



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:47 AM UTC

PDB ID : 7JOQ / pdb_00007joq
Title : Structure of NV1 small terminase
Authors : Cingolani, G.; Lokareddy, R.
Deposited on : 2020-08-07
Resolution : 3.95 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

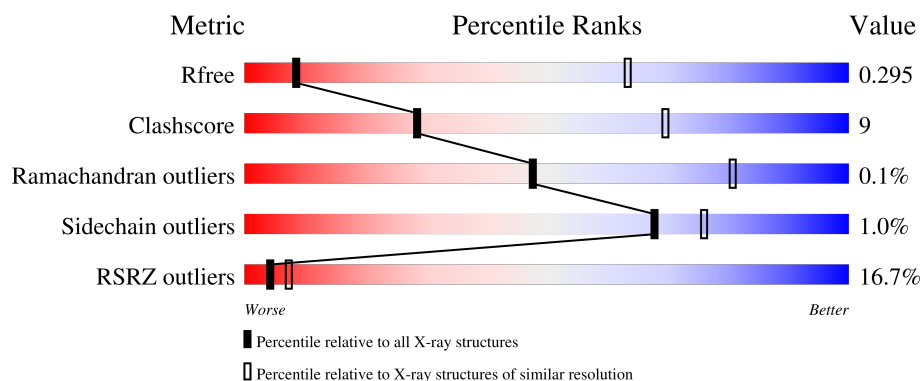
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.95 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.



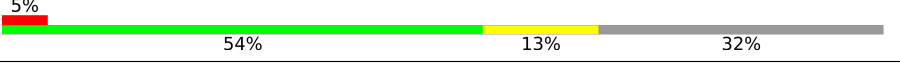
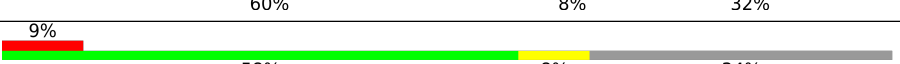
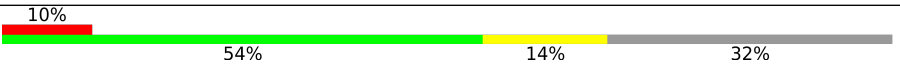
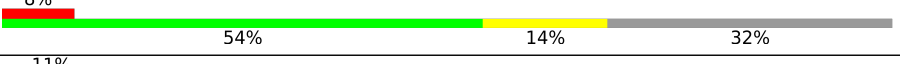
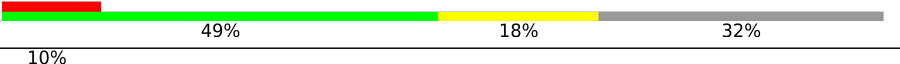
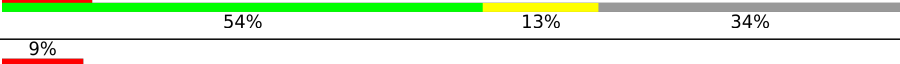
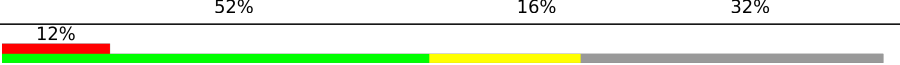
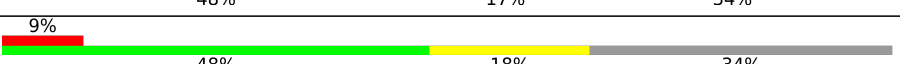
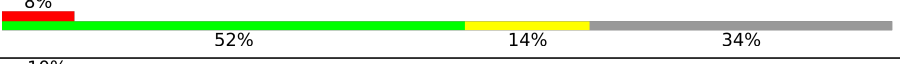
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	0	157	11% 55% 13% 32%
1	1	157	9% 56% 10% 34%
1	2	157	8% 53% 15% 32%
1	3	157	15% 52% 16% 32%
1	4	157	11% 48% 18% 34%

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Mol	Chain	Length	Quality of chain
1	5	157	
1	6	157	
1	7	157	
1	8	157	
1	9	157	
1	A	157	
1	AA	157	
1	AB	157	
1	AC	157	
1	AD	157	
1	AE	157	
1	AF	157	
1	AG	157	
1	AH	157	
1	AI	157	
1	AJ	157	
1	B	157	
1	C	157	
1	D	157	
1	E	157	
1	F	157	
1	G	157	
1	H	157	
1	I	157	
1	J	157	

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Mol	Chain	Length	Quality of chain
1	K	157	11% 52% 15% 32%
1	L	157	11% 49% 17% 34%
1	M	157	15% 58% 10% 32%
1	N	157	11% 50% 18% 32%
1	O	157	11% 55% 11% 34%
1	P	157	16% 52% 15% 32%
1	Q	157	15% 52% 16% 32%
1	R	157	8% 54% 11% 34%
1	S	157	10% 51% 17% 32%
1	T	157	9% 55% 13% 32%
1	U	157	20% 52% 13% 34%
1	V	157	11% 55% 12% 32%
1	W	157	12% 58% 10% 32%
1	X	157	13% 56% 11% 33%
1	Y	157	7% 54% 13% 32%
1	Z	157	6% 53% 15% 32%
1	a	157	6% 54% 11% 34%
1	b	157	13% 55% 13% 32%
1	c	157	10% 52% 15% 32%
1	d	157	15% 55% 11% 34%
1	e	157	11% 57% 11% 32%
1	ee	157	17% 56% 12% 32%
1	f	157	11% 58% 10% 32%
1	ff	157	15% 48% 20% 32%
1	g	157	14% 54% 12% 34%

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Mol	Chain	Length	Quality of chain
1	gg	157	
1	h	157	
1	hh	157	
1	i	157	
1	ii	157	
1	j	157	
1	jj	157	
1	k	157	
1	kk	157	
1	l	157	
1	ll	157	
1	m	157	
1	mm	157	
1	n	157	
1	o	157	
1	p	157	
1	q	157	
1	r	157	
1	s	157	
1	t	157	
1	u	157	
1	v	157	
1	w	157	
1	x	157	
1	y	157	

