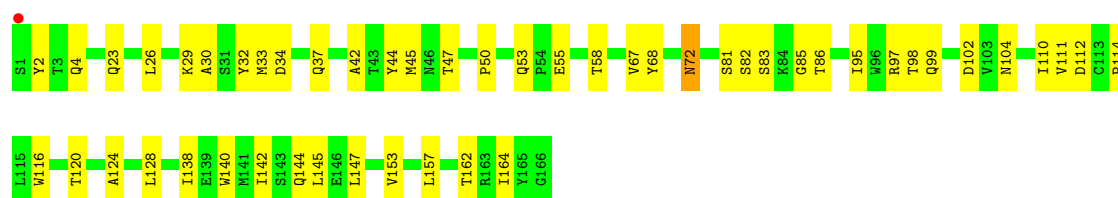


- Molecule 1: coat protein

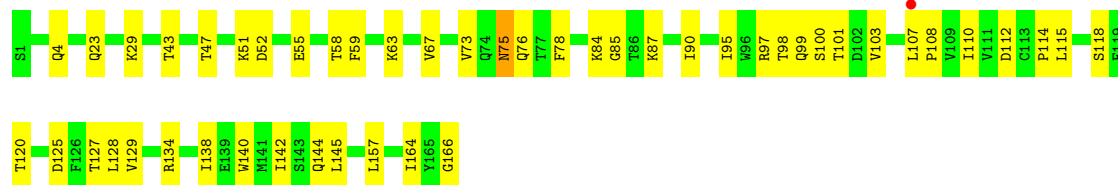


- Molecule 1: coat protein

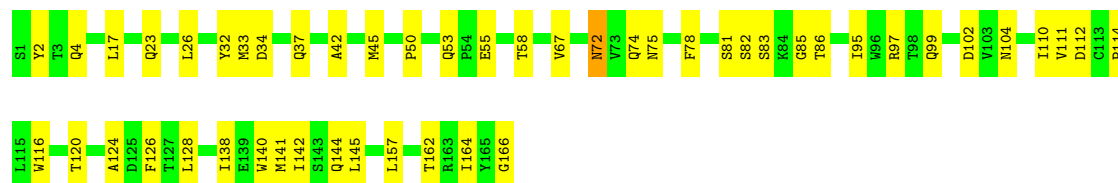




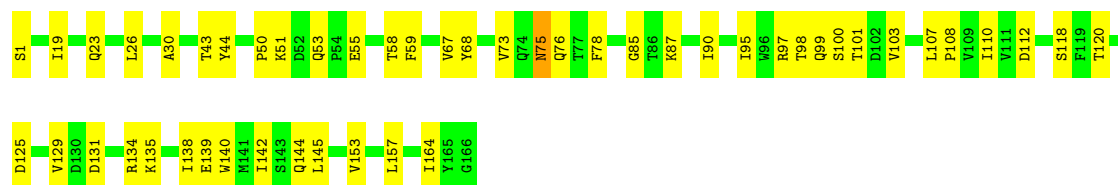
- Molecule 1: coat protein



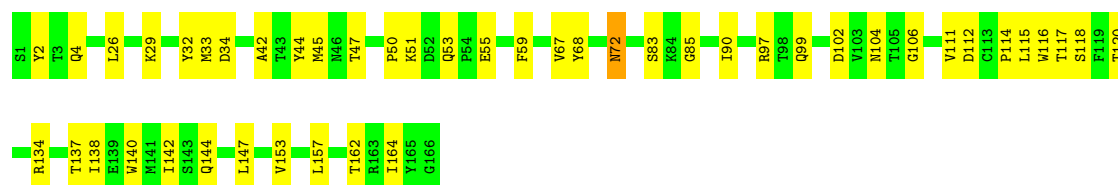
- Molecule 1: coat protein



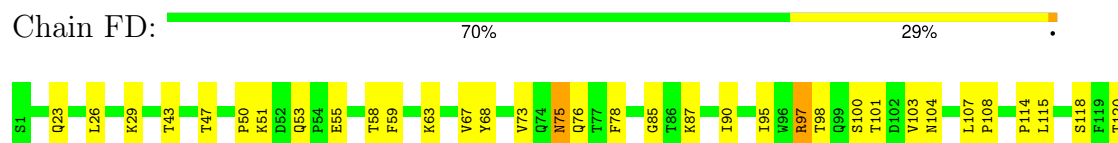
- Molecule 1: coat protein



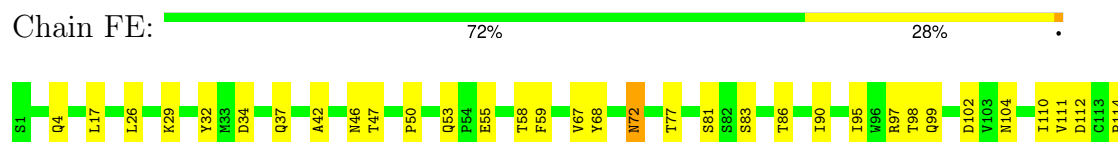
- Molecule 1: coat protein



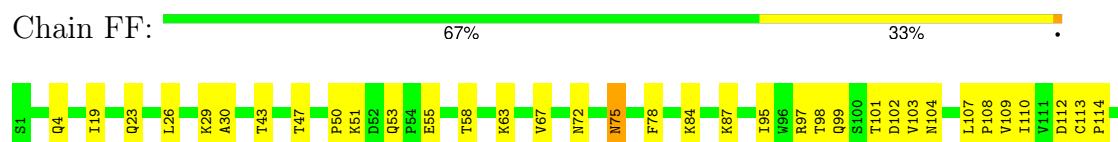
- Molecule 1: coat protein



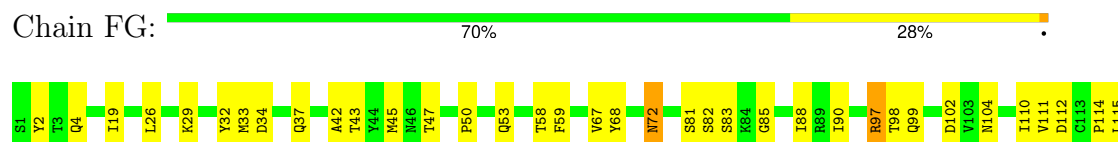
- Molecule 1: coat protein



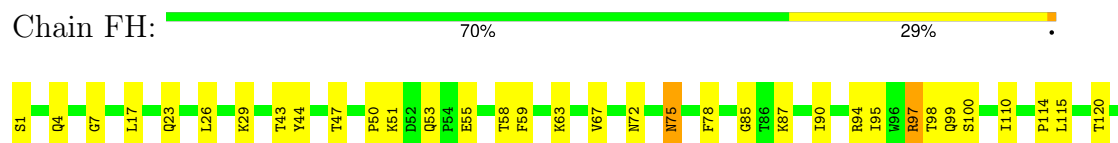
- Molecule 1: coat protein



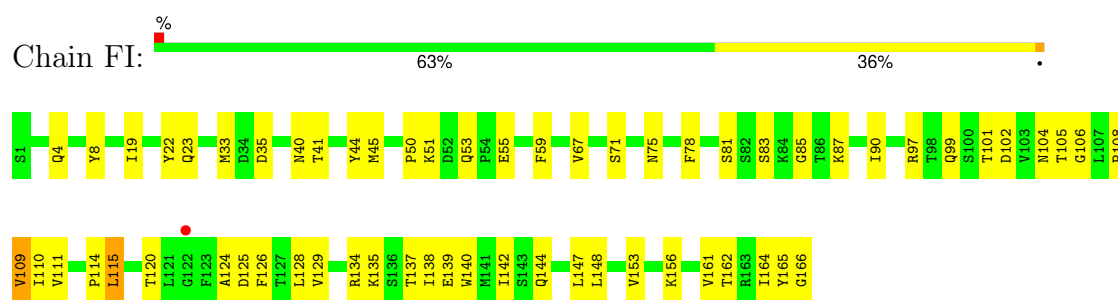
- Molecule 1: coat protein



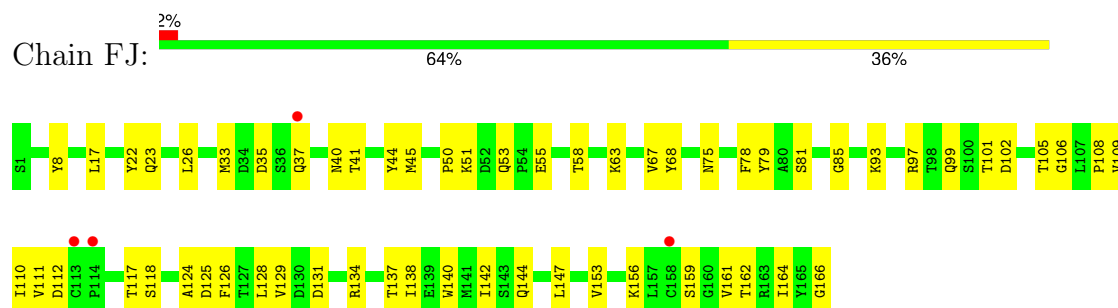
- Molecule 1: coat protein



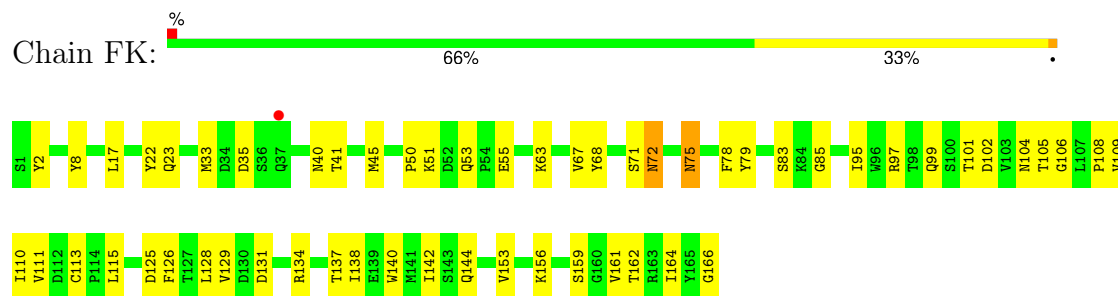
- Molecule 1: coat protein



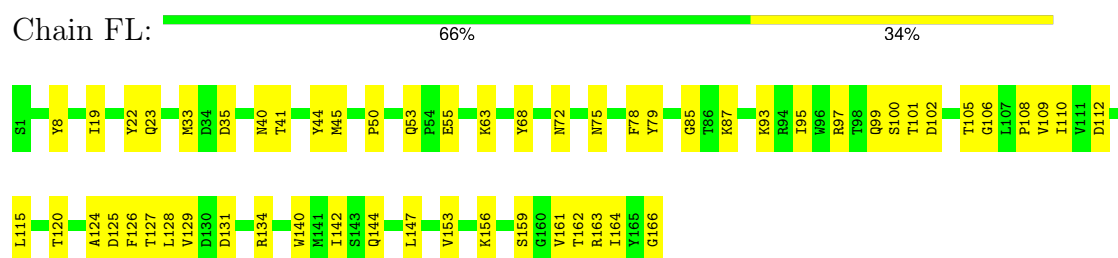
- Molecule 1: coat protein



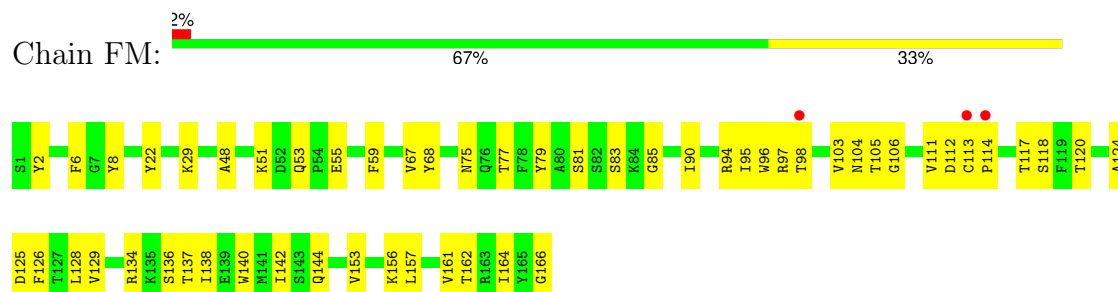
- Molecule 1: coat protein



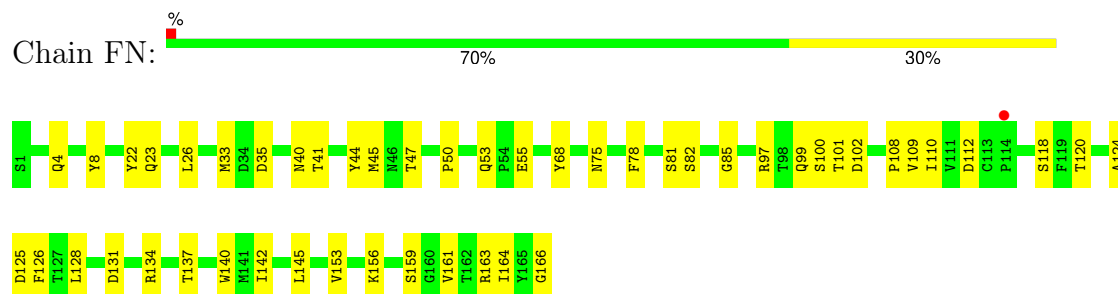
- Molecule 1: coat protein



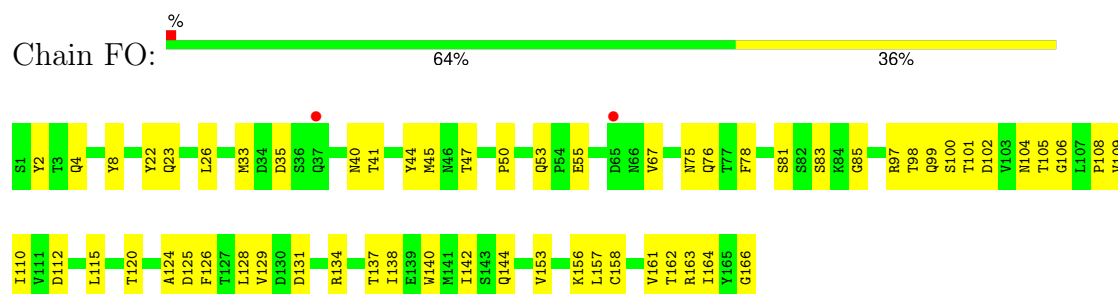
- Molecule 1: coat protein



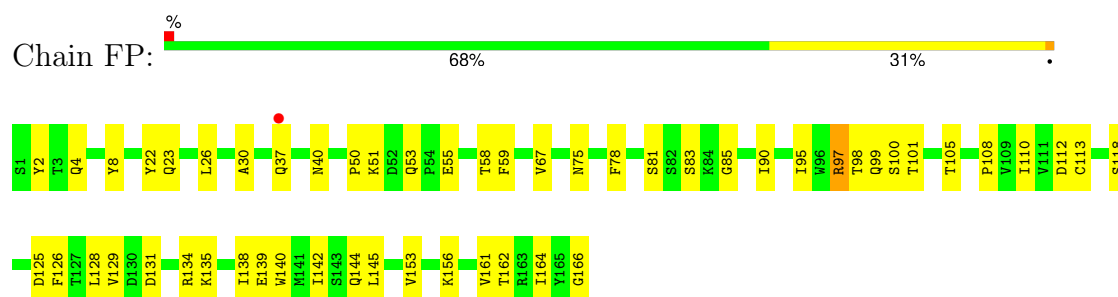
- Molecule 1: coat protein



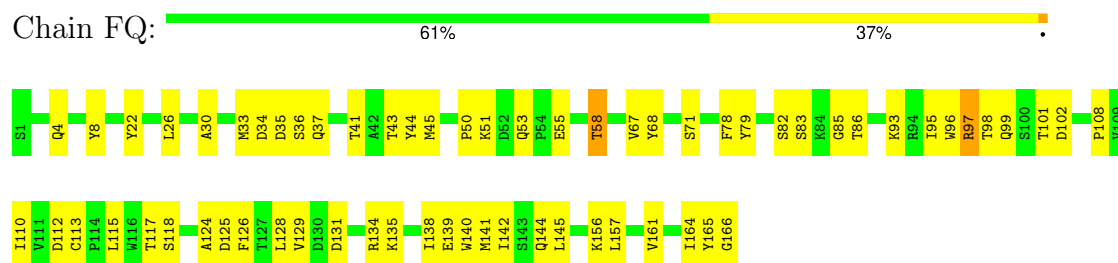
- Molecule 1: coat protein



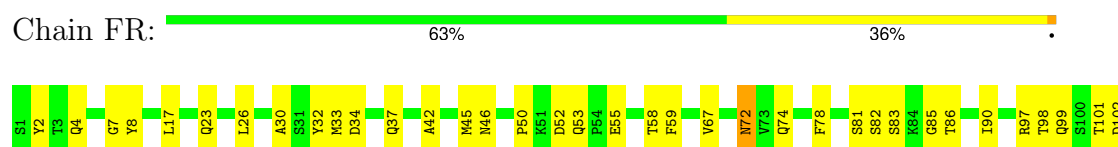
- Molecule 1: coat protein



- Molecule 1: coat protein

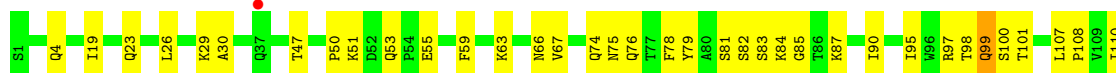


- Molecule 1: coat protein





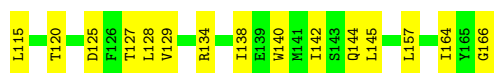
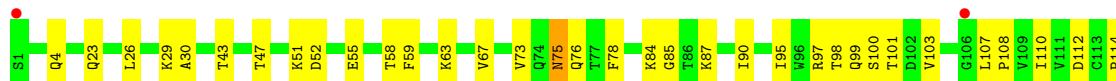
- Molecule 1: coat protein