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Mol	Chain	Length	Quality of chain
1	z	157	10% 48% 20% 32%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 62617 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 Small Terminase subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	107	Total	C	N	O	S	0	0	0
			788	498	142	147	1			
1	A	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	B	103	Total	C	N	O	S	0	0	0
			759	478	138	142	1			
1	C	106	Total	C	N	O	S	0	0	0
			776	489	141	145	1			
1	D	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	E	104	Total	C	N	O	S	0	0	0
			766	483	139	143	1			
1	F	106	Total	C	N	O	S	0	0	0
			776	489	141	145	1			
1	G	105	Total	C	N	O	S	0	0	0
			773	487	140	145	1			
1	H	103	Total	C	N	O	S	0	0	0
			755	475	137	142	1			
1	J	107	Total	C	N	O	S	0	0	0
			788	498	142	147	1			
1	K	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	L	103	Total	C	N	O	S	0	0	0
			759	478	138	142	1			
1	M	106	Total	C	N	O	S	0	0	0
			776	489	141	145	1			
1	N	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	O	104	Total	C	N	O	S	0	0	0
			766	483	139	143	1			
1	P	106	Total	C	N	O	S	0	0	0
			776	489	141	145	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	106	Total	C	N	O	S	0	0	0
			781	493	141	146	1			
1	R	103	Total	C	N	O	S	0	0	0
			755	475	137	142	1			
1	S	107	Total	C	N	O	S	0	0	0
			788	498	142	147	1			
1	T	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	U	103	Total	C	N	O	S	0	0	0
			759	478	138	142	1			
1	V	106	Total	C	N	O	S	0	0	0
			776	489	141	145	1			
1	W	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	X	105	Total	C	N	O	S	0	0	0
			771	486	140	144	1			
1	Y	106	Total	C	N	O	S	0	0	0
			776	489	141	145	1			
1	Z	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	a	103	Total	C	N	O	S	0	0	0
			755	475	137	142	1			
1	b	107	Total	C	N	O	S	0	0	0
			788	498	142	147	1			
1	c	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	d	103	Total	C	N	O	S	0	0	0
			759	478	138	142	1			
1	e	106	Total	C	N	O	S	0	0	0
			776	489	141	145	1			
1	f	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	g	104	Total	C	N	O	S	0	0	0
			766	483	139	143	1			
1	h	106	Total	C	N	O	S	0	0	0
			776	489	141	145	1			
1	i	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	j	103	Total	C	N	O	S	0	0	0
			755	475	137	142	1			
1	k	107	Total	C	N	O	S	0	0	0
			788	498	142	147	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	l	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	m	103	Total	C	N	O	S	0	0	0
			759	478	138	142	1			
1	n	106	Total	C	N	O	S	0	0	0
			776	489	141	145	1			
1	o	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	p	105	Total	C	N	O	S	0	0	0
			771	486	140	144	1			
1	q	106	Total	C	N	O	S	0	0	0
			776	489	141	145	1			
1	r	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	s	103	Total	C	N	O	S	0	0	0
			755	475	137	142	1			
1	t	107	Total	C	N	O	S	0	0	0
			788	498	142	147	1			
1	u	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	v	103	Total	C	N	O	S	0	0	0
			759	478	138	142	1			
1	w	106	Total	C	N	O	S	0	0	0
			776	489	141	145	1			
1	x	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	y	104	Total	C	N	O	S	0	0	0
			766	483	139	143	1			
1	z	106	Total	C	N	O	S	0	0	0
			776	489	141	145	1			
1	0	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	1	103	Total	C	N	O	S	0	0	0
			755	475	137	142	1			
1	2	107	Total	C	N	O	S	0	0	0
			788	498	142	147	1			
1	3	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	4	103	Total	C	N	O	S	0	0	0
			759	478	138	142	1			
1	5	106	Total	C	N	O	S	0	0	0
			776	489	141	145	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	6	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	7	104	Total	C	N	O	S	0	0	0
			766	483	139	143	1			
1	8	106	Total	C	N	O	S	0	0	0
			776	489	141	145	1			
1	9	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	AA	103	Total	C	N	O	S	0	0	0
			755	475	137	142	1			
1	AB	107	Total	C	N	O	S	0	0	0
			788	498	142	147	1			
1	AC	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	AD	103	Total	C	N	O	S	0	0	0
			759	478	138	142	1			
1	AE	106	Total	C	N	O	S	0	0	0
			776	489	141	145	1			
1	AF	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	AG	104	Total	C	N	O	S	0	0	0
			766	483	139	143	1			
1	AH	106	Total	C	N	O	S	0	0	0
			776	489	141	145	1			
1	AI	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	AJ	103	Total	C	N	O	S	0	0	0
			755	475	137	142	1			
1	ee	107	Total	C	N	O	S	0	0	0
			788	498	142	147	1			
1	ff	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	gg	103	Total	C	N	O	S	0	0	0
			759	478	138	142	1			
1	hh	106	Total	C	N	O	S	0	0	0
			776	489	141	145	1			
1	ii	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	jj	104	Total	C	N	O	S	0	0	0
			764	481	139	143	1			
1	kk	106	Total	C	N	O	S	0	0	0
			776	489	141	145	1			

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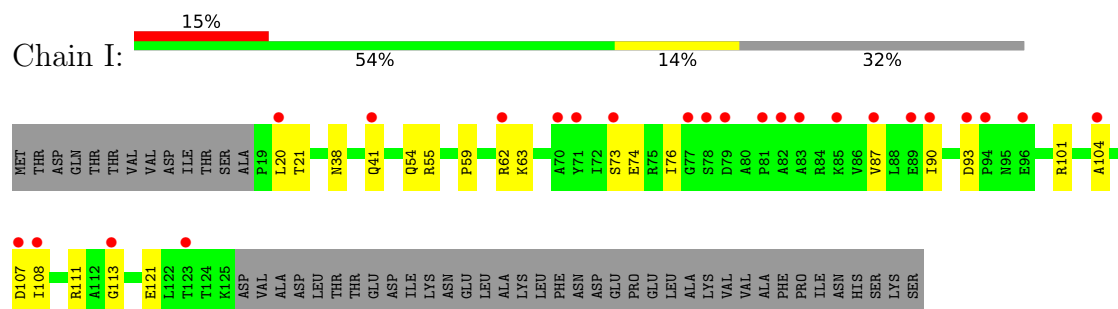
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			779	492	141	145	1			
1	mm	103	Total	C	N	O	S	0	0	0
			755	475	137	142	1			

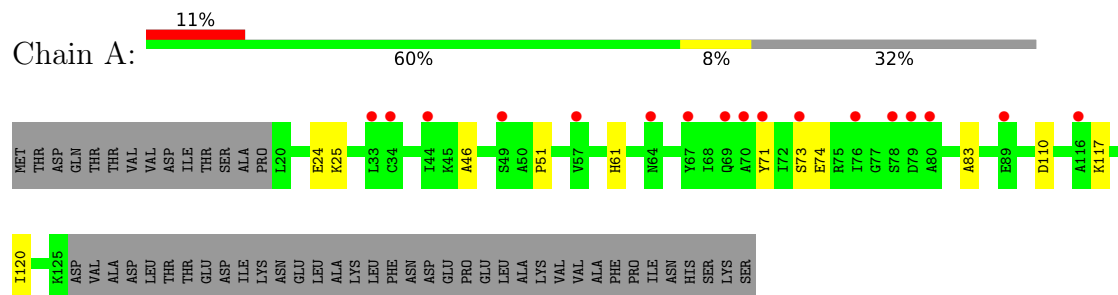
3 Residue-property plots [i](#)

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.

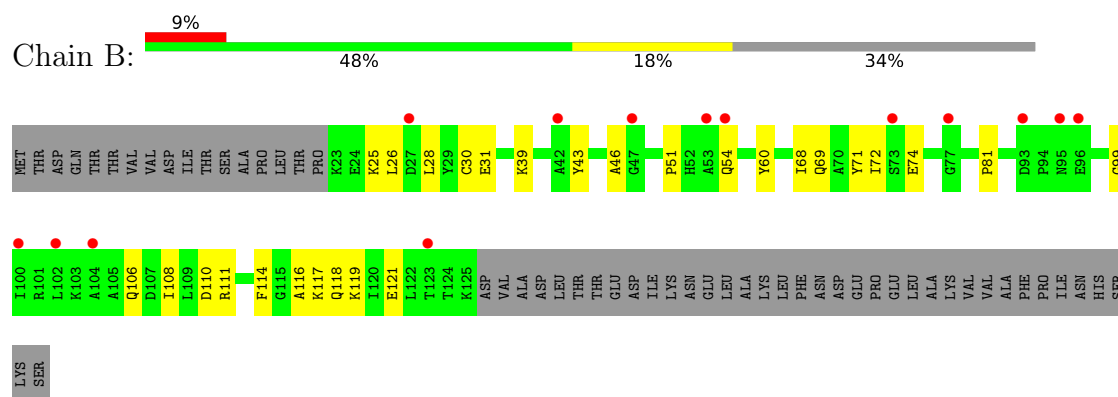
- Molecule 1: Small Terminase subunit



- Molecule 1: Small Terminase subunit

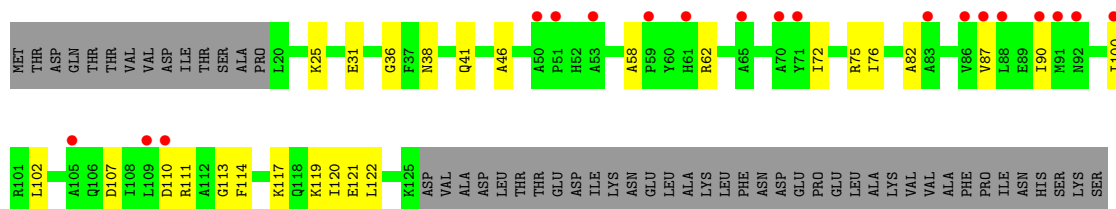


- Molecule 1: Small Terminase subunit

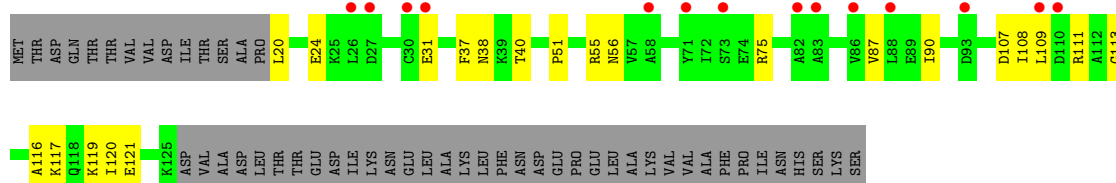


- Molecule 1: Small Terminase subunit

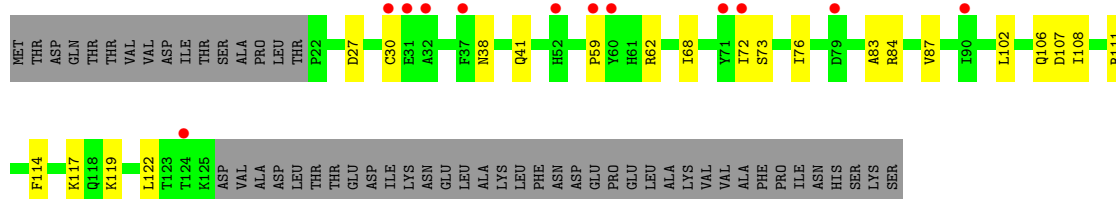




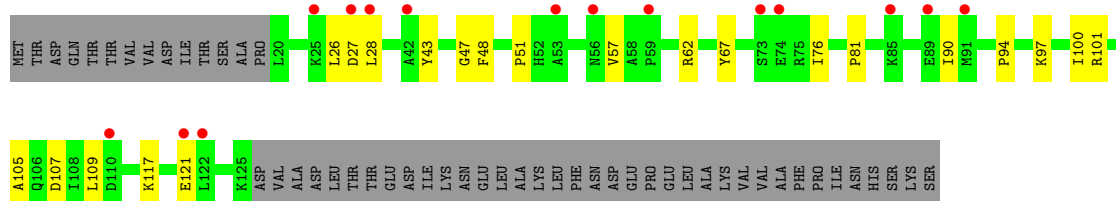
• Molecule 1: Small Terminase subunit



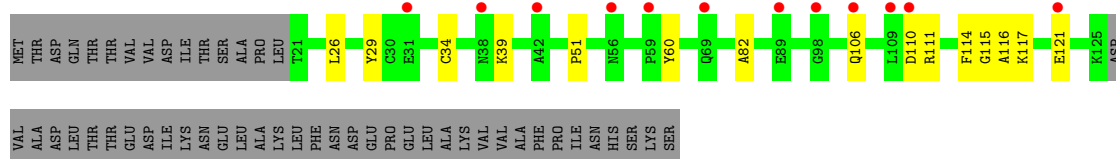
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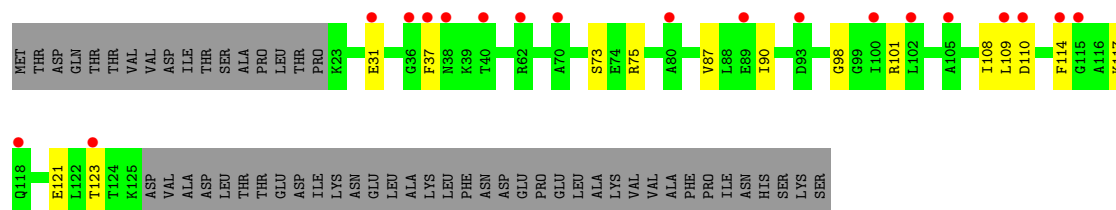
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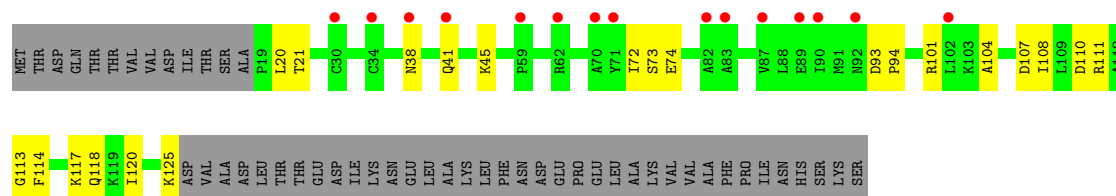
• Molecule 1: Small Terminase subunit



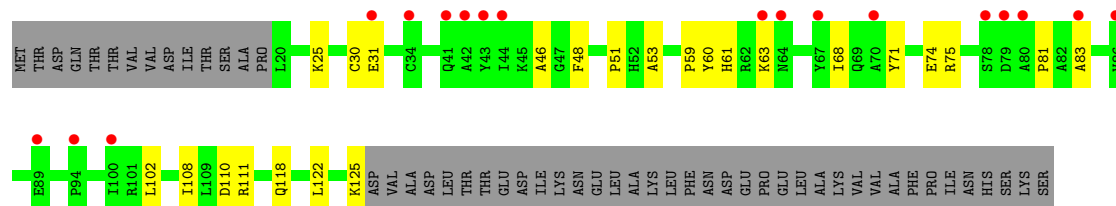
• Molecule 1: Small Terminase subunit



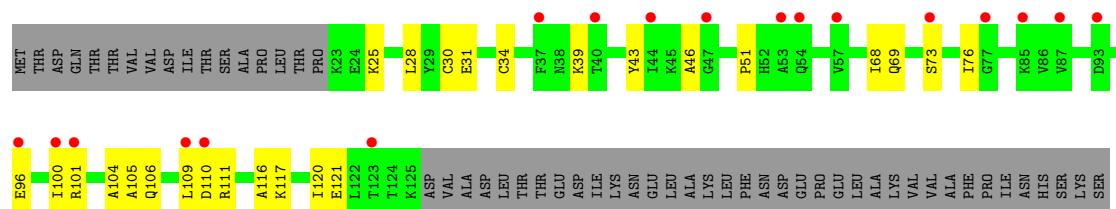
- Molecule 1: Small Terminase subunit



- Molecule 1: Small Terminase subunit

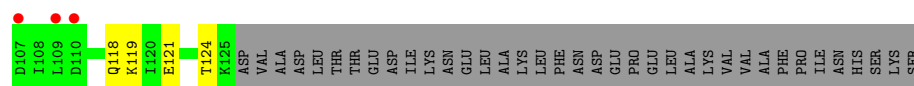


- Molecule 1: Small Terminase subunit

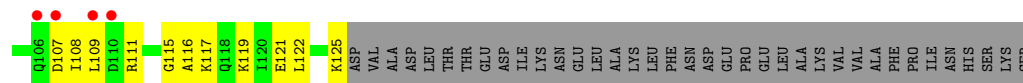


- Molecule 1: Small Terminase subunit

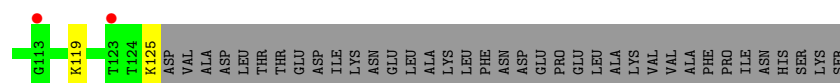
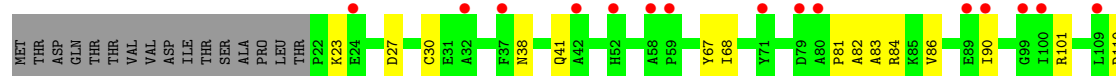