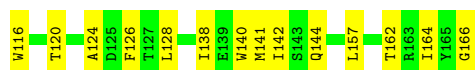
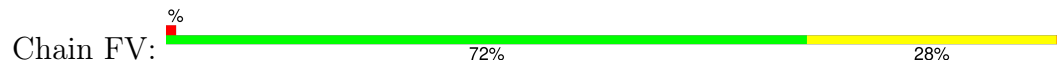
- Molecule 1: coat protein



- Molecule 1: coat protein

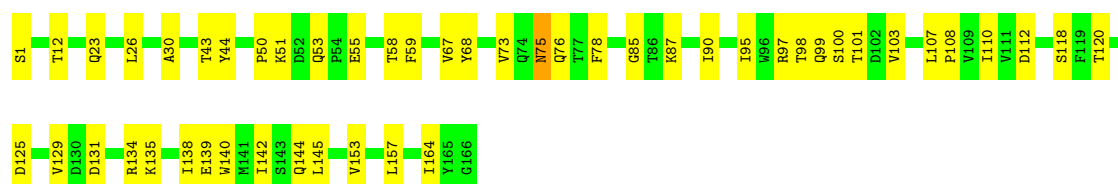


- Molecule 1: coat protein



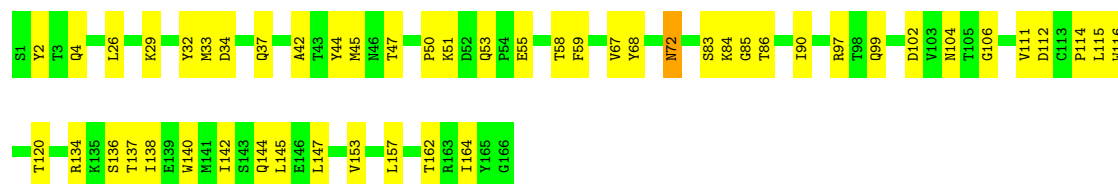
- Molecule 1: coat protein





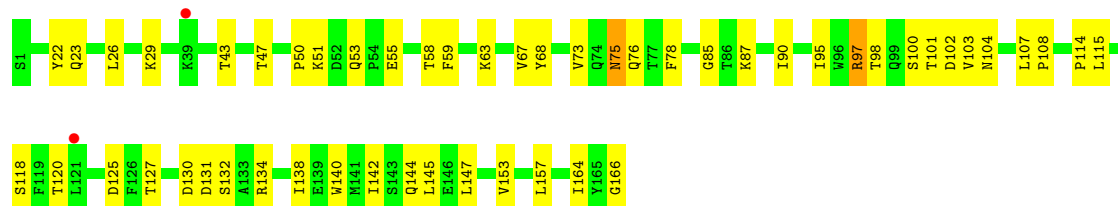
- Molecule 1: coat protein

Chain FX: 70% 30% .



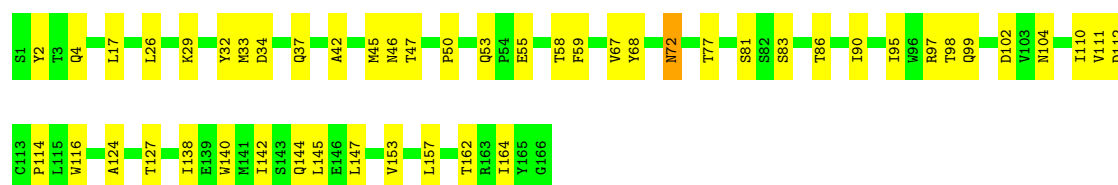
- Molecule 1: coat protein

Chain FY: 69% 30% .



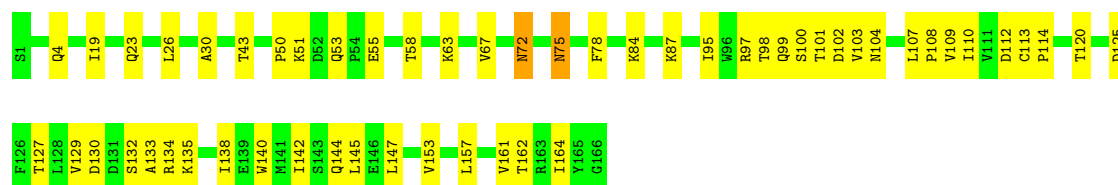
- Molecule 1: coat protein

Chain FZ: 70% 29% .

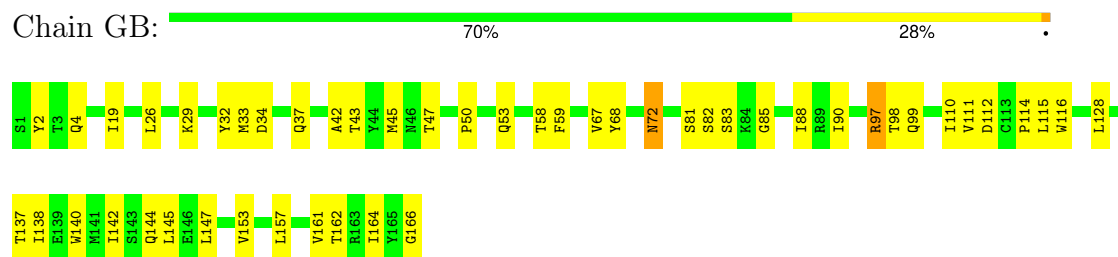


- Molecule 1: coat protein

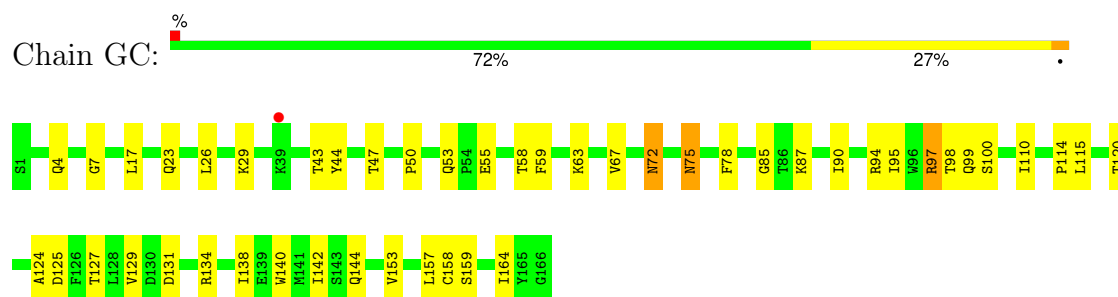
Chain GA: 67% 31% .



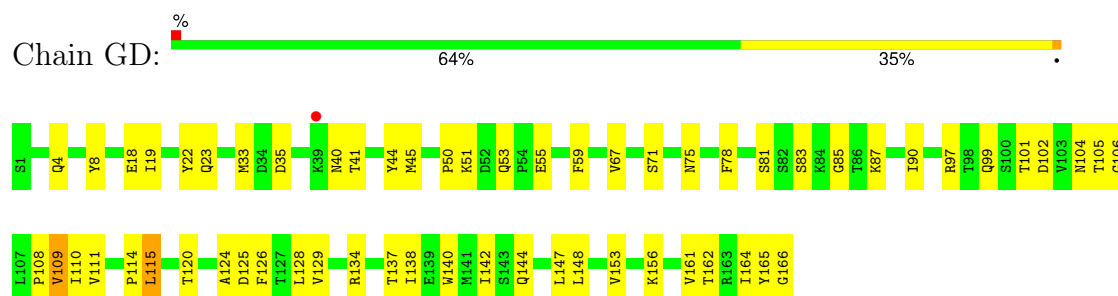
- Molecule 1: coat protein



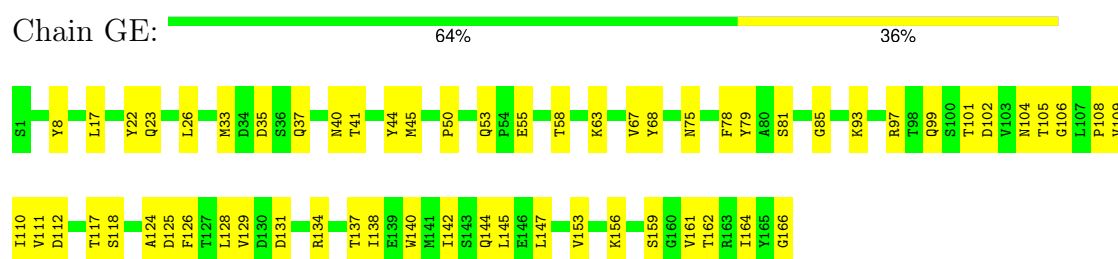
- Molecule 1: coat protein



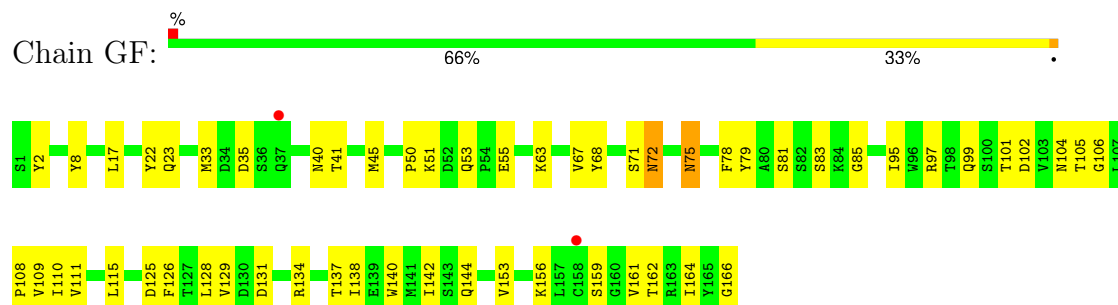
- Molecule 1: coat protein



- Molecule 1: coat protein

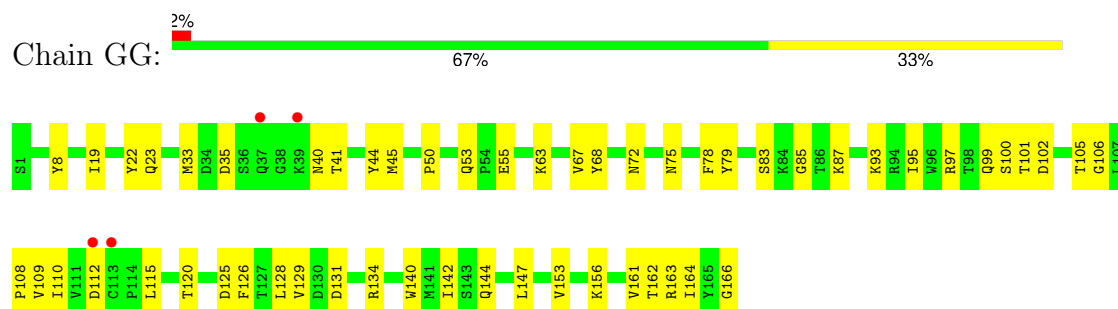


- Molecule 1: coat protein

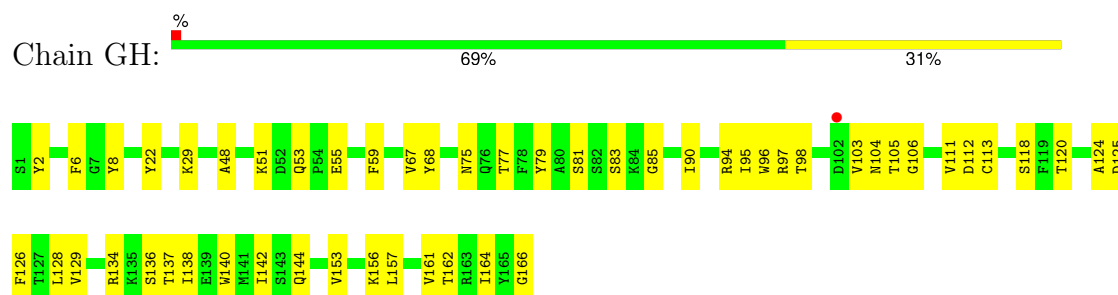




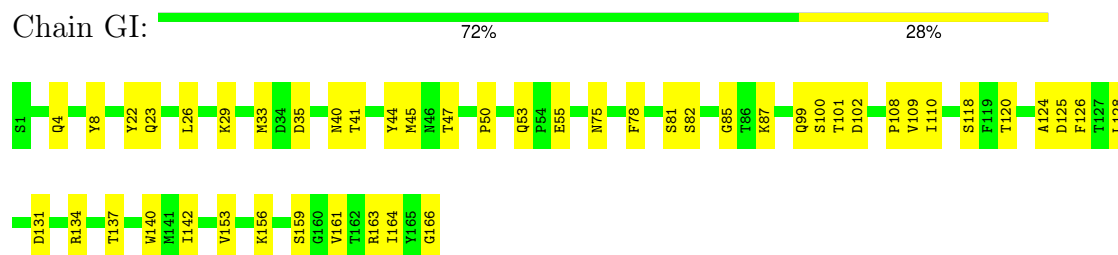
- Molecule 1: coat protein



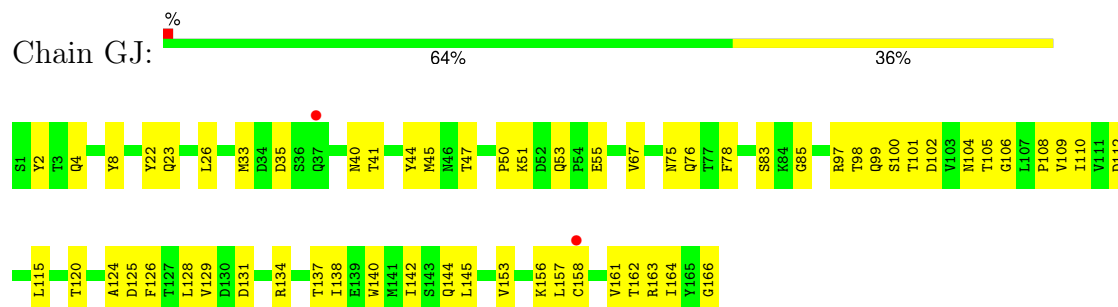
- Molecule 1: coat protein



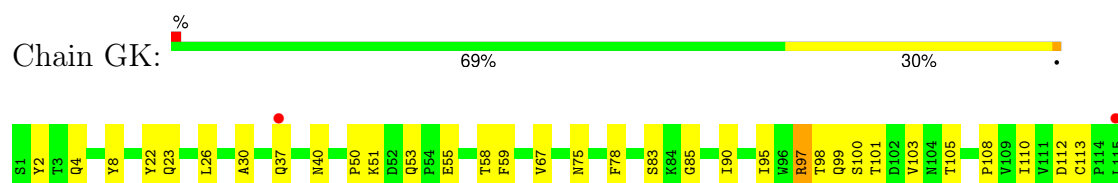
- Molecule 1: coat protein



- Molecule 1: coat protein



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- Molecule 1: coat protein



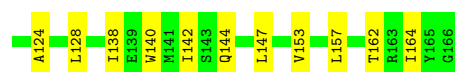
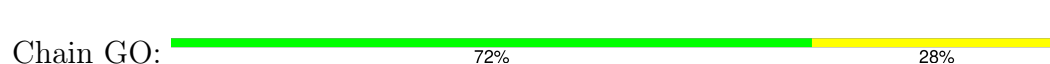
- Molecule 1: coat protein



- Molecule 1: coat protein

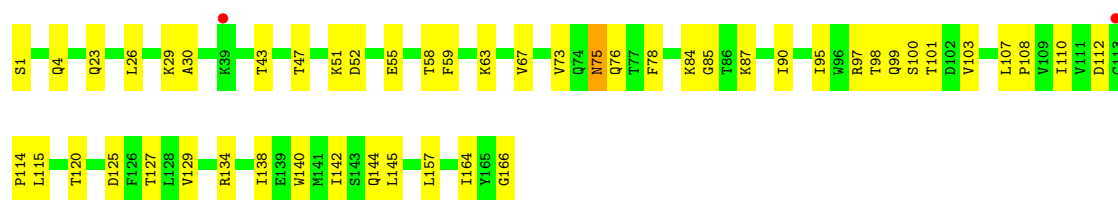


- Molecule 1: coat protein

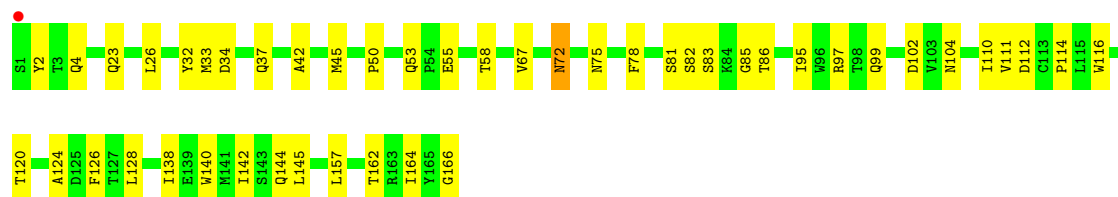
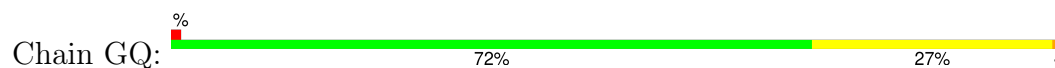


- Molecule 1: coat protein

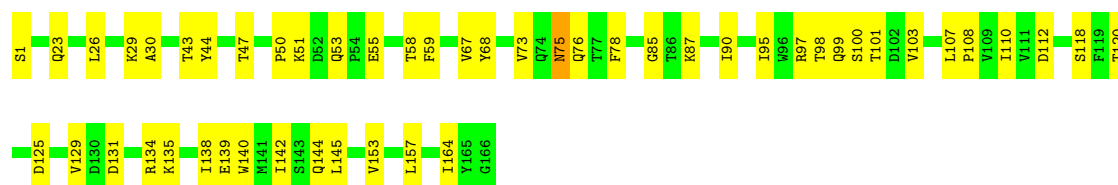




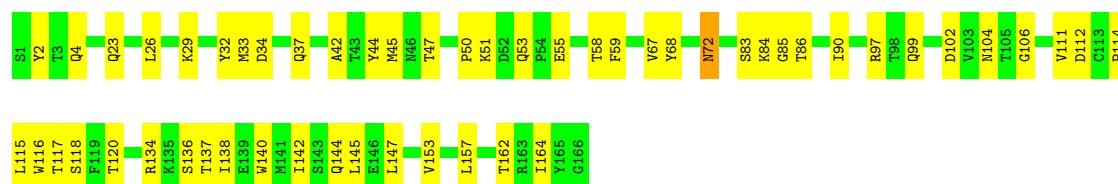
- Molecule 1: coat protein



- Molecule 1: coat protein



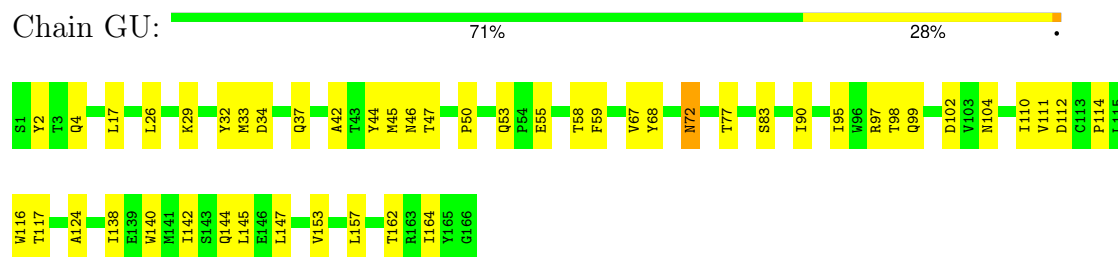
- Molecule 1: coat protein



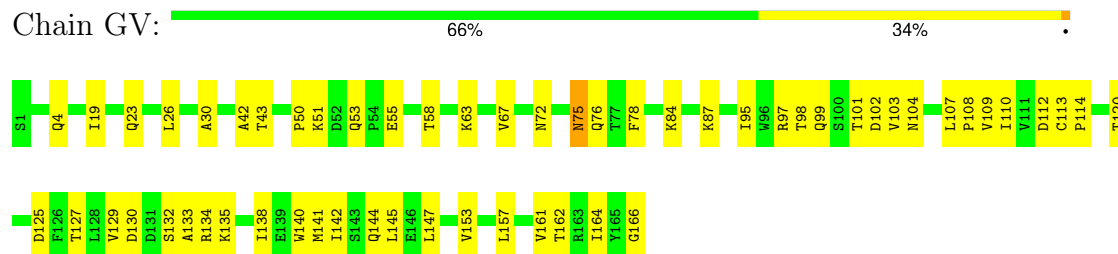
- Molecule 1: coat protein



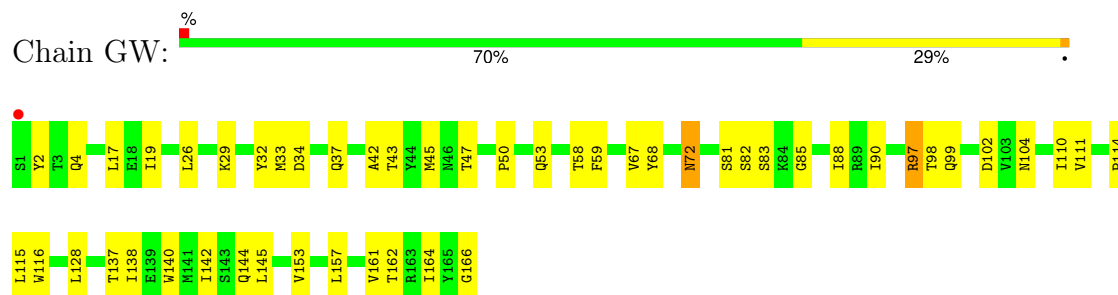
- Molecule 1: coat protein



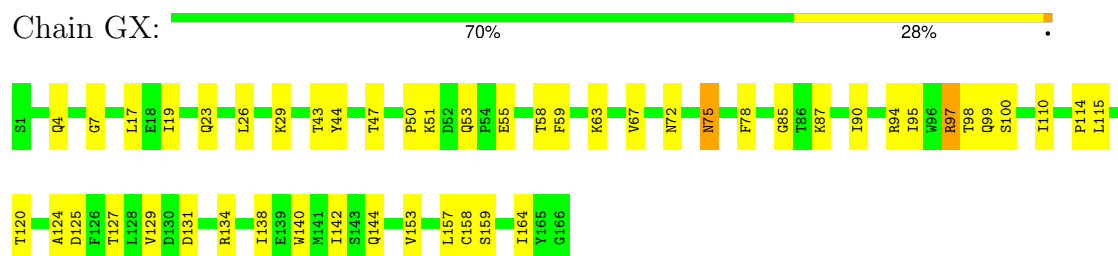
- Molecule 1: coat protein



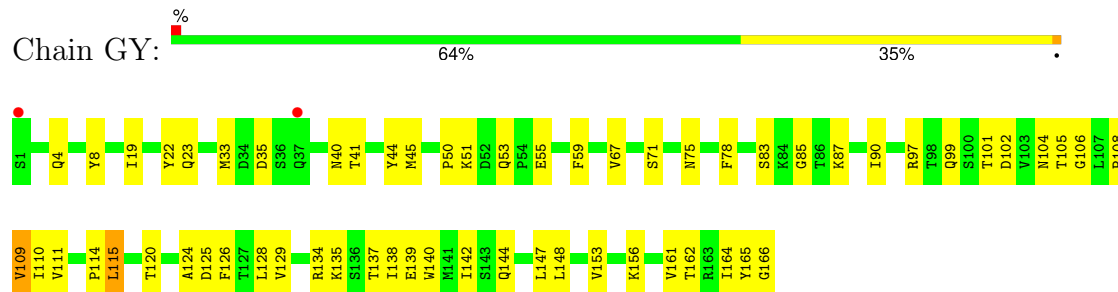
- Molecule 1: coat protein



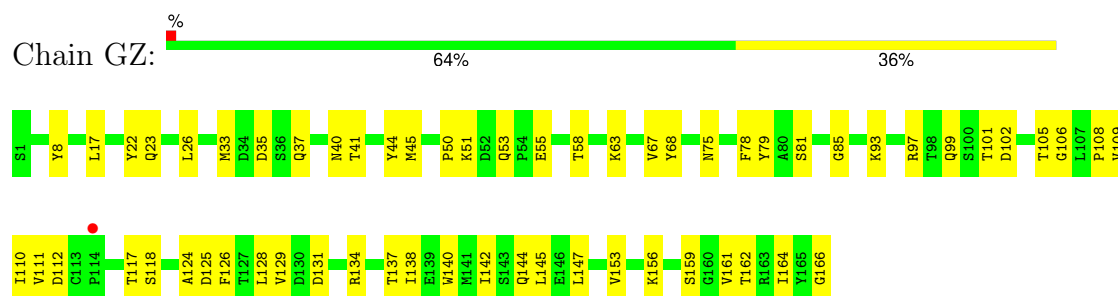
- Molecule 1: coat protein



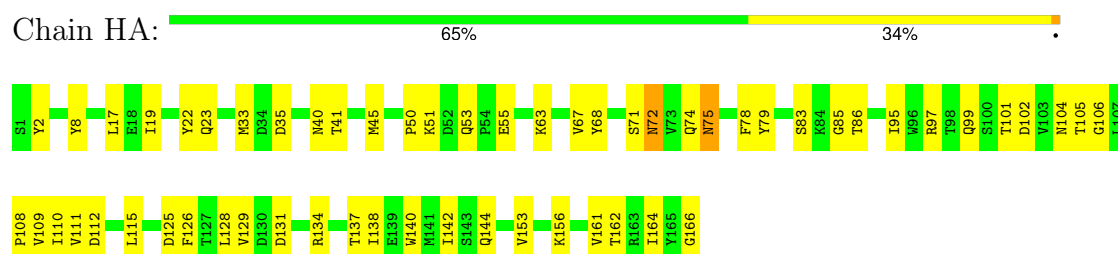
- Molecule 1: coat protein



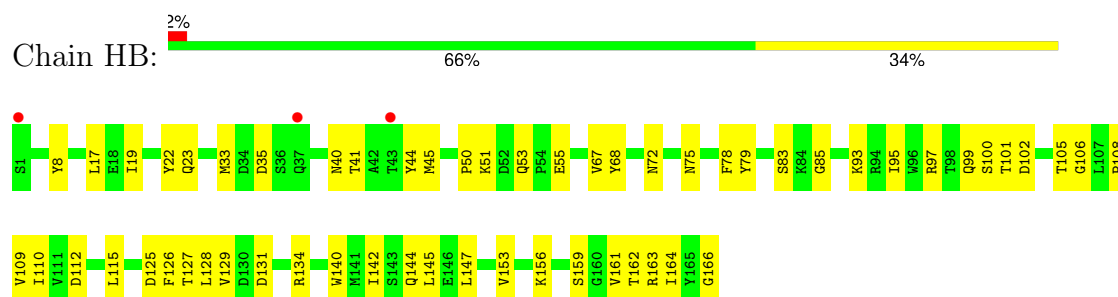
- Molecule 1: coat protein



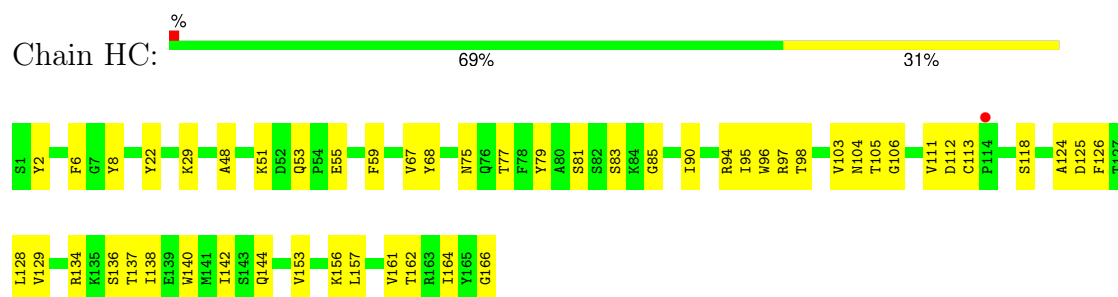
- Molecule 1: coat protein



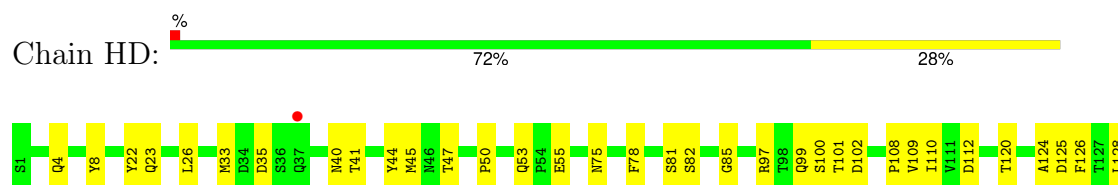
- Molecule 1: coat protein



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- Molecule 1: coat protein





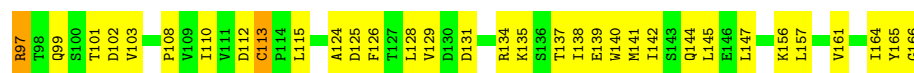
- Molecule 1: coat protein



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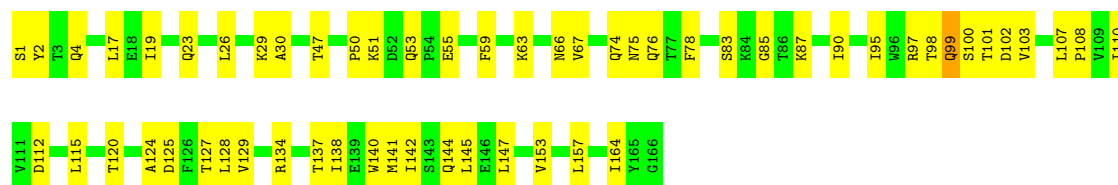