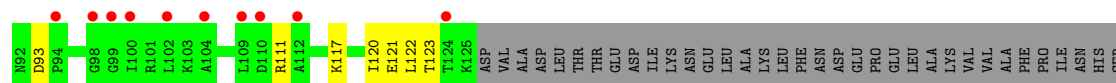
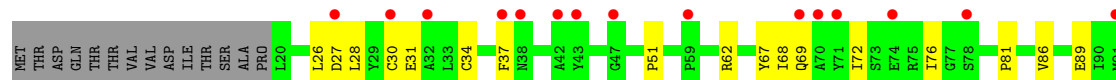
• Molecule 1: Small Terminase subunit



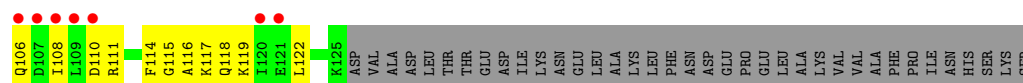
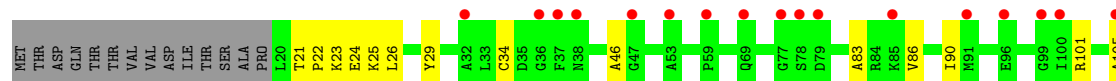
• Molecule 1: Small Terminase subunit



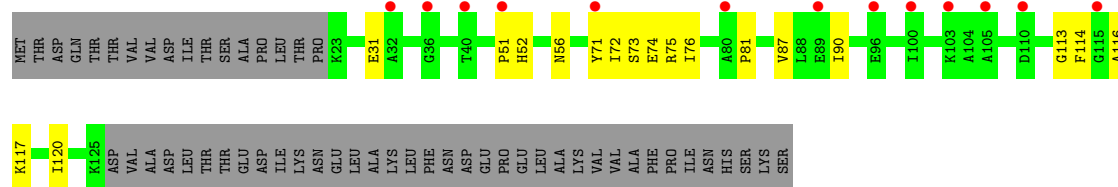
• Molecule 1: Small Terminase subunit



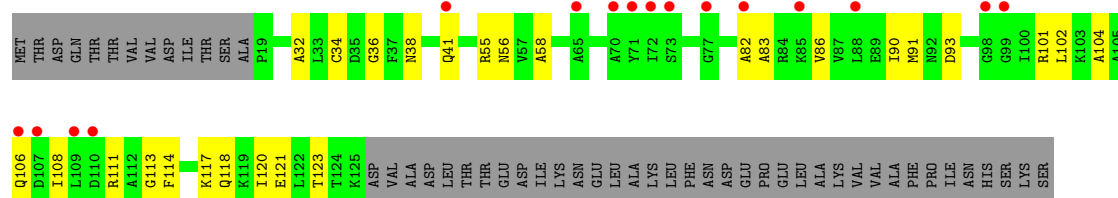
• Molecule 1: Small Terminase subunit



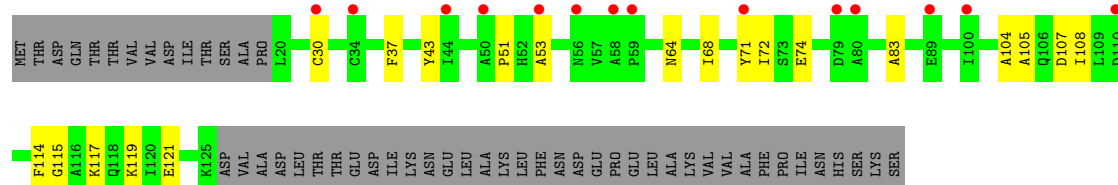
• Molecule 1: Small Terminase subunit



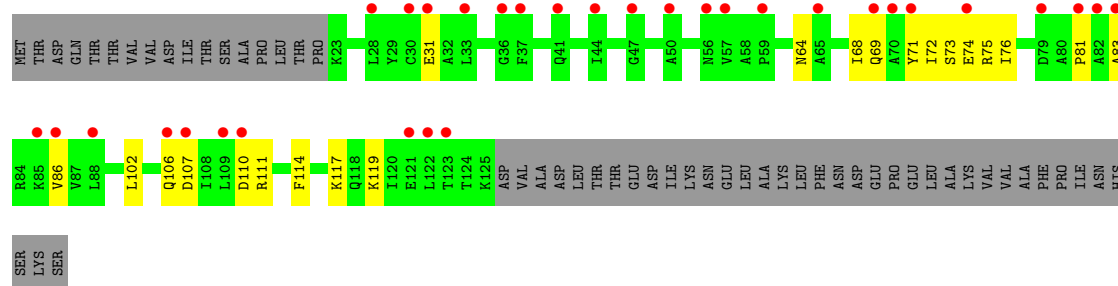
• Molecule 1: Small Terminase subunit



• Molecule 1: Small Terminase subunit



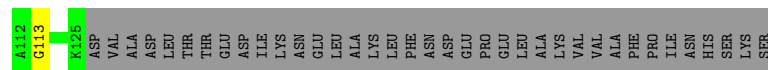
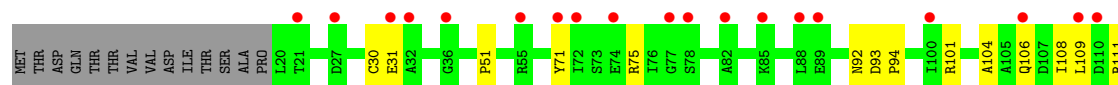
• Molecule 1: Small Terminase subunit



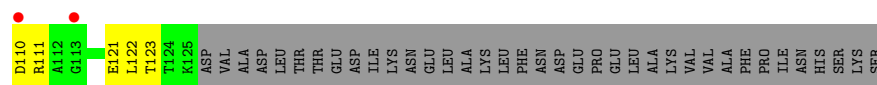
• Molecule 1: Small Terminase subunit



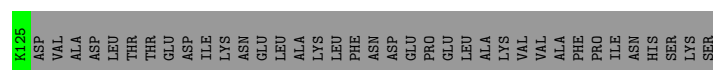
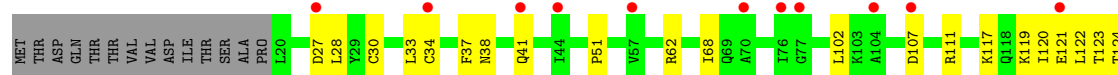
- Molecule 1: Small Terminase subunit