- Molecule 1: coat protein



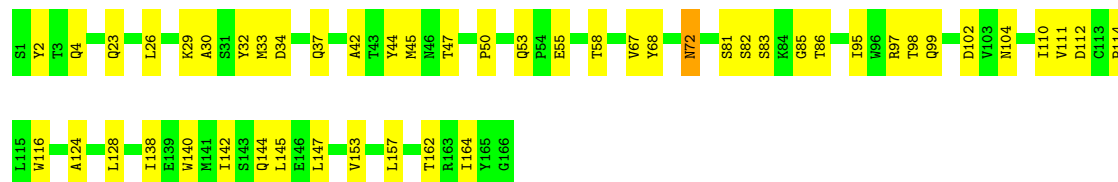
- Molecule 1: coat protein





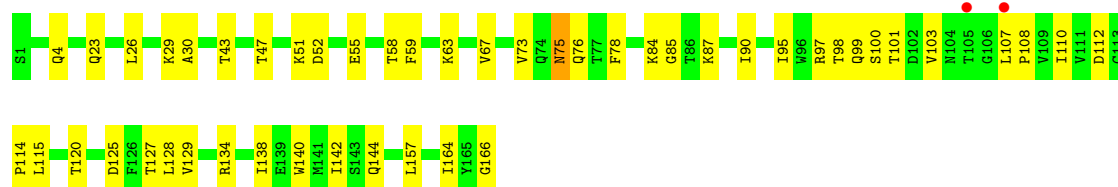
- Molecule 1: coat protein

Chain HJ: 70% 29% .



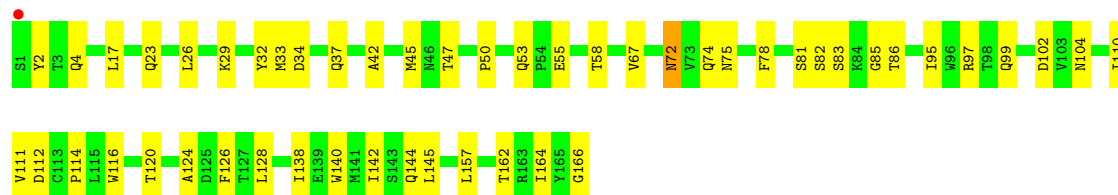
- Molecule 1: coat protein

Chain HK: 71% 28% .



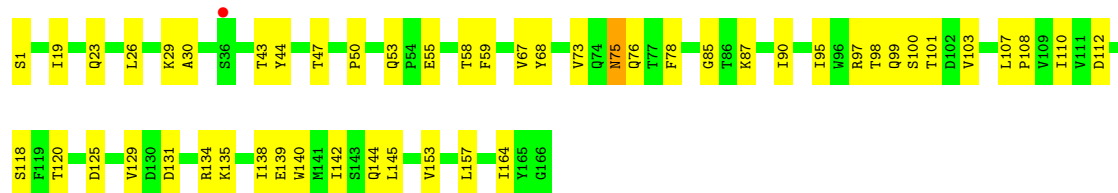
- Molecule 1: coat protein

Chain HL: 70% 30% .

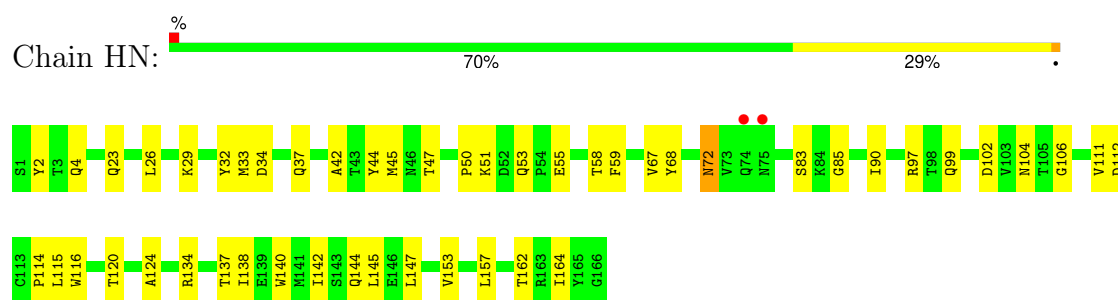


- Molecule 1: coat protein

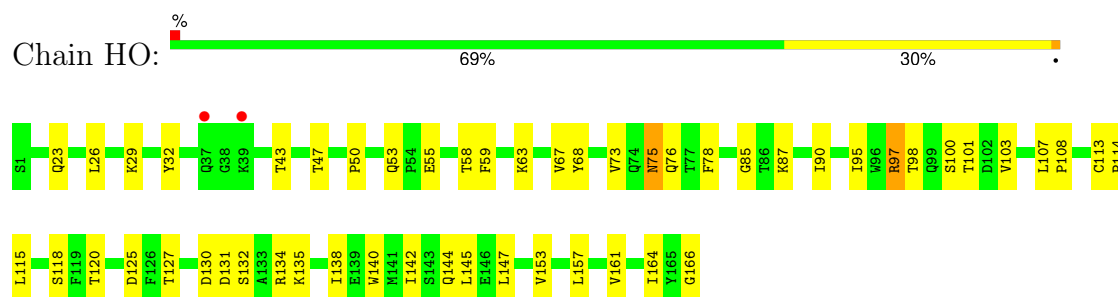
Chain HM: 70% 30% .



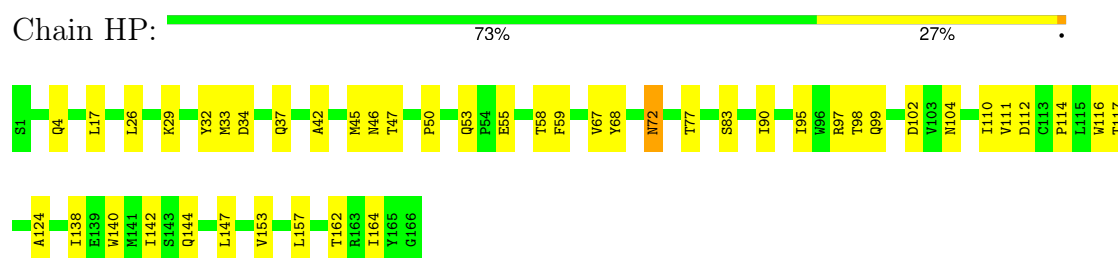
- Molecule 1: coat protein



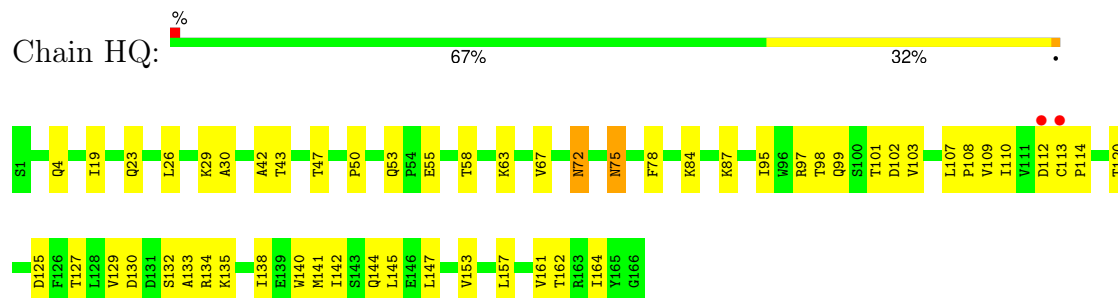
- Molecule 1: coat protein



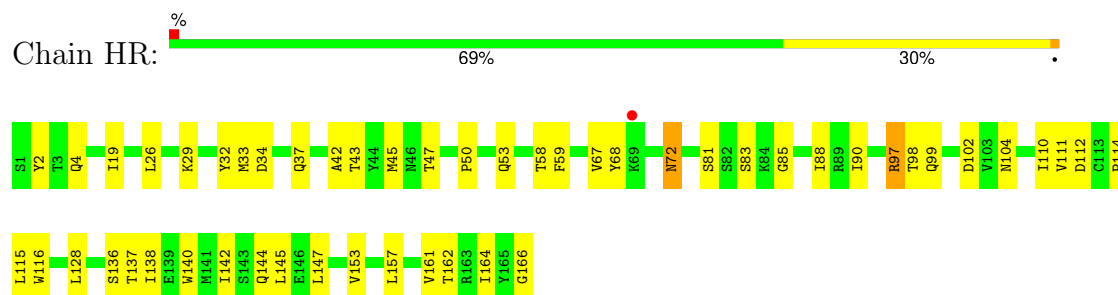
- Molecule 1: coat protein



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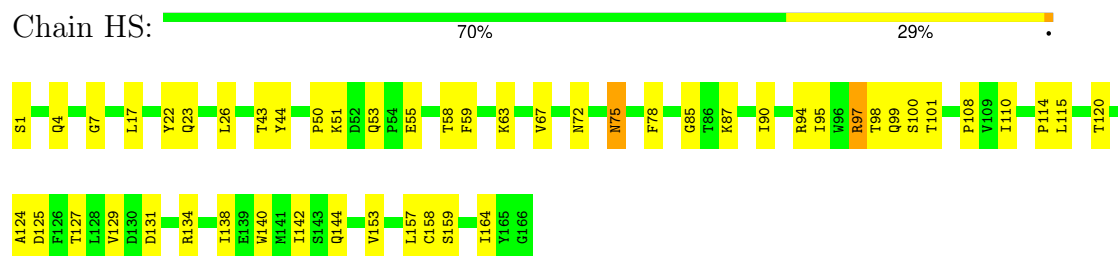


- Molecule 1: coat protein

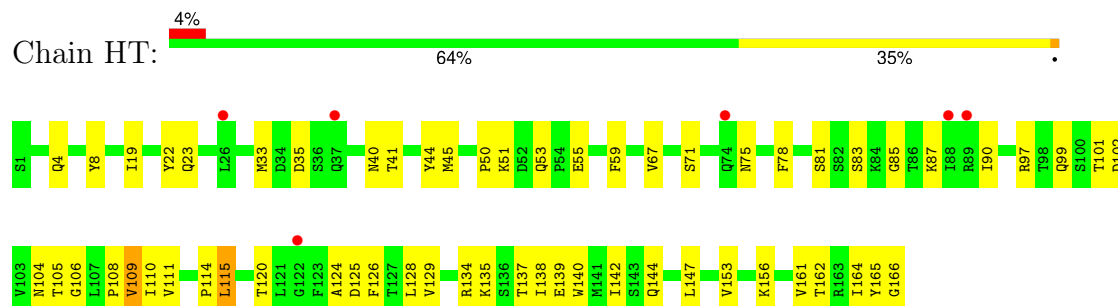




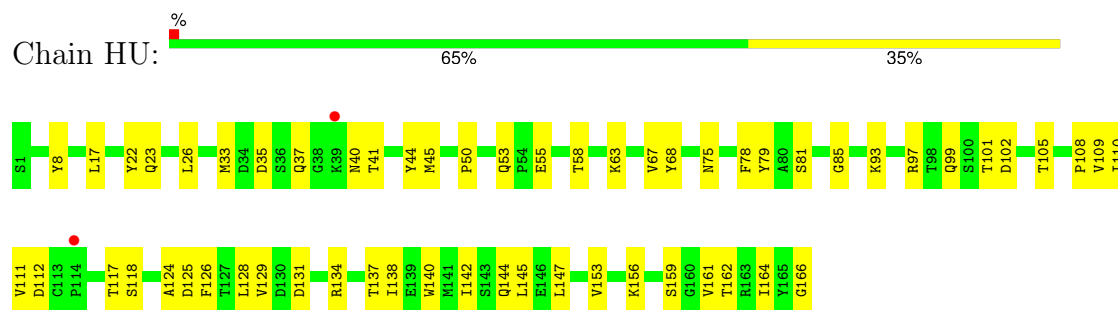
- Molecule 1: coat protein



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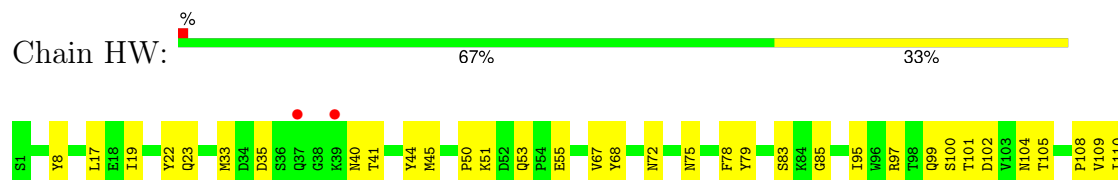
- Molecule 1: coat protein



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- Molecule 1: coat protein

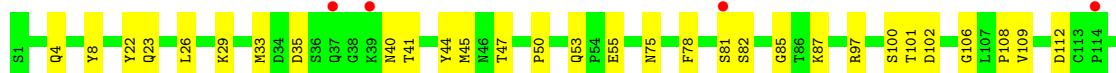
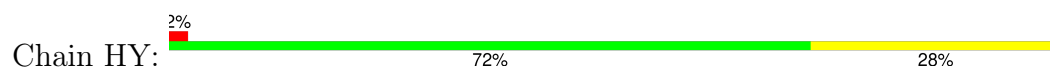




- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein

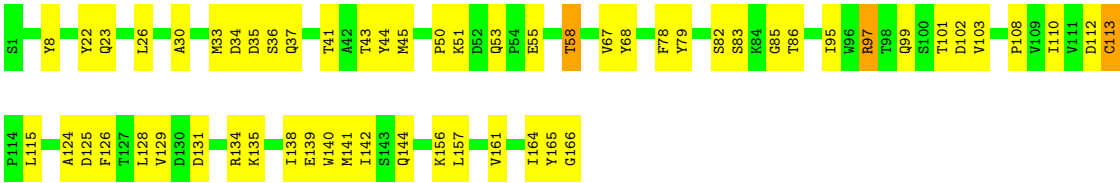


- Molecule 1: coat protein



- Molecule 1: coat protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	325.47Å 298.52Å 417.12Å 90.00° 100.00° 90.00°	Depositor
Resolution (Å)	49.32 – 3.59 49.32 – 3.59	Depositor EDS
% Data completeness (in resolution range)	93.0 (49.32-3.59) 93.9 (49.32-3.59)	Depositor EDS
$R_{merge}$	0.47	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.278 , 0.283 0.281 , 0.286	Depositor DCC
$R_{free}$ test set	10000 reflections (1.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	101.9	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 40.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	275100	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	AA	0.44	0/1337	0.64	2/1814 (0.1%)
1	AB	0.46	0/1337	0.67	2/1814 (0.1%)
1	AC	0.43	0/1337	0.62	0/1814
1	AD	0.46	0/1337	0.69	2/1814 (0.1%)
1	AE	0.43	0/1337	0.64	0/1814
1	AF	0.46	0/1337	0.65	0/1814
1	AG	0.44	0/1337	0.65	1/1814 (0.1%)
1	AH	0.47	0/1337	0.65	2/1814 (0.1%)
1	AI	0.44	0/1337	0.65	0/1814
1	AJ	0.46	0/1337	0.68	1/1814 (0.1%)
1	AK	0.45	0/1337	0.64	1/1814 (0.1%)
1	AL	0.48	0/1337	0.68	1/1814 (0.1%)
1	AM	0.45	0/1337	0.66	2/1814 (0.1%)
1	AN	0.45	0/1337	0.65	0/1814
1	AO	0.44	0/1337	0.64	1/1814 (0.1%)
1	AP	0.44	0/1337	0.66	1/1814 (0.1%)
1	AQ	0.46	0/1337	0.65	0/1814
1	AR	0.44	0/1337	0.62	0/1814
1	AS	0.44	0/1337	0.67	1/1814 (0.1%)
1	AT	0.46	0/1337	0.67	0/1814
1	AU	0.45	0/1337	0.66	2/1814 (0.1%)
1	AV	0.44	0/1337	0.64	2/1814 (0.1%)
1	AW	0.46	0/1337	0.67	2/1814 (0.1%)
1	AX	0.43	0/1337	0.62	0/1814
1	AY	0.46	0/1337	0.69	2/1814 (0.1%)
1	AZ	0.43	0/1337	0.64	0/1814
1	BA	0.46	0/1337	0.66	0/1814
1	BB	0.44	0/1337	0.65	1/1814 (0.1%)
1	BC	0.47	0/1337	0.66	2/1814 (0.1%)
1	BD	0.44	0/1337	0.65	0/1814
1	BE	0.47	0/1337	0.68	1/1814 (0.1%)
1	BF	0.45	0/1337	0.64	1/1814 (0.1%)
1	BG	0.48	0/1337	0.68	1/1814 (0.1%)
1	BH	0.45	0/1337	0.66	2/1814 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	BI	0.45	0/1337	0.65	0/1814
1	BJ	0.44	0/1337	0.64	1/1814 (0.1%)
1	BK	0.44	0/1337	0.66	1/1814 (0.1%)
1	BL	0.46	0/1337	0.65	0/1814
1	BM	0.44	0/1337	0.62	0/1814
1	BN	0.44	0/1337	0.66	1/1814 (0.1%)
1	BO	0.46	0/1337	0.67	0/1814
1	BP	0.45	0/1337	0.66	2/1814 (0.1%)
1	BQ	0.44	0/1337	0.64	1/1814 (0.1%)
1	BR	0.46	0/1337	0.67	2/1814 (0.1%)
1	BS	0.43	0/1337	0.62	0/1814
1	BT	0.46	0/1337	0.69	2/1814 (0.1%)
1	BU	0.43	0/1337	0.64	0/1814
1	BV	0.46	0/1337	0.65	0/1814
1	BW	0.44	0/1337	0.65	1/1814 (0.1%)
1	BX	0.47	0/1337	0.66	2/1814 (0.1%)
1	BY	0.44	0/1337	0.65	0/1814
1	BZ	0.47	0/1337	0.68	1/1814 (0.1%)
1	CA	0.45	0/1337	0.64	1/1814 (0.1%)
1	CB	0.48	0/1337	0.68	1/1814 (0.1%)
1	CC	0.46	0/1337	0.66	2/1814 (0.1%)
1	CD	0.45	0/1337	0.65	0/1814
1	CE	0.44	0/1337	0.64	1/1814 (0.1%)
1	CF	0.44	0/1337	0.66	1/1814 (0.1%)
1	CG	0.46	0/1337	0.65	0/1814
1	CH	0.44	0/1337	0.62	0/1814
1	CI	0.44	0/1337	0.67	1/1814 (0.1%)
1	CJ	0.46	0/1337	0.67	0/1814
1	CK	0.45	0/1337	0.66	2/1814 (0.1%)
1	CL	0.44	0/1337	0.64	2/1814 (0.1%)
1	CM	0.46	0/1337	0.67	2/1814 (0.1%)
1	CN	0.43	0/1337	0.62	0/1814
1	CO	0.46	0/1337	0.69	2/1814 (0.1%)
1	CP	0.43	0/1337	0.64	0/1814
1	CQ	0.46	0/1337	0.65	0/1814
1	CR	0.44	0/1337	0.65	1/1814 (0.1%)
1	CS	0.47	0/1337	0.65	2/1814 (0.1%)
1	CT	0.44	0/1337	0.65	0/1814
1	CU	0.46	0/1337	0.68	1/1814 (0.1%)
1	CV	0.45	0/1337	0.64	1/1814 (0.1%)
1	CW	0.48	0/1337	0.68	1/1814 (0.1%)
1	CX	0.45	0/1337	0.66	2/1814 (0.1%)
1	CY	0.45	0/1337	0.65	0/1814

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	CZ	0.44	0/1337	0.64	1/1814 (0.1%)
1	DA	0.44	0/1337	0.66	1/1814 (0.1%)
1	DB	0.47	0/1337	0.65	0/1814
1	DC	0.44	0/1337	0.62	0/1814
1	DD	0.44	0/1337	0.67	1/1814 (0.1%)
1	DE	0.45	0/1337	0.67	0/1814
1	DF	0.45	0/1337	0.66	2/1814 (0.1%)
1	DG	0.44	0/1337	0.64	2/1814 (0.1%)
1	DH	0.46	0/1337	0.67	2/1814 (0.1%)
1	DI	0.43	0/1337	0.62	0/1814
1	DJ	0.46	0/1337	0.69	2/1814 (0.1%)
1	DK	0.43	0/1337	0.64	0/1814
1	DL	0.46	0/1337	0.66	0/1814
1	DM	0.44	0/1337	0.65	1/1814 (0.1%)
1	DN	0.47	0/1337	0.65	2/1814 (0.1%)
1	DO	0.44	0/1337	0.65	0/1814
1	DP	0.46	0/1337	0.68	1/1814 (0.1%)
1	DQ	0.45	0/1337	0.64	1/1814 (0.1%)
1	DR	0.48	0/1337	0.68	1/1814 (0.1%)
1	DS	0.45	0/1337	0.66	2/1814 (0.1%)
1	DT	0.45	0/1337	0.65	0/1814
1	DU	0.44	0/1337	0.64	1/1814 (0.1%)
1	DV	0.44	0/1337	0.66	1/1814 (0.1%)
1	DW	0.46	0/1337	0.65	0/1814
1	DX	0.44	0/1337	0.62	0/1814
1	DY	0.44	0/1337	0.67	1/1814 (0.1%)
1	DZ	0.46	0/1337	0.67	0/1814
1	EA	0.45	0/1337	0.66	2/1814 (0.1%)
1	EB	0.44	0/1337	0.64	2/1814 (0.1%)
1	EC	0.46	0/1337	0.67	2/1814 (0.1%)
1	ED	0.42	0/1337	0.62	0/1814
1	EE	0.46	0/1337	0.69	2/1814 (0.1%)
1	EF	0.43	0/1337	0.64	0/1814
1	EG	0.45	0/1337	0.66	0/1814
1	EH	0.44	0/1337	0.65	1/1814 (0.1%)
1	EI	0.47	0/1337	0.66	2/1814 (0.1%)
1	EJ	0.44	0/1337	0.65	0/1814
1	EK	0.46	0/1337	0.68	2/1814 (0.1%)
1	EL	0.45	0/1337	0.64	1/1814 (0.1%)
1	EM	0.48	0/1337	0.68	1/1814 (0.1%)
1	EN	0.46	0/1337	0.66	2/1814 (0.1%)
1	EO	0.45	0/1337	0.65	0/1814
1	EP	0.44	0/1337	0.64	1/1814 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	EQ	0.44	0/1337	0.66	1/1814 (0.1%)
1	ER	0.47	0/1337	0.65	0/1814
1	ES	0.44	0/1337	0.62	0/1814
1	ET	0.44	0/1337	0.67	1/1814 (0.1%)
1	EU	0.46	0/1337	0.67	0/1814
1	EV	0.45	0/1337	0.66	2/1814 (0.1%)
1	EW	0.44	0/1337	0.64	2/1814 (0.1%)
1	EX	0.46	0/1337	0.67	2/1814 (0.1%)
1	EY	0.43	0/1337	0.62	0/1814
1	EZ	0.46	0/1337	0.69	2/1814 (0.1%)
1	FA	0.43	0/1337	0.64	0/1814
1	FB	0.46	0/1337	0.66	0/1814
1	FC	0.44	0/1337	0.65	1/1814 (0.1%)
1	FD	0.47	0/1337	0.65	2/1814 (0.1%)
1	FE	0.44	0/1337	0.65	0/1814
1	FF	0.46	0/1337	0.68	1/1814 (0.1%)
1	FG	0.45	0/1337	0.64	1/1814 (0.1%)
1	FH	0.48	0/1337	0.68	1/1814 (0.1%)
1	FI	0.45	0/1337	0.66	2/1814 (0.1%)
1	FJ	0.45	0/1337	0.65	0/1814
1	FK	0.44	0/1337	0.64	1/1814 (0.1%)
1	FL	0.44	0/1337	0.66	1/1814 (0.1%)
1	FM	0.47	0/1337	0.65	0/1814
1	FN	0.44	0/1337	0.62	0/1814
1	FO	0.44	0/1337	0.67	1/1814 (0.1%)
1	FP	0.46	0/1337	0.67	0/1814
1	FQ	0.45	0/1337	0.65	2/1814 (0.1%)
1	FR	0.44	0/1337	0.64	2/1814 (0.1%)
1	FS	0.46	0/1337	0.67	2/1814 (0.1%)
1	FT	0.42	0/1337	0.62	0/1814
1	FU	0.46	0/1337	0.69	2/1814 (0.1%)
1	FV	0.43	0/1337	0.64	0/1814
1	FW	0.45	0/1337	0.66	0/1814
1	FX	0.44	0/1337	0.65	1/1814 (0.1%)
1	FY	0.47	0/1337	0.65	2/1814 (0.1%)
1	FZ	0.44	0/1337	0.65	0/1814
1	GA	0.46	0/1337	0.68	1/1814 (0.1%)
1	GB	0.45	0/1337	0.64	1/1814 (0.1%)
1	GC	0.48	0/1337	0.68	1/1814 (0.1%)
1	GD	0.45	0/1337	0.66	2/1814 (0.1%)
1	GE	0.45	0/1337	0.65	0/1814
1	GF	0.44	0/1337	0.64	1/1814 (0.1%)
1	GG	0.44	0/1337	0.66	1/1814 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	GH	0.47	0/1337	0.65	0/1814
1	GI	0.44	0/1337	0.62	0/1814
1	GJ	0.44	0/1337	0.67	1/1814 (0.1%)
1	GK	0.46	0/1337	0.67	0/1814
1	GL	0.45	0/1337	0.65	2/1814 (0.1%)
1	GM	0.44	0/1337	0.64	1/1814 (0.1%)
1	GN	0.46	0/1337	0.67	2/1814 (0.1%)
1	GO	0.43	0/1337	0.62	0/1814
1	GP	0.46	0/1337	0.69	2/1814 (0.1%)
1	GQ	0.43	0/1337	0.64	0/1814
1	GR	0.46	0/1337	0.65	0/1814
1	GS	0.44	0/1337	0.65	1/1814 (0.1%)
1	GT	0.47	0/1337	0.65	2/1814 (0.1%)
1	GU	0.44	0/1337	0.65	0/1814
1	GV	0.46	0/1337	0.68	1/1814 (0.1%)
1	GW	0.45	0/1337	0.64	1/1814 (0.1%)
1	GX	0.48	0/1337	0.68	1/1814 (0.1%)
1	GY	0.45	0/1337	0.66	2/1814 (0.1%)
1	GZ	0.45	0/1337	0.65	0/1814
1	HA	0.44	0/1337	0.64	1/1814 (0.1%)
1	HB	0.44	0/1337	0.66	1/1814 (0.1%)
1	HC	0.47	0/1337	0.65	0/1814
1	HD	0.44	0/1337	0.62	0/1814
1	HE	0.44	0/1337	0.67	1/1814 (0.1%)
1	HF	0.46	0/1337	0.67	0/1814
1	HG	0.45	0/1337	0.66	2/1814 (0.1%)
1	HH	0.44	0/1337	0.64	2/1814 (0.1%)
1	HI	0.46	0/1337	0.67	2/1814 (0.1%)
1	HJ	0.43	0/1337	0.62	0/1814
1	HK	0.46	0/1337	0.69	2/1814 (0.1%)
1	HL	0.43	0/1337	0.64	0/1814
1	HM	0.46	0/1337	0.65	0/1814
1	HN	0.44	0/1337	0.65	1/1814 (0.1%)
1	HO	0.47	0/1337	0.65	2/1814 (0.1%)
1	HP	0.44	0/1337	0.65	0/1814
1	HQ	0.46	0/1337	0.68	1/1814 (0.1%)
1	HR	0.45	0/1337	0.64	1/1814 (0.1%)
1	HS	0.48	0/1337	0.68	1/1814 (0.1%)
1	HT	0.46	0/1337	0.66	2/1814 (0.1%)
1	HU	0.45	0/1337	0.65	0/1814
1	HV	0.44	0/1337	0.64	1/1814 (0.1%)
1	HW	0.44	0/1337	0.66	1/1814 (0.1%)
1	HX	0.47	0/1337	0.65	0/1814

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	HY	0.44	0/1337	0.62	0/1814
1	HZ	0.44	0/1337	0.67	1/1814 (0.1%)
1	IA	0.46	0/1337	0.67	0/1814
1	IB	0.45	0/1337	0.66	2/1814 (0.1%)
All	All	0.45	0/280770	0.65	189/380940 (0.0%)

There are no bond length outliers.

The worst 5 of 189 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	GX	63	LYS	CD-CE-NZ	6.53	126.72	111.70
1	EM	63	LYS	CD-CE-NZ	6.52	126.70	111.70
1	BG	63	LYS	CD-CE-NZ	6.52	126.69	111.70
1	FH	63	LYS	CD-CE-NZ	6.52	126.69	111.70
1	HS	63	LYS	CD-CE-NZ	6.52	126.69	111.70

There are no chirality outliers.

There are no planarity outliers.

## 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	AA	1310	0	1289	65	0
1	AB	1310	0	1289	69	0
1	AC	1310	0	1289	50	0
1	AD	1310	0	1289	51	0
1	AE	1310	0	1289	52	0
1	AF	1310	0	1289	50	0
1	AG	1310	0	1289	54	0
1	AH	1310	0	1289	50	0
1	AI	1310	0	1289	57	0
1	AJ	1310	0	1289	56	0
1	AK	1310	0	1289	58	0
1	AL	1310	0	1289	52	0
1	AM	1310	0	1289	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AN	1310	0	1289	67	0
1	AO	1310	0	1289	66	0
1	AP	1310	0	1289	62	0
1	AQ	1310	0	1289	62	0
1	AR	1310	0	1289	45	0
1	AS	1310	0	1289	76	0
1	AT	1310	0	1289	63	0
1	AU	1310	0	1289	74	0
1	AV	1310	0	1289	68	0
1	AW	1310	0	1289	66	0
1	AX	1310	0	1289	51	0
1	AY	1310	0	1289	48	0
1	AZ	1310	0	1289	55	0
1	BA	1310	0	1289	54	0
1	BB	1310	0	1289	52	0
1	BC	1310	0	1289	45	0
1	BD	1310	0	1289	44	0
1	BE	1310	0	1289	53	0
1	BF	1310	0	1289	54	0
1	BG	1310	0	1289	48	0
1	BH	1310	0	1289	64	0
1	BI	1310	0	1289	62	0
1	BJ	1310	0	1289	64	0
1	BK	1310	0	1289	65	0
1	BL	1310	0	1289	60	0
1	BM	1310	0	1289	47	0
1	BN	1310	0	1289	70	0
1	BO	1310	0	1289	57	0
1	BP	1310	0	1289	69	0
1	BQ	1310	0	1289	65	0
1	BR	1310	0	1289	63	0
1	BS	1310	0	1289	52	0
1	BT	1310	0	1289	51	0
1	BU	1310	0	1289	55	1
1	BV	1310	0	1289	53	0
1	BW	1310	0	1289	49	0
1	BX	1310	0	1289	48	0
1	BY	1310	0	1289	46	0
1	BZ	1310	0	1289	50	0
1	CA	1310	0	1289	52	0
1	CB	1310	0	1289	50	0
1	CC	1310	0	1289	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CD	1310	0	1289	66	1
1	CE	1310	0	1289	67	0
1	CF	1310	0	1289	64	0
1	CG	1310	0	1289	62	0
1	CH	1310	0	1289	47	0
1	CI	1310	0	1289	71	0
1	CJ	1310	0	1289	57	1
1	CK	1310	0	1289	63	0
1	CL	1310	0	1289	69	0
1	CM	1310	0	1289	68	0
1	CN	1310	0	1289	54	0
1	CO	1310	0	1289	50	0
1	CP	1310	0	1289	54	0
1	CQ	1310	0	1289	52	0
1	CR	1310	0	1289	55	0
1	CS	1310	0	1289	49	0
1	CT	1310	0	1289	44	0
1	CU	1310	0	1289	49	0
1	CV	1310	0	1289	56	0
1	CW	1310	0	1289	48	0
1	CX	1310	0	1289	62	0
1	CY	1310	0	1289	63	0
1	CZ	1310	0	1289	64	0
1	DA	1310	0	1289	63	0
1	DB	1310	0	1289	60	0
1	DC	1310	0	1289	48	1
1	DD	1310	0	1289	70	0
1	DE	1310	0	1289	59	0
1	DF	1310	0	1289	72	0
1	DG	1310	0	1289	75	0
1	DH	1310	0	1289	75	0
1	DI	1310	0	1289	51	0
1	DJ	1310	0	1289	49	0
1	DK	1310	0	1289	57	0
1	DL	1310	0	1289	53	0
1	DM	1310	0	1289	48	0
1	DN	1310	0	1289	51	0
1	DO	1310	0	1289	48	0
1	DP	1310	0	1289	49	0
1	DQ	1310	0	1289	54	0
1	DR	1310	0	1289	50	0
1	DS	1310	0	1289	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DT	1310	0	1289	65	0
1	DU	1310	0	1289	64	0
1	DV	1310	0	1289	64	0
1	DW	1310	0	1289	62	0
1	DX	1310	0	1289	48	0
1	DY	1310	0	1289	72	0
1	DZ	1310	0	1289	56	0
1	EA	1310	0	1289	59	0
1	EB	1310	0	1289	68	0
1	EC	1310	0	1289	67	0
1	ED	1310	0	1289	54	0
1	EE	1310	0	1289	50	0
1	EF	1310	0	1289	54	0
1	EG	1310	0	1289	52	0
1	EH	1310	0	1289	54	0
1	EI	1310	0	1289	48	0
1	EJ	1310	0	1289	46	0
1	EK	1310	0	1289	49	0
1	EL	1310	0	1289	53	0
1	EM	1310	0	1289	46	0
1	EN	1310	0	1289	65	0
1	EO	1310	0	1289	61	0
1	EP	1310	0	1289	63	0
1	EQ	1310	0	1289	64	0
1	ER	1310	0	1289	63	0
1	ES	1310	0	1289	50	0
1	ET	1310	0	1289	73	0
1	EU	1310	0	1289	61	0
1	EV	1310	0	1289	71	0
1	EW	1310	0	1289	68	0
1	EX	1310	0	1289	70	0
1	EY	1310	0	1289	54	0
1	EZ	1310	0	1289	49	0
1	FA	1310	0	1289	55	0
1	FB	1310	0	1289	51	0
1	FC	1310	0	1289	47	0
1	FD	1310	0	1289	48	0
1	FE	1310	0	1289	47	0
1	FF	1310	0	1289	51	0
1	FG	1310	0	1289	53	0
1	FH	1310	0	1289	48	0
1	FI	1310	0	1289	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	FJ	1310	0	1289	64	0
1	FK	1310	0	1289	65	0
1	FL	1310	0	1289	65	0
1	FM	1310	0	1289	63	0
1	FN	1310	0	1289	47	0
1	FO	1310	0	1289	71	0
1	FP	1310	0	1289	56	0
1	FQ	1310	0	1289	64	0
1	FR	1310	0	1289	74	0
1	FS	1310	0	1289	71	0
1	FT	1310	0	1289	51	0
1	FU	1310	0	1289	50	0
1	FV	1310	0	1289	53	0
1	FW	1310	0	1289	51	1
1	FX	1310	0	1289	52	0
1	FY	1310	0	1289	50	0
1	FZ	1310	0	1289	55	0
1	GA	1310	0	1289	53	0
1	GB	1310	0	1289	54	0
1	GC	1310	0	1289	48	0
1	GD	1310	0	1289	63	1
1	GE	1310	0	1289	66	0
1	GF	1310	0	1289	64	0
1	GG	1310	0	1289	60	0
1	GH	1310	0	1289	61	0
1	GI	1310	0	1289	47	0
1	GJ	1310	0	1289	76	0
1	GK	1310	0	1289	60	0
1	GL	1310	0	1289	67	0
1	GM	1310	0	1289	66	0
1	GN	1310	0	1289	61	0
1	GO	1310	0	1289	50	0
1	GP	1310	0	1289	50	0
1	GQ	1310	0	1289	51	0
1	GR	1310	0	1289	52	0
1	GS	1310	0	1289	51	0
1	GT	1310	0	1289	48	0
1	GU	1310	0	1289	48	0
1	GV	1310	0	1289	51	0
1	GW	1310	0	1289	54	0
1	GX	1310	0	1289	48	0
1	GY	1310	0	1289	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	GZ	1310	0	1289	65	0
1	HA	1310	0	1289	67	0
1	HB	1310	0	1289	68	0
1	HC	1310	0	1289	59	0
1	HD	1310	0	1289	44	0
1	HE	1310	0	1289	69	0
1	HF	1310	0	1289	55	0
1	HG	1310	0	1289	76	0
1	HH	1310	0	1289	67	0
1	HI	1310	0	1289	77	0
1	HJ	1310	0	1289	52	0
1	HK	1310	0	1289	48	0
1	HL	1310	0	1289	55	0
1	HM	1310	0	1289	53	0
1	HN	1310	0	1289	51	0
1	HO	1310	0	1289	50	0
1	HP	1310	0	1289	45	0
1	HQ	1310	0	1289	51	0
1	HR	1310	0	1289	54	0
1	HS	1310	0	1289	48	0
1	HT	1310	0	1289	61	0
1	HU	1310	0	1289	62	0
1	HV	1310	0	1289	65	0
1	HW	1310	0	1289	63	0
1	HX	1310	0	1289	60	0
1	HY	1310	0	1289	46	0
1	HZ	1310	0	1289	66	0
1	IA	1310	0	1289	55	0
1	IB	1310	0	1289	58	0
All	All	275100	0	270690	8493	3

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 16.

The worst 5 of 8493 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:EB:162:THR:HB	1:HH:34:ASP:HB3	1.26	1.14
1:AA:162:THR:HB	1:DG:34:ASP:HB3	1.36	1.07
1:AV:34:ASP:HB3	1:BQ:162:THR:HB	1.37	1.02
1:AA:155:SER:OG	1:DG:51:LYS:NZ	1.92	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AI:162:THR:HB	1:AK:34:ASP:HB3	1.44	1.00

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CD:14:LYS:NZ	1:FW:12:THR:OG1[1_455]	2.03	0.17
1:CJ:9:THR:OG1	1:DC:13:GLU:OE2[2_444]	2.07	0.13
1:BU:18:GLU:OE1	1:GD:18:GLU:OE1[1_455]	2.18	0.02