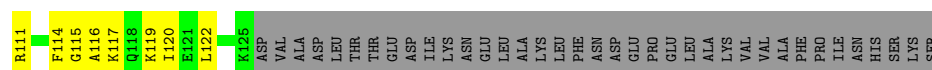
- Molecule 1: Small Terminase subunit



- Molecule 1: Small Terminase subunit



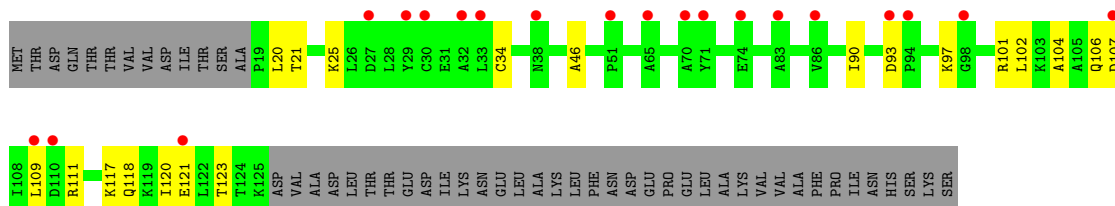
- Molecule 1: Small Terminase subunit



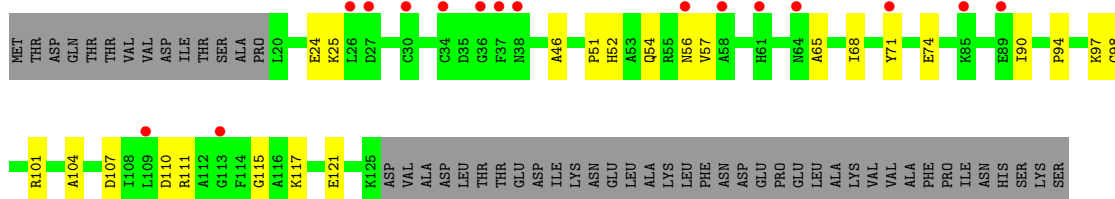
- Molecule 1: Small Terminase subunit



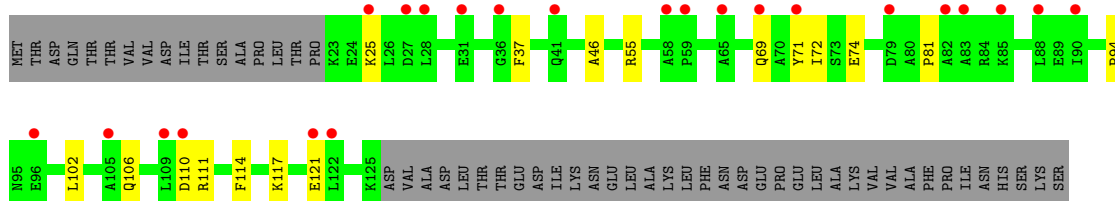
- Molecule 1: Small Terminase subunit



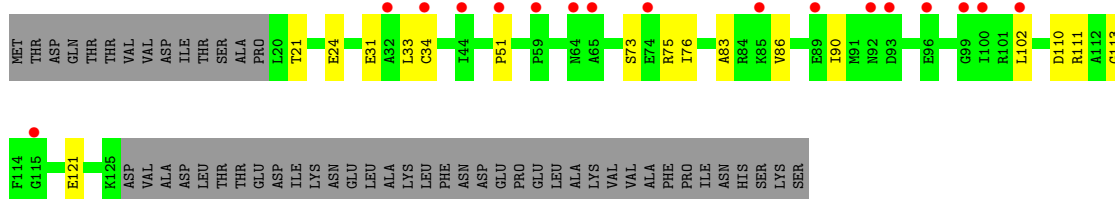
- Molecule 1: Small Terminase subunit



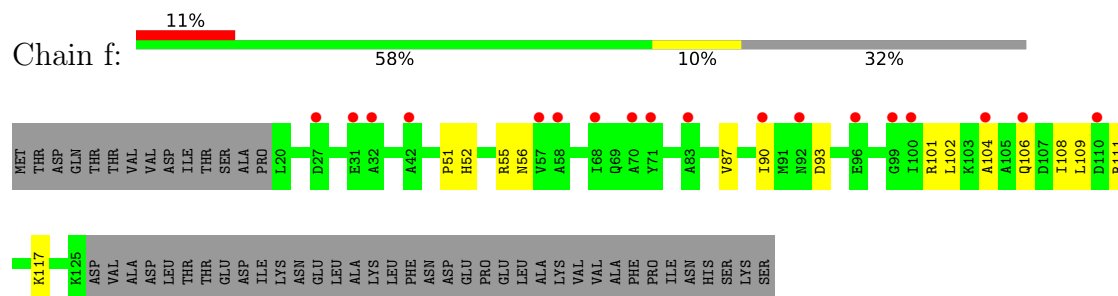
- Molecule 1: Small Terminase subunit



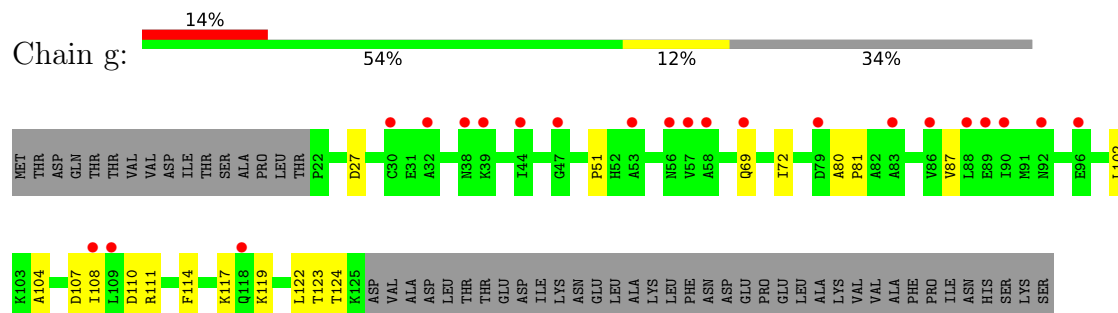
- Molecule 1: Small Terminase subunit



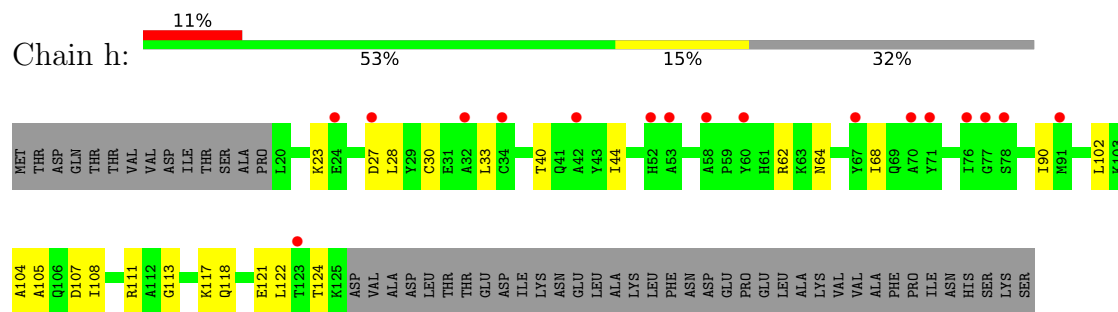
- Molecule 1: Small Terminase subunit



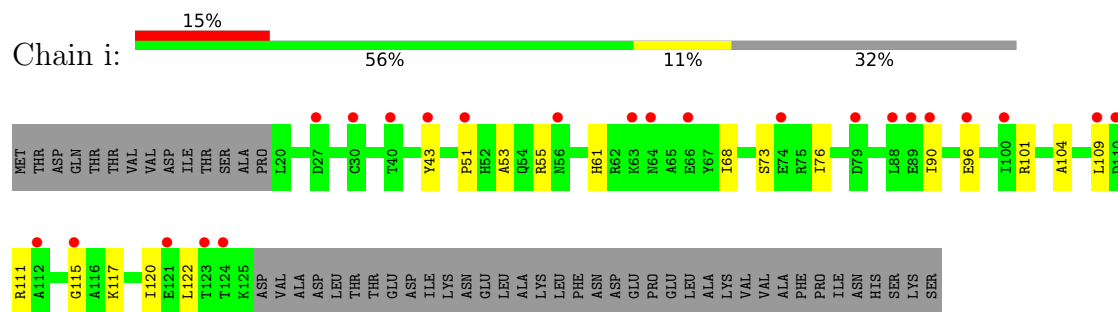
- Molecule 1: Small Terminase subunit



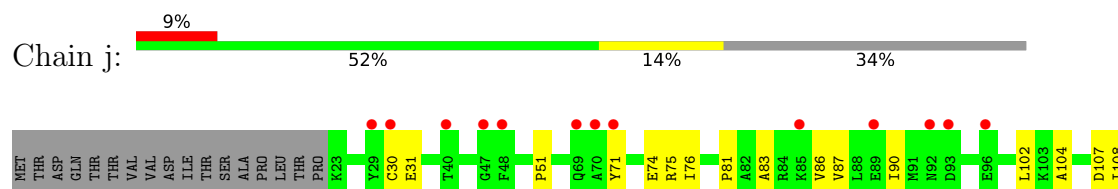
- Molecule 1: Small Terminase subunit

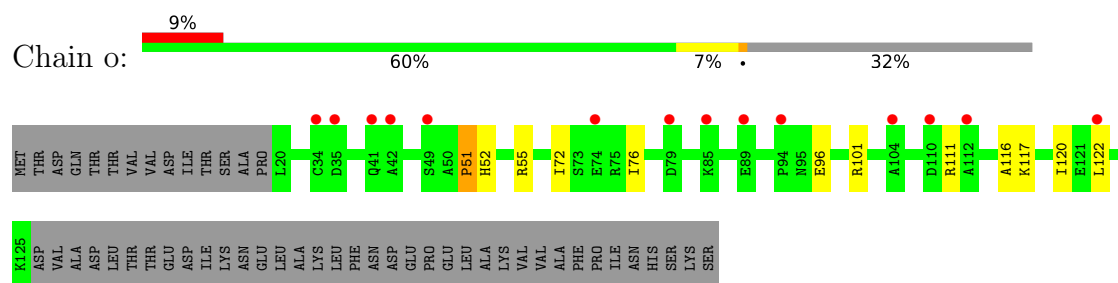


- Molecule 1: Small Terminase subunit

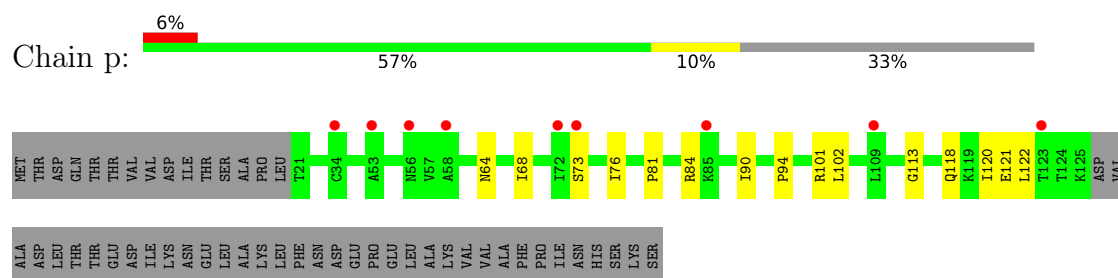


- Molecule 1: Small Terminase subunit

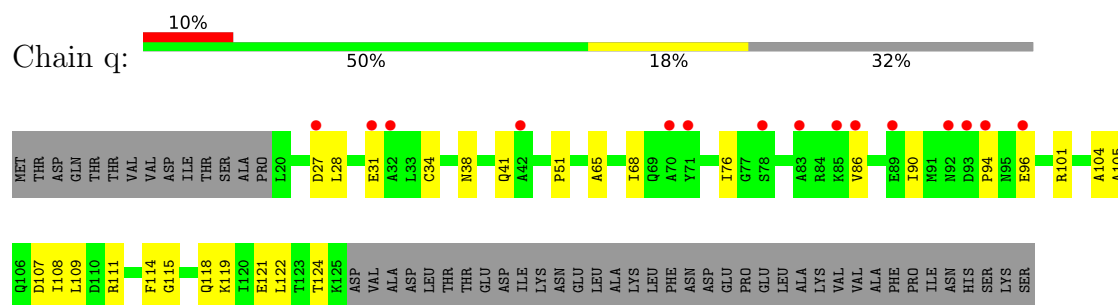




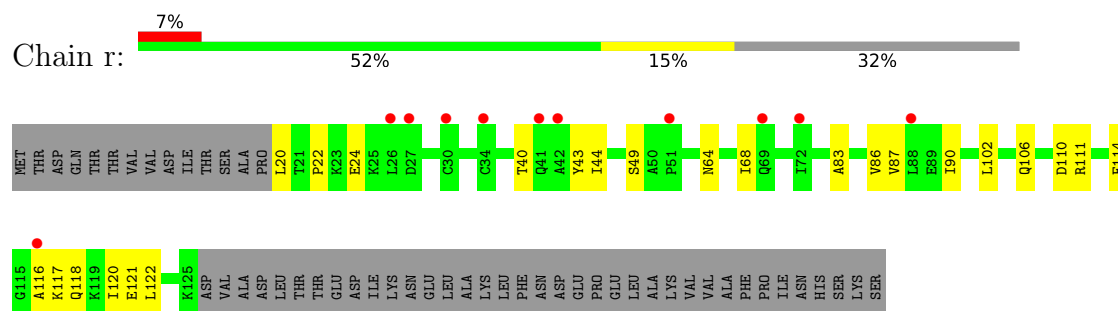
• Molecule 1: Small Terminase subunit



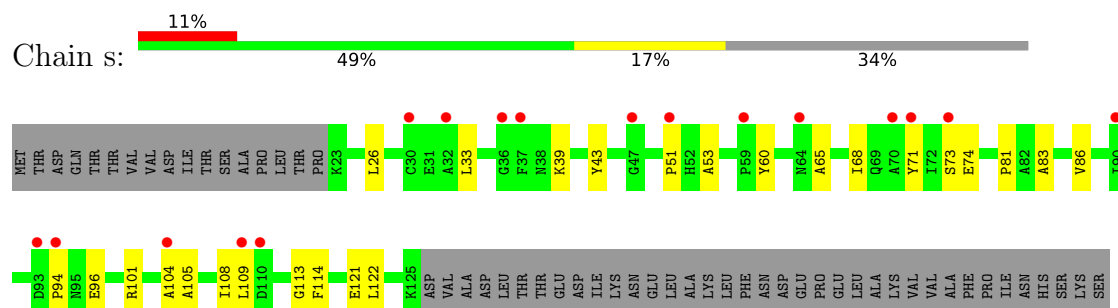
• Molecule 1: Small Terminase subunit



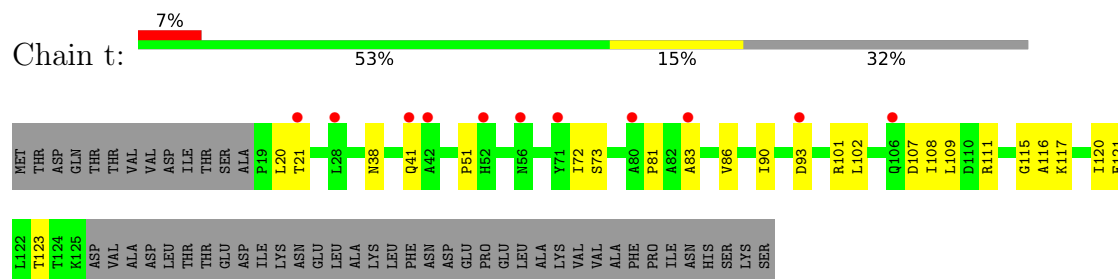
• Molecule 1: Small Terminase subunit



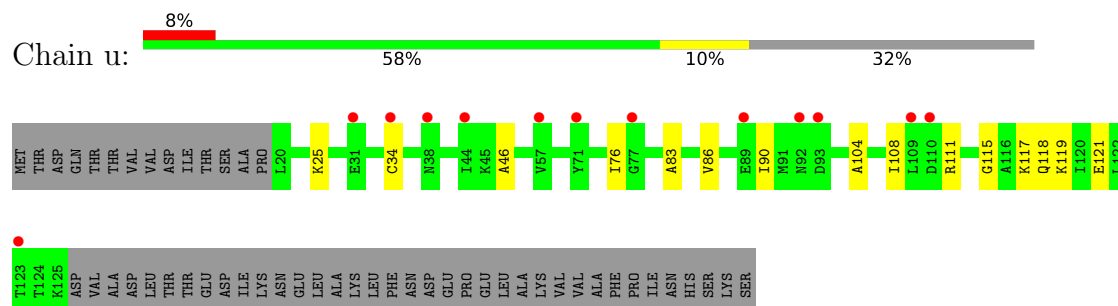
• Molecule 1: Small Terminase subunit



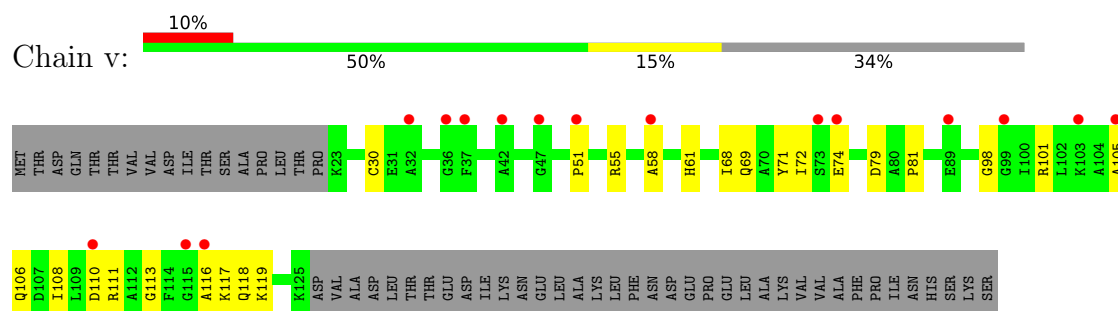