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	AB	164/166 (99%)	160 (98%)	4 (2%)	0	100	100
1	AC	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	AD	164/166 (99%)	155 (94%)	9 (6%)	0	100	100
1	AE	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	AF	164/166 (99%)	159 (97%)	5 (3%)	0	100	100
1	AG	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	AH	164/166 (99%)	157 (96%)	7 (4%)	0	100	100
1	AI	164/166 (99%)	162 (99%)	2 (1%)	0	100	100
1	AJ	164/166 (99%)	156 (95%)	8 (5%)	0	100	100
1	AK	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	AL	164/166 (99%)	159 (97%)	5 (3%)	0	100	100
1	AM	164/166 (99%)	164 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AN	164/166 (99%)	164 (100%)	0	0	100	100
1	AO	164/166 (99%)	164 (100%)	0	0	100	100
1	AP	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	AQ	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	AR	164/166 (99%)	164 (100%)	0	0	100	100
1	AS	164/166 (99%)	164 (100%)	0	0	100	100
1	AT	164/166 (99%)	164 (100%)	0	0	100	100
1	AU	164/166 (99%)	164 (100%)	0	0	100	100
1	AV	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	AW	164/166 (99%)	160 (98%)	4 (2%)	0	100	100
1	AX	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	AY	164/166 (99%)	155 (94%)	9 (6%)	0	100	100
1	AZ	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	BA	164/166 (99%)	159 (97%)	5 (3%)	0	100	100
1	BB	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	BC	164/166 (99%)	157 (96%)	7 (4%)	0	100	100
1	BD	164/166 (99%)	162 (99%)	2 (1%)	0	100	100
1	BE	164/166 (99%)	156 (95%)	8 (5%)	0	100	100
1	BF	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	BG	164/166 (99%)	159 (97%)	5 (3%)	0	100	100
1	BH	164/166 (99%)	164 (100%)	0	0	100	100
1	BI	164/166 (99%)	164 (100%)	0	0	100	100
1	BJ	164/166 (99%)	164 (100%)	0	0	100	100
1	BK	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	BL	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	BM	164/166 (99%)	164 (100%)	0	0	100	100
1	BN	164/166 (99%)	164 (100%)	0	0	100	100
1	BO	164/166 (99%)	164 (100%)	0	0	100	100
1	BP	164/166 (99%)	164 (100%)	0	0	100	100
1	BQ	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	BR	164/166 (99%)	160 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BS	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	BT	164/166 (99%)	155 (94%)	9 (6%)	0	100	100
1	BU	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	BV	164/166 (99%)	159 (97%)	5 (3%)	0	100	100
1	BW	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	BX	164/166 (99%)	157 (96%)	7 (4%)	0	100	100
1	BY	164/166 (99%)	162 (99%)	2 (1%)	0	100	100
1	BZ	164/166 (99%)	156 (95%)	8 (5%)	0	100	100
1	CA	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	CB	164/166 (99%)	158 (96%)	5 (3%)	1 (1%)	25	64
1	CC	164/166 (99%)	164 (100%)	0	0	100	100
1	CD	164/166 (99%)	164 (100%)	0	0	100	100
1	CE	164/166 (99%)	164 (100%)	0	0	100	100
1	CF	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	CG	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	CH	164/166 (99%)	164 (100%)	0	0	100	100
1	CI	164/166 (99%)	164 (100%)	0	0	100	100
1	CJ	164/166 (99%)	164 (100%)	0	0	100	100
1	CK	164/166 (99%)	164 (100%)	0	0	100	100
1	CL	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	CM	164/166 (99%)	160 (98%)	4 (2%)	0	100	100
1	CN	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	CO	164/166 (99%)	155 (94%)	9 (6%)	0	100	100
1	CP	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	CQ	164/166 (99%)	159 (97%)	5 (3%)	0	100	100
1	CR	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	CS	164/166 (99%)	157 (96%)	7 (4%)	0	100	100
1	CT	164/166 (99%)	162 (99%)	2 (1%)	0	100	100
1	CU	164/166 (99%)	156 (95%)	8 (5%)	0	100	100
1	CV	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	CW	164/166 (99%)	158 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CX	164/166 (99%)	164 (100%)	0	0	100	100
1	CY	164/166 (99%)	164 (100%)	0	0	100	100
1	CZ	164/166 (99%)	164 (100%)	0	0	100	100
1	DA	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	DB	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	DC	164/166 (99%)	164 (100%)	0	0	100	100
1	DD	164/166 (99%)	164 (100%)	0	0	100	100
1	DE	164/166 (99%)	164 (100%)	0	0	100	100
1	DF	164/166 (99%)	164 (100%)	0	0	100	100
1	DG	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	DH	164/166 (99%)	160 (98%)	4 (2%)	0	100	100
1	DI	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	DJ	164/166 (99%)	155 (94%)	9 (6%)	0	100	100
1	DK	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	DL	164/166 (99%)	158 (96%)	6 (4%)	0	100	100
1	DM	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	DN	164/166 (99%)	157 (96%)	7 (4%)	0	100	100
1	DO	164/166 (99%)	162 (99%)	2 (1%)	0	100	100
1	DP	164/166 (99%)	156 (95%)	8 (5%)	0	100	100
1	DQ	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	DR	164/166 (99%)	158 (96%)	6 (4%)	0	100	100
1	DS	164/166 (99%)	164 (100%)	0	0	100	100
1	DT	164/166 (99%)	164 (100%)	0	0	100	100
1	DU	164/166 (99%)	164 (100%)	0	0	100	100
1	DV	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	DW	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	DX	164/166 (99%)	164 (100%)	0	0	100	100
1	DY	164/166 (99%)	164 (100%)	0	0	100	100
1	DZ	164/166 (99%)	164 (100%)	0	0	100	100
1	EA	164/166 (99%)	164 (100%)	0	0	100	100
1	EB	164/166 (99%)	161 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EC	164/166 (99%)	160 (98%)	4 (2%)	0	100	100
1	ED	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	EE	164/166 (99%)	155 (94%)	9 (6%)	0	100	100
1	EF	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	EG	164/166 (99%)	159 (97%)	5 (3%)	0	100	100
1	EH	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	EI	164/166 (99%)	157 (96%)	7 (4%)	0	100	100
1	EJ	164/166 (99%)	162 (99%)	2 (1%)	0	100	100
1	EK	164/166 (99%)	156 (95%)	8 (5%)	0	100	100
1	EL	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	EM	164/166 (99%)	159 (97%)	4 (2%)	1 (1%)	25	64
1	EN	164/166 (99%)	164 (100%)	0	0	100	100
1	EO	164/166 (99%)	164 (100%)	0	0	100	100
1	EP	164/166 (99%)	164 (100%)	0	0	100	100
1	EQ	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	ER	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	ES	164/166 (99%)	164 (100%)	0	0	100	100
1	ET	164/166 (99%)	164 (100%)	0	0	100	100
1	EU	164/166 (99%)	164 (100%)	0	0	100	100
1	EV	164/166 (99%)	164 (100%)	0	0	100	100
1	EW	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	EX	164/166 (99%)	160 (98%)	4 (2%)	0	100	100
1	EY	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	EZ	164/166 (99%)	155 (94%)	9 (6%)	0	100	100
1	FA	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	FB	164/166 (99%)	159 (97%)	5 (3%)	0	100	100
1	FC	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	FD	164/166 (99%)	157 (96%)	7 (4%)	0	100	100
1	FE	164/166 (99%)	162 (99%)	2 (1%)	0	100	100
1	FF	164/166 (99%)	156 (95%)	8 (5%)	0	100	100
1	FG	164/166 (99%)	161 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	FH	164/166 (99%)	160 (98%)	4 (2%)	0	100	100
1	FI	164/166 (99%)	164 (100%)	0	0	100	100
1	FJ	164/166 (99%)	164 (100%)	0	0	100	100
1	FK	164/166 (99%)	164 (100%)	0	0	100	100
1	FL	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	FM	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	FN	164/166 (99%)	164 (100%)	0	0	100	100
1	FO	164/166 (99%)	164 (100%)	0	0	100	100
1	FP	164/166 (99%)	164 (100%)	0	0	100	100
1	FQ	164/166 (99%)	164 (100%)	0	0	100	100
1	FR	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	FS	164/166 (99%)	160 (98%)	4 (2%)	0	100	100
1	FT	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	FU	164/166 (99%)	155 (94%)	9 (6%)	0	100	100
1	FV	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	FW	164/166 (99%)	159 (97%)	5 (3%)	0	100	100
1	FX	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	FY	164/166 (99%)	157 (96%)	7 (4%)	0	100	100
1	FZ	164/166 (99%)	162 (99%)	2 (1%)	0	100	100
1	GA	164/166 (99%)	156 (95%)	8 (5%)	0	100	100
1	GB	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	GC	164/166 (99%)	159 (97%)	5 (3%)	0	100	100
1	GD	164/166 (99%)	164 (100%)	0	0	100	100
1	GE	164/166 (99%)	164 (100%)	0	0	100	100
1	GF	164/166 (99%)	164 (100%)	0	0	100	100
1	GG	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	GH	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	GI	164/166 (99%)	164 (100%)	0	0	100	100
1	GJ	164/166 (99%)	164 (100%)	0	0	100	100
1	GK	164/166 (99%)	164 (100%)	0	0	100	100
1	GL	164/166 (99%)	164 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	GM	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	GN	164/166 (99%)	160 (98%)	4 (2%)	0	100	100
1	GO	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	GP	164/166 (99%)	155 (94%)	9 (6%)	0	100	100
1	GQ	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	GR	164/166 (99%)	159 (97%)	5 (3%)	0	100	100
1	GS	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	GT	164/166 (99%)	157 (96%)	7 (4%)	0	100	100
1	GU	164/166 (99%)	162 (99%)	2 (1%)	0	100	100
1	GV	164/166 (99%)	156 (95%)	8 (5%)	0	100	100
1	GW	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	GX	164/166 (99%)	158 (96%)	6 (4%)	0	100	100
1	GY	164/166 (99%)	164 (100%)	0	0	100	100
1	GZ	164/166 (99%)	164 (100%)	0	0	100	100
1	HA	164/166 (99%)	164 (100%)	0	0	100	100
1	HB	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	HC	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	HD	164/166 (99%)	164 (100%)	0	0	100	100
1	HE	164/166 (99%)	164 (100%)	0	0	100	100
1	HF	164/166 (99%)	164 (100%)	0	0	100	100
1	HG	164/166 (99%)	164 (100%)	0	0	100	100
1	HH	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	HI	164/166 (99%)	160 (98%)	4 (2%)	0	100	100
1	HJ	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	HK	164/166 (99%)	155 (94%)	9 (6%)	0	100	100
1	HL	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	HM	164/166 (99%)	159 (97%)	5 (3%)	0	100	100
1	HN	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	HO	164/166 (99%)	157 (96%)	7 (4%)	0	100	100
1	HP	164/166 (99%)	162 (99%)	2 (1%)	0	100	100
1	HQ	164/166 (99%)	156 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	HR	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	HS	164/166 (99%)	159 (97%)	5 (3%)	0	100	100
1	HT	164/166 (99%)	164 (100%)	0	0	100	100
1	HU	164/166 (99%)	164 (100%)	0	0	100	100
1	HV	164/166 (99%)	164 (100%)	0	0	100	100
1	HW	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	HX	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	HY	164/166 (99%)	164 (100%)	0	0	100	100
1	HZ	164/166 (99%)	164 (100%)	0	0	100	100
1	IA	164/166 (99%)	164 (100%)	0	0	100	100
1	IB	164/166 (99%)	164 (100%)	0	0	100	100
All	All	34440/34860 (99%)	33906 (98%)	532 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CB	106	GLY
1	EM	106	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	AB	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	AC	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	AD	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	AE	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	AF	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	AG	147/147 (100%)	145 (99%)	2 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AH	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	AI	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	AJ	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	AK	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	AL	147/147 (100%)	144 (98%)	3 (2%)	55	79
1	AM	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	AN	147/147 (100%)	147 (100%)	0	100	100
1	AO	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	AP	147/147 (100%)	147 (100%)	0	100	100
1	AQ	147/147 (100%)	147 (100%)	0	100	100
1	AR	147/147 (100%)	147 (100%)	0	100	100
1	AS	147/147 (100%)	147 (100%)	0	100	100
1	AT	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	AU	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	AV	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	AW	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	AX	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	AY	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	AZ	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	BA	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	BB	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	BC	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	BD	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	BE	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	BF	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	BG	147/147 (100%)	144 (98%)	3 (2%)	55	79
1	BH	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	BI	147/147 (100%)	147 (100%)	0	100	100
1	BJ	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	BK	147/147 (100%)	147 (100%)	0	100	100
1	BL	147/147 (100%)	147 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BM	147/147 (100%)	147 (100%)	0	100	100
1	BN	147/147 (100%)	147 (100%)	0	100	100
1	BO	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	BP	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	BQ	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	BR	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	BS	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	BT	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	BU	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	BV	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	BW	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	BX	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	BY	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	BZ	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	CA	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	CB	147/147 (100%)	144 (98%)	3 (2%)	55	79
1	CC	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	CD	147/147 (100%)	147 (100%)	0	100	100
1	CE	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	CF	147/147 (100%)	147 (100%)	0	100	100
1	CG	147/147 (100%)	147 (100%)	0	100	100
1	CH	147/147 (100%)	147 (100%)	0	100	100
1	CI	147/147 (100%)	147 (100%)	0	100	100
1	CJ	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	CK	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	CL	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	CM	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	CN	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	CO	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	CP	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	CQ	147/147 (100%)	146 (99%)	1 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CR	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	CS	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	CT	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	CU	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	CV	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	CW	147/147 (100%)	144 (98%)	3 (2%)	55	79
1	CX	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	CY	147/147 (100%)	147 (100%)	0	100	100
1	CZ	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	DA	147/147 (100%)	147 (100%)	0	100	100
1	DB	147/147 (100%)	147 (100%)	0	100	100
1	DC	147/147 (100%)	147 (100%)	0	100	100
1	DD	147/147 (100%)	147 (100%)	0	100	100
1	DE	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	DF	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	DG	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	DH	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	DI	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	DJ	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	DK	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	DL	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	DM	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	DN	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	DO	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	DP	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	DQ	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	DR	147/147 (100%)	144 (98%)	3 (2%)	55	79
1	DS	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	DT	147/147 (100%)	147 (100%)	0	100	100
1	DU	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	DV	147/147 (100%)	147 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DW	147/147 (100%)	147 (100%)	0	100	100
1	DX	147/147 (100%)	147 (100%)	0	100	100
1	DY	147/147 (100%)	147 (100%)	0	100	100
1	DZ	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	EA	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	EB	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	EC	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	ED	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	EE	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	EF	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	EG	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	EH	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	EI	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	EJ	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	EK	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	EL	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	EM	147/147 (100%)	144 (98%)	3 (2%)	55	79
1	EN	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	EO	147/147 (100%)	147 (100%)	0	100	100
1	EP	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	EQ	147/147 (100%)	147 (100%)	0	100	100
1	ER	147/147 (100%)	147 (100%)	0	100	100
1	ES	147/147 (100%)	147 (100%)	0	100	100
1	ET	147/147 (100%)	147 (100%)	0	100	100
1	EU	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	EV	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	EW	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	EX	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	EY	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	EZ	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	FA	147/147 (100%)	146 (99%)	1 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FB	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	FC	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	FD	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	FE	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	FF	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	FG	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	FH	147/147 (100%)	144 (98%)	3 (2%)	55	79
1	FI	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	FJ	147/147 (100%)	147 (100%)	0	100	100
1	FK	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	FL	147/147 (100%)	147 (100%)	0	100	100
1	FM	147/147 (100%)	147 (100%)	0	100	100
1	FN	147/147 (100%)	147 (100%)	0	100	100
1	FO	147/147 (100%)	147 (100%)	0	100	100
1	FP	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	FQ	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	FR	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	FS	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	FT	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	FU	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	FV	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	FW	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	FX	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	FY	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	FZ	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	GA	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	GB	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	GC	147/147 (100%)	144 (98%)	3 (2%)	55	79
1	GD	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	GE	147/147 (100%)	147 (100%)	0	100	100
1	GF	147/147 (100%)	145 (99%)	2 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GG	147/147 (100%)	147 (100%)	0	100	100
1	GH	147/147 (100%)	147 (100%)	0	100	100
1	GI	147/147 (100%)	147 (100%)	0	100	100
1	GJ	147/147 (100%)	147 (100%)	0	100	100
1	GK	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	GL	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	GM	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	GN	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	GO	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	GP	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	GQ	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	GR	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	GS	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	GT	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	GU	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	GV	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	GW	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	GX	147/147 (100%)	144 (98%)	3 (2%)	55	79
1	GY	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	GZ	147/147 (100%)	147 (100%)	0	100	100
1	HA	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	HB	147/147 (100%)	147 (100%)	0	100	100
1	HC	147/147 (100%)	147 (100%)	0	100	100
1	HD	147/147 (100%)	147 (100%)	0	100	100
1	HE	147/147 (100%)	147 (100%)	0	100	100
1	HF	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	HG	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	HH	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	HI	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	HJ	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	HK	147/147 (100%)	146 (99%)	1 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	HL	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	HM	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	HN	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	HO	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	HP	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	HQ	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	HR	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	HS	147/147 (100%)	144 (98%)	3 (2%)	55	79
1	HT	147/147 (100%)	146 (99%)	1 (1%)	84	93
1	HU	147/147 (100%)	147 (100%)	0	100	100
1	HV	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	HW	147/147 (100%)	147 (100%)	0	100	100
1	HX	147/147 (100%)	147 (100%)	0	100	100
1	HY	147/147 (100%)	147 (100%)	0	100	100
1	HZ	147/147 (100%)	147 (100%)	0	100	100
1	IA	147/147 (100%)	145 (99%)	2 (1%)	67	85
1	IB	147/147 (100%)	145 (99%)	2 (1%)	67	85
All	All	30870/30870 (100%)	30610 (99%)	260 (1%)	81	91

5 of 260 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	HF	113	CYS
1	HK	75	ASN
1	CX	109	VAL
1	CW	72	ASN
1	HO	75	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
1	EX	75	ASN
1	GL	144	GLN
1	EZ	144	GLN
1	FS	144	GLN