- Molecule 1: Small Terminase subunit



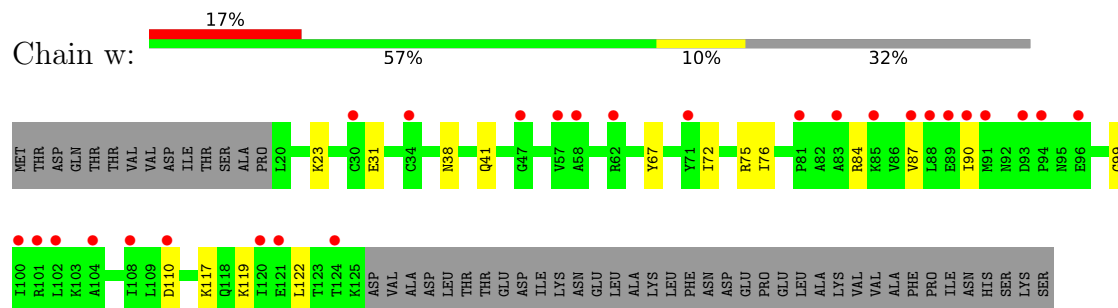
- Molecule 1: Small Terminase subunit



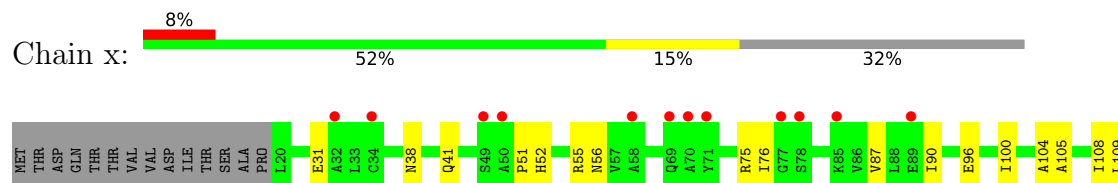
- Molecule 1: Small Terminase subunit

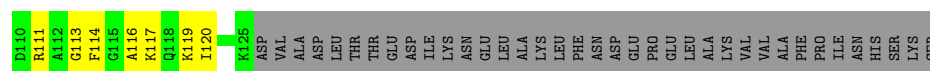


- Molecule 1: Small Terminase subunit

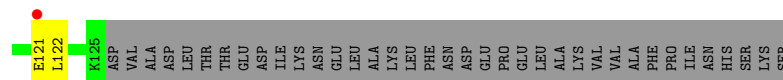
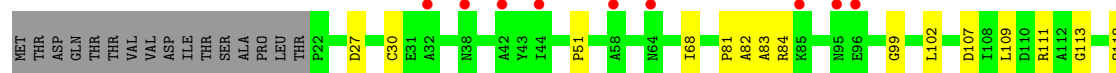


- Molecule 1: Small Terminase subunit

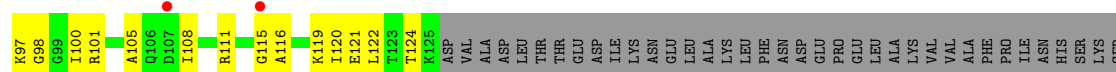




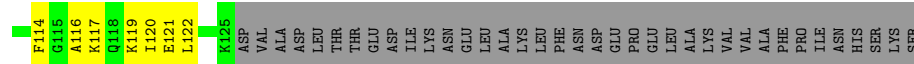
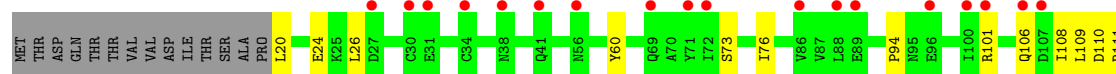
- Molecule 1: Small Terminase subunit



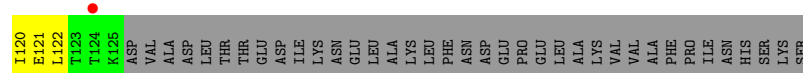
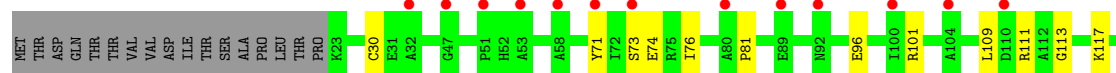
- Molecule 1: Small Terminase subunit