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Mol	Chain	Res	Type
1	GT	144	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides 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.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	166/166 (100%)	-0.16	2 (1%) 79 66	76, 102, 127, 158	0
1	AB	166/166 (100%)	-0.19	0 100 100	80, 103, 133, 171	0
1	AC	166/166 (100%)	-0.30	0 100 100	77, 99, 128, 154	0
1	AD	166/166 (100%)	-0.24	1 (0%) 89 81	76, 101, 136, 166	0
1	AE	166/166 (100%)	-0.34	1 (0%) 89 81	75, 99, 125, 158	0
1	AF	166/166 (100%)	-0.26	2 (1%) 79 66	75, 100, 137, 171	0
1	AG	166/166 (100%)	-0.10	0 100 100	75, 98, 123, 150	0
1	AH	166/166 (100%)	-0.11	1 (0%) 89 81	75, 97, 135, 166	0
1	AI	166/166 (100%)	-0.20	0 100 100	76, 97, 123, 140	0
1	AJ	166/166 (100%)	-0.20	3 (1%) 68 53	76, 97, 127, 170	0
1	AK	166/166 (100%)	-0.22	1 (0%) 89 81	76, 96, 121, 156	0
1	AL	166/166 (100%)	-0.18	1 (0%) 89 81	76, 97, 133, 170	0
1	AM	166/166 (100%)	-0.16	0 100 100	78, 105, 138, 151	0
1	AN	166/166 (100%)	-0.18	2 (1%) 79 66	81, 104, 137, 156	0
1	AO	166/166 (100%)	-0.20	0 100 100	80, 100, 136, 151	0
1	AP	166/166 (100%)	-0.25	0 100 100	75, 103, 133, 149	0
1	AQ	166/166 (100%)	-0.23	0 100 100	76, 101, 138, 162	0
1	AR	166/166 (100%)	-0.21	0 100 100	77, 100, 138, 153	0
1	AS	166/166 (100%)	-0.06	5 (3%) 50 34	76, 97, 138, 150	0
1	AT	166/166 (100%)	-0.16	1 (0%) 89 81	76, 98, 134, 178	0
1	AU	166/166 (100%)	0.21	3 (1%) 68 53	79, 100, 130, 148	0
1	AV	166/166 (100%)	-0.13	0 100 100	76, 102, 127, 158	0
1	AW	166/166 (100%)	-0.20	0 100 100	80, 103, 133, 171	0
1	AX	166/166 (100%)	-0.24	0 100 100	77, 99, 128, 154	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AY	166/166 (100%)	-0.15	3 (1%) 68 53	76, 101, 136, 166	0
1	AZ	166/166 (100%)	-0.32	0 100 100	75, 99, 125, 158	0
1	BA	166/166 (100%)	-0.22	0 100 100	75, 100, 137, 171	0
1	BB	166/166 (100%)	-0.36	0 100 100	75, 98, 123, 150	0
1	BC	166/166 (100%)	-0.26	0 100 100	75, 97, 135, 166	0
1	BD	166/166 (100%)	-0.22	0 100 100	76, 97, 123, 140	0
1	BE	166/166 (100%)	-0.22	0 100 100	76, 97, 127, 170	0
1	BF	166/166 (100%)	-0.31	0 100 100	76, 96, 121, 156	0
1	BG	166/166 (100%)	-0.27	0 100 100	76, 97, 133, 170	0
1	BH	166/166 (100%)	-0.05	2 (1%) 79 66	78, 105, 138, 151	0
1	BI	166/166 (100%)	-0.07	1 (0%) 89 81	81, 104, 137, 156	0
1	BJ	166/166 (100%)	-0.15	1 (0%) 89 81	80, 100, 136, 151	0
1	BK	166/166 (100%)	-0.21	3 (1%) 68 53	75, 103, 133, 149	0
1	BL	166/166 (100%)	-0.20	1 (0%) 89 81	76, 101, 138, 162	0
1	BM	166/166 (100%)	-0.13	3 (1%) 68 53	77, 100, 138, 153	0
1	BN	166/166 (100%)	-0.20	3 (1%) 68 53	76, 97, 138, 150	0
1	BO	166/166 (100%)	-0.24	1 (0%) 89 81	76, 98, 134, 178	0
1	BP	166/166 (100%)	-0.08	0 100 100	79, 100, 130, 148	0
1	BQ	166/166 (100%)	-0.16	0 100 100	76, 102, 127, 158	0
1	BR	166/166 (100%)	-0.25	0 100 100	80, 103, 133, 171	0
1	BS	166/166 (100%)	-0.18	0 100 100	77, 99, 128, 154	0
1	BT	166/166 (100%)	-0.27	0 100 100	76, 101, 136, 166	0
1	BU	166/166 (100%)	-0.15	0 100 100	75, 99, 125, 158	0
1	BV	166/166 (100%)	-0.18	0 100 100	75, 100, 137, 171	0
1	BW	166/166 (100%)	-0.27	0 100 100	75, 98, 123, 150	0
1	BX	166/166 (100%)	-0.19	0 100 100	75, 97, 135, 166	0
1	BY	166/166 (100%)	-0.19	1 (0%) 89 81	76, 97, 123, 140	0
1	BZ	166/166 (100%)	-0.27	0 100 100	76, 97, 127, 170	0
1	CA	166/166 (100%)	-0.28	0 100 100	76, 96, 121, 156	0
1	CB	166/166 (100%)	-0.23	0 100 100	76, 97, 133, 170	0
1	CC	166/166 (100%)	-0.16	1 (0%) 89 81	78, 105, 138, 151	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	CD	166/166 (100%)	-0.20	0 100 100	81, 104, 137, 156	0
1	CE	166/166 (100%)	-0.25	0 100 100	80, 100, 136, 151	0
1	CF	166/166 (100%)	-0.17	1 (0%) 89 81	75, 103, 133, 149	0
1	CG	166/166 (100%)	-0.17	1 (0%) 89 81	76, 101, 138, 162	0
1	CH	166/166 (100%)	-0.07	1 (0%) 89 81	77, 100, 138, 153	0
1	CI	166/166 (100%)	-0.06	3 (1%) 68 53	76, 97, 138, 150	0
1	CJ	166/166 (100%)	-0.14	1 (0%) 89 81	76, 98, 134, 178	0
1	CK	166/166 (100%)	-0.10	0 100 100	79, 100, 130, 148	0
1	CL	166/166 (100%)	-0.04	3 (1%) 68 53	76, 102, 127, 158	0
1	CM	166/166 (100%)	-0.12	0 100 100	80, 103, 133, 171	0
1	CN	166/166 (100%)	-0.26	0 100 100	77, 99, 128, 154	0
1	CO	166/166 (100%)	-0.20	1 (0%) 89 81	76, 101, 136, 166	0
1	CP	166/166 (100%)	-0.30	0 100 100	75, 99, 125, 158	0
1	CQ	166/166 (100%)	-0.20	0 100 100	75, 100, 137, 171	0
1	CR	166/166 (100%)	-0.28	0 100 100	75, 98, 123, 150	0
1	CS	166/166 (100%)	-0.27	1 (0%) 89 81	75, 97, 135, 166	0
1	CT	166/166 (100%)	-0.19	0 100 100	76, 97, 123, 140	0
1	CU	166/166 (100%)	-0.27	0 100 100	76, 97, 127, 170	0
1	CV	166/166 (100%)	-0.21	0 100 100	76, 96, 121, 156	0
1	CW	166/166 (100%)	-0.17	0 100 100	76, 97, 133, 170	0
1	CX	166/166 (100%)	-0.20	1 (0%) 89 81	78, 105, 138, 151	0
1	CY	166/166 (100%)	-0.18	0 100 100	81, 104, 137, 156	0
1	CZ	166/166 (100%)	-0.19	1 (0%) 89 81	80, 100, 136, 151	0
1	DA	166/166 (100%)	-0.29	1 (0%) 89 81	75, 103, 133, 149	0
1	DB	166/166 (100%)	-0.17	0 100 100	76, 101, 138, 162	0
1	DC	166/166 (100%)	-0.12	1 (0%) 89 81	77, 100, 138, 153	0
1	DD	166/166 (100%)	-0.15	1 (0%) 89 81	76, 97, 138, 150	0
1	DE	166/166 (100%)	-0.10	2 (1%) 79 66	76, 98, 134, 178	0
1	DF	166/166 (100%)	-0.06	0 100 100	79, 100, 130, 148	0
1	DG	166/166 (100%)	-0.25	1 (0%) 89 81	76, 102, 127, 158	0
1	DH	166/166 (100%)	-0.26	2 (1%) 79 66	80, 103, 133, 171	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	DI	166/166 (100%)	-0.17	1 (0%) 89 81	77, 99, 128, 154	0
1	DJ	166/166 (100%)	-0.06	0 100 100	76, 101, 136, 166	0
1	DK	166/166 (100%)	-0.30	0 100 100	75, 99, 125, 158	0
1	DL	166/166 (100%)	-0.24	0 100 100	75, 100, 137, 171	0
1	DM	166/166 (100%)	-0.18	1 (0%) 89 81	75, 98, 123, 150	0
1	DN	166/166 (100%)	-0.16	1 (0%) 89 81	75, 97, 135, 166	0
1	DO	166/166 (100%)	-0.12	0 100 100	76, 97, 123, 140	0
1	DP	166/166 (100%)	-0.13	1 (0%) 89 81	76, 97, 127, 170	0
1	DQ	166/166 (100%)	-0.28	1 (0%) 89 81	76, 96, 121, 156	0
1	DR	166/166 (100%)	-0.26	0 100 100	76, 97, 133, 170	0
1	DS	166/166 (100%)	0.08	4 (2%) 59 42	78, 105, 138, 151	0
1	DT	166/166 (100%)	-0.04	2 (1%) 79 66	81, 104, 137, 156	0
1	DU	166/166 (100%)	-0.22	0 100 100	80, 100, 136, 151	0
1	DV	166/166 (100%)	-0.17	1 (0%) 89 81	75, 103, 133, 149	0
1	DW	166/166 (100%)	-0.14	1 (0%) 89 81	76, 101, 138, 162	0
1	DX	166/166 (100%)	-0.09	1 (0%) 89 81	77, 100, 138, 153	0
1	DY	166/166 (100%)	-0.14	1 (0%) 89 81	76, 97, 138, 150	0
1	DZ	166/166 (100%)	-0.27	1 (0%) 89 81	76, 98, 134, 178	0
1	EA	166/166 (100%)	-0.20	0 100 100	79, 100, 130, 148	0
1	EB	166/166 (100%)	-0.24	0 100 100	76, 102, 127, 158	0
1	EC	166/166 (100%)	-0.18	0 100 100	80, 103, 133, 171	0
1	ED	166/166 (100%)	-0.22	2 (1%) 79 66	77, 99, 128, 154	0
1	EE	166/166 (100%)	-0.33	0 100 100	76, 101, 136, 166	0
1	EF	166/166 (100%)	-0.35	1 (0%) 89 81	75, 99, 125, 158	0
1	EG	166/166 (100%)	-0.25	0 100 100	75, 100, 137, 171	0
1	EH	166/166 (100%)	-0.26	0 100 100	75, 98, 123, 150	0
1	EI	166/166 (100%)	-0.13	0 100 100	75, 97, 135, 166	0
1	EJ	166/166 (100%)	-0.18	0 100 100	76, 97, 123, 140	0
1	EK	166/166 (100%)	-0.11	0 100 100	76, 97, 127, 170	0
1	EL	166/166 (100%)	-0.22	1 (0%) 89 81	76, 96, 121, 156	0
1	EM	166/166 (100%)	-0.23	1 (0%) 89 81	76, 97, 133, 170	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	EN	166/166 (100%)	-0.17	1 (0%) 89 81	78, 105, 138, 151	0
1	EO	166/166 (100%)	-0.21	1 (0%) 89 81	81, 104, 137, 156	0
1	EP	166/166 (100%)	-0.26	1 (0%) 89 81	80, 100, 136, 151	0
1	EQ	166/166 (100%)	-0.16	1 (0%) 89 81	75, 103, 133, 149	0
1	ER	166/166 (100%)	-0.22	1 (0%) 89 81	76, 101, 138, 162	0
1	ES	166/166 (100%)	-0.27	0 100 100	77, 100, 138, 153	0
1	ET	166/166 (100%)	-0.05	2 (1%) 79 66	76, 97, 138, 150	0
1	EU	166/166 (100%)	-0.16	2 (1%) 79 66	76, 98, 134, 178	0
1	EV	166/166 (100%)	-0.09	0 100 100	79, 100, 130, 148	0
1	EW	166/166 (100%)	-0.22	1 (0%) 89 81	76, 102, 127, 158	0
1	EX	166/166 (100%)	-0.14	2 (1%) 79 66	80, 103, 133, 171	0
1	EY	166/166 (100%)	-0.29	1 (0%) 89 81	77, 99, 128, 154	0
1	EZ	166/166 (100%)	-0.20	1 (0%) 89 81	76, 101, 136, 166	0
1	FA	166/166 (100%)	-0.30	0 100 100	75, 99, 125, 158	0
1	FB	166/166 (100%)	-0.29	0 100 100	75, 100, 137, 171	0
1	FC	166/166 (100%)	-0.28	0 100 100	75, 98, 123, 150	0
1	FD	166/166 (100%)	-0.35	0 100 100	75, 97, 135, 166	0
1	FE	166/166 (100%)	-0.26	0 100 100	76, 97, 123, 140	0
1	FF	166/166 (100%)	-0.18	0 100 100	76, 97, 127, 170	0
1	FG	166/166 (100%)	-0.29	0 100 100	76, 96, 121, 156	0
1	FH	166/166 (100%)	-0.31	0 100 100	76, 97, 133, 170	0
1	FI	166/166 (100%)	-0.10	1 (0%) 89 81	78, 105, 138, 151	0
1	FJ	166/166 (100%)	0.04	4 (2%) 59 42	81, 104, 137, 156	0
1	FK	166/166 (100%)	-0.22	1 (0%) 89 81	80, 100, 136, 151	0
1	FL	166/166 (100%)	-0.23	0 100 100	75, 103, 133, 149	0
1	FM	166/166 (100%)	-0.16	3 (1%) 68 53	76, 101, 138, 162	0
1	FN	166/166 (100%)	-0.22	1 (0%) 89 81	77, 100, 138, 153	0
1	FO	166/166 (100%)	-0.17	2 (1%) 79 66	76, 97, 138, 150	0
1	FP	166/166 (100%)	-0.19	1 (0%) 89 81	76, 98, 134, 178	0
1	FQ	166/166 (100%)	-0.23	0 100 100	79, 100, 130, 148	0
1	FR	166/166 (100%)	-0.23	0 100 100	76, 102, 127, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	FS	166/166 (100%)	-0.18	1 (0%) 89 81	80, 103, 133, 171	0
1	FT	166/166 (100%)	-0.14	0 100 100	77, 99, 128, 154	0
1	FU	166/166 (100%)	-0.17	2 (1%) 79 66	76, 101, 136, 166	0
1	FV	166/166 (100%)	-0.07	1 (0%) 89 81	75, 99, 125, 158	0
1	FW	166/166 (100%)	-0.24	0 100 100	75, 100, 137, 171	0
1	FX	166/166 (100%)	-0.35	0 100 100	75, 98, 123, 150	0
1	FY	166/166 (100%)	-0.22	2 (1%) 79 66	75, 97, 135, 166	0
1	FZ	166/166 (100%)	-0.26	0 100 100	76, 97, 123, 140	0
1	GA	166/166 (100%)	-0.12	0 100 100	76, 97, 127, 170	0
1	GB	166/166 (100%)	-0.22	0 100 100	76, 96, 121, 156	0
1	GC	166/166 (100%)	-0.18	1 (0%) 89 81	76, 97, 133, 170	0
1	GD	166/166 (100%)	-0.24	1 (0%) 89 81	78, 105, 138, 151	0
1	GE	166/166 (100%)	-0.24	0 100 100	81, 104, 137, 156	0
1	GF	166/166 (100%)	-0.24	2 (1%) 79 66	80, 100, 136, 151	0
1	GG	166/166 (100%)	-0.20	4 (2%) 59 42	75, 103, 133, 149	0
1	GH	166/166 (100%)	-0.19	1 (0%) 89 81	76, 101, 138, 162	0
1	GI	166/166 (100%)	-0.21	0 100 100	77, 100, 138, 153	0
1	GJ	166/166 (100%)	0.09	2 (1%) 79 66	76, 97, 138, 150	0
1	GK	166/166 (100%)	0.08	2 (1%) 79 66	76, 98, 134, 178	0
1	GL	166/166 (100%)	-0.05	1 (0%) 89 81	79, 100, 130, 148	0
1	GM	166/166 (100%)	-0.08	1 (0%) 89 81	76, 102, 127, 158	0
1	GN	166/166 (100%)	-0.14	2 (1%) 79 66	80, 103, 133, 171	0
1	GO	166/166 (100%)	-0.28	0 100 100	77, 99, 128, 154	0
1	GP	166/166 (100%)	-0.20	2 (1%) 79 66	76, 101, 136, 166	0
1	GQ	166/166 (100%)	-0.18	1 (0%) 89 81	75, 99, 125, 158	0
1	GR	166/166 (100%)	-0.26	0 100 100	75, 100, 137, 171	0
1	GS	166/166 (100%)	-0.28	0 100 100	75, 98, 123, 150	0
1	GT	166/166 (100%)	-0.15	2 (1%) 79 66	75, 97, 135, 166	0
1	GU	166/166 (100%)	-0.23	0 100 100	76, 97, 123, 140	0
1	GV	166/166 (100%)	-0.20	0 100 100	76, 97, 127, 170	0
1	GW	166/166 (100%)	-0.15	1 (0%) 89 81	76, 96, 121, 156	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	GX	166/166 (100%)	-0.17	0 100 100	76, 97, 133, 170	0
1	GY	166/166 (100%)	-0.16	2 (1%) 79 66	78, 105, 138, 151	0
1	GZ	166/166 (100%)	-0.17	1 (0%) 89 81	81, 104, 137, 156	0
1	HA	166/166 (100%)	-0.16	0 100 100	80, 100, 136, 151	0
1	HB	166/166 (100%)	-0.22	3 (1%) 68 53	75, 103, 133, 149	0
1	HC	166/166 (100%)	-0.07	1 (0%) 89 81	76, 101, 138, 162	0
1	HD	166/166 (100%)	-0.10	1 (0%) 89 81	77, 100, 138, 153	0
1	HE	166/166 (100%)	-0.02	5 (3%) 50 34	76, 97, 138, 150	0
1	HF	166/166 (100%)	-0.02	4 (2%) 59 42	76, 98, 134, 178	0
1	HG	166/166 (100%)	0.04	0 100 100	79, 100, 130, 148	0
1	HH	166/166 (100%)	-0.23	0 100 100	76, 102, 127, 158	0
1	HI	166/166 (100%)	-0.23	0 100 100	80, 103, 133, 171	0
1	HJ	166/166 (100%)	-0.20	0 100 100	77, 99, 128, 154	0
1	HK	166/166 (100%)	-0.16	2 (1%) 79 66	76, 101, 136, 166	0
1	HL	166/166 (100%)	-0.37	1 (0%) 89 81	75, 99, 125, 158	0
1	HM	166/166 (100%)	-0.27	1 (0%) 89 81	75, 100, 137, 171	0
1	HN	166/166 (100%)	-0.29	2 (1%) 79 66	75, 98, 123, 150	0
1	HO	166/166 (100%)	-0.22	2 (1%) 79 66	75, 97, 135, 166	0
1	HP	166/166 (100%)	-0.23	0 100 100	76, 97, 123, 140	0
1	HQ	166/166 (100%)	-0.17	2 (1%) 79 66	76, 97, 127, 170	0
1	HR	166/166 (100%)	-0.30	1 (0%) 89 81	76, 96, 121, 156	0
1	HS	166/166 (100%)	-0.35	0 100 100	76, 97, 133, 170	0
1	HT	166/166 (100%)	-0.04	6 (3%) 42 28	78, 105, 138, 151	0
1	HU	166/166 (100%)	-0.10	2 (1%) 79 66	81, 104, 137, 156	0
1	HV	166/166 (100%)	-0.19	0 100 100	80, 100, 136, 151	0
1	HW	166/166 (100%)	-0.14	2 (1%) 79 66	75, 103, 133, 149	0
1	HX	166/166 (100%)	-0.14	1 (0%) 89 81	76, 101, 138, 162	0
1	HY	166/166 (100%)	-0.21	4 (2%) 59 42	77, 100, 138, 153	0
1	HZ	166/166 (100%)	-0.20	3 (1%) 68 53	76, 97, 138, 150	0
1	IA	166/166 (100%)	-0.21	2 (1%) 79 66	76, 98, 134, 178	0
1	IB	166/166 (100%)	-0.24	0 100 100	79, 100, 130, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	34860/34860 (100%)	-0.19	190 (0%) 91 83	75, 100, 135, 178	0

The worst 5 of 190 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	EU	37	GLN	5.2
1	DE	37	GLN	5.0
1	CF	37	GLN	4.8
1	GJ	37	GLN	4.7
1	FO	37	GLN	4.6

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.