- Molecule 1: Small Terminase subunit

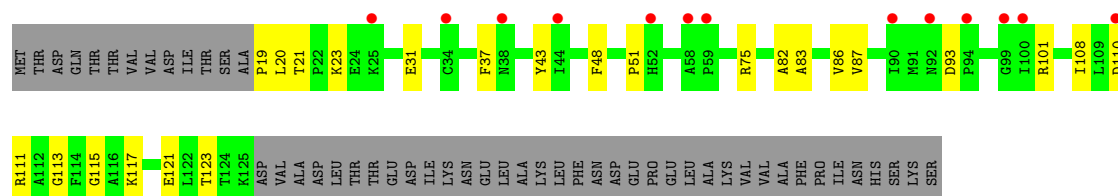


- Molecule 1: Small Terminase subunit

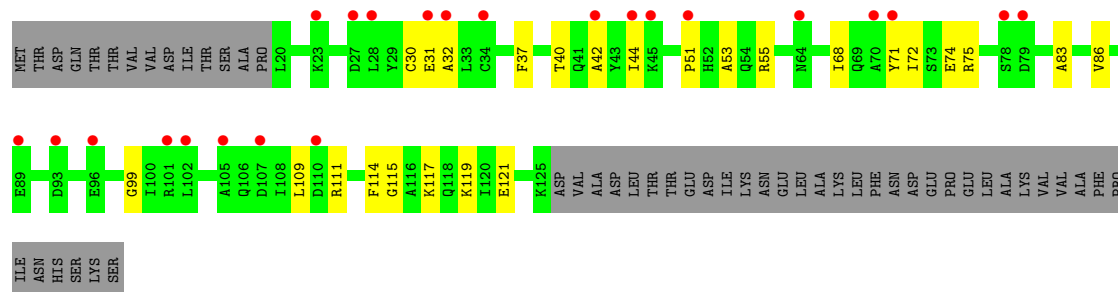


- Molecule 1: Small Terminase subunit

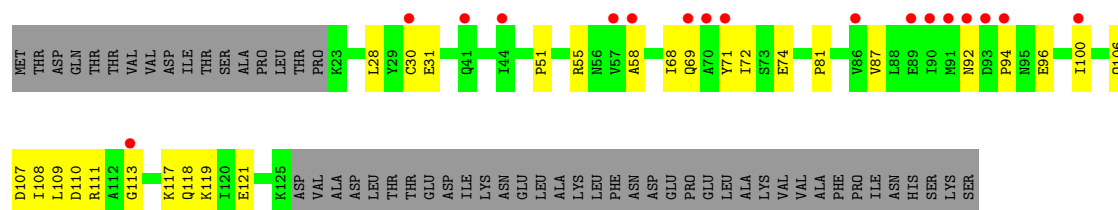




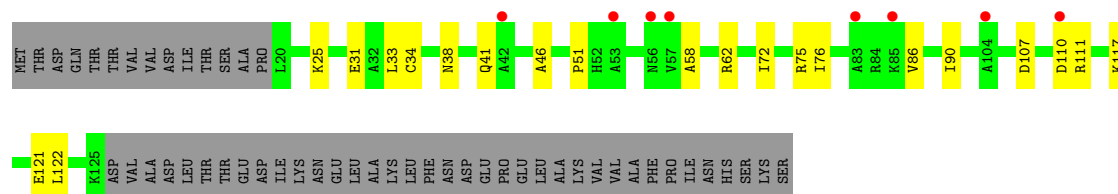
• Molecule 1: Small Terminase subunit



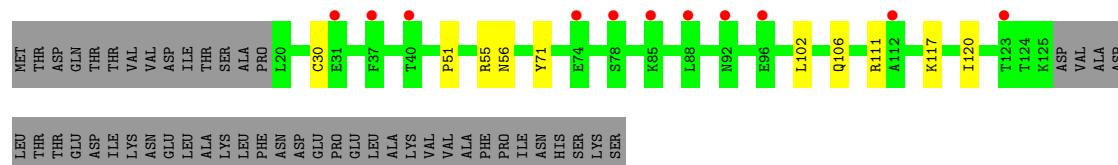
• Molecule 1: Small Terminase subunit



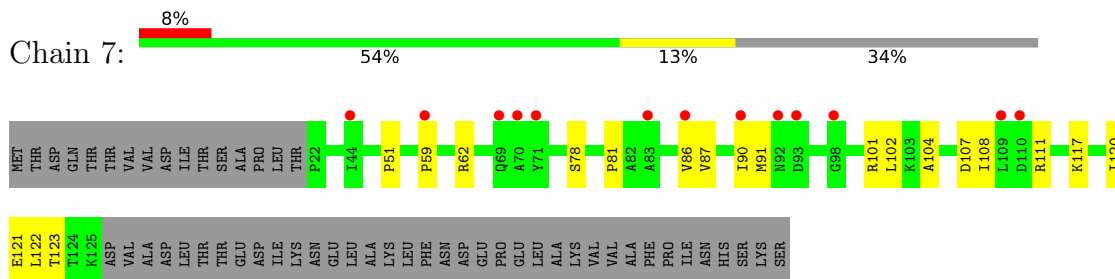
• Molecule 1: Small Terminase subunit



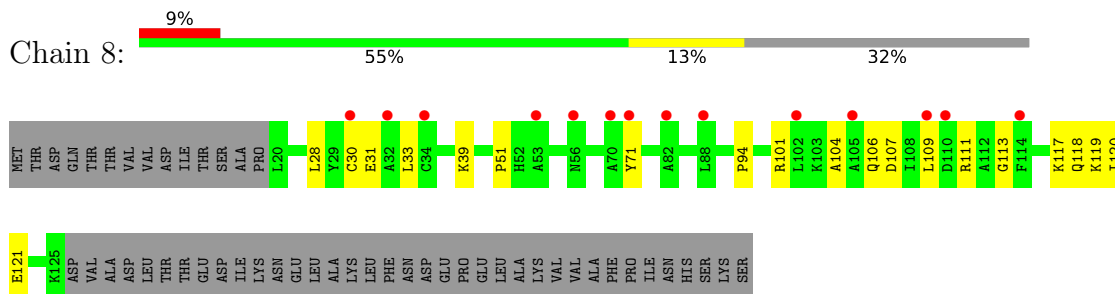
• Molecule 1: Small Terminase subunit



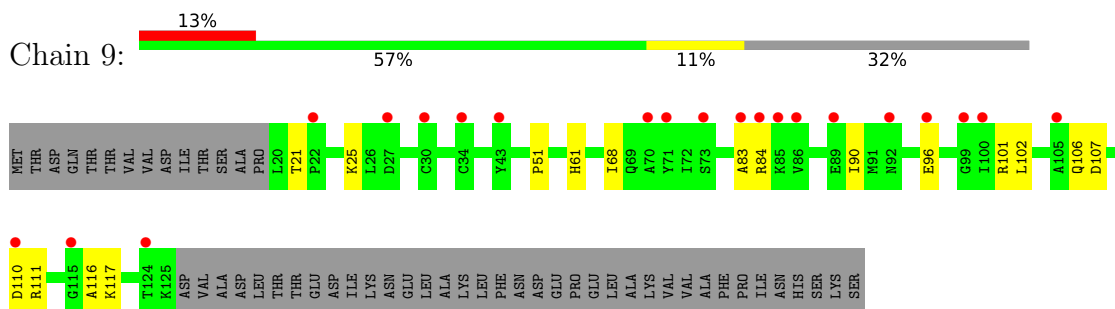
- Molecule 1: Small Terminase subunit



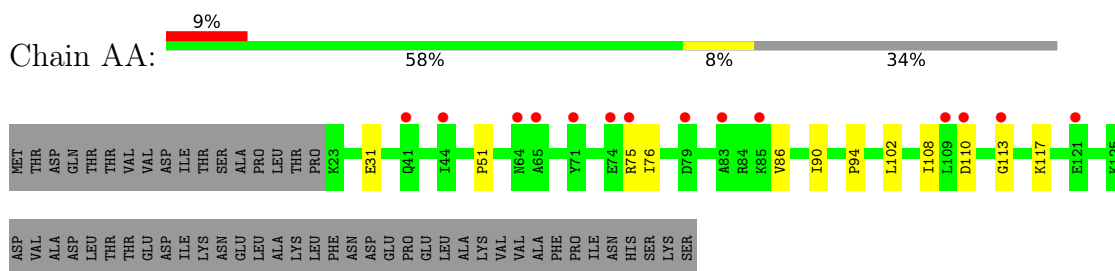
- Molecule 1: Small Terminase subunit



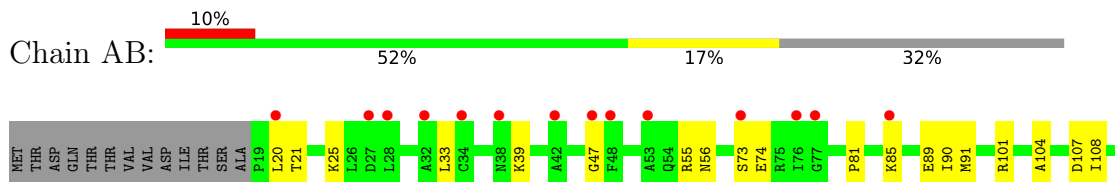
- Molecule 1: Small Terminase subunit

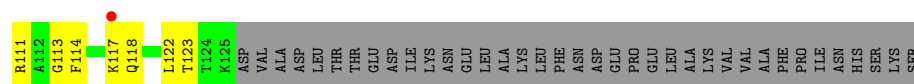


- Molecule 1: Small Terminase subunit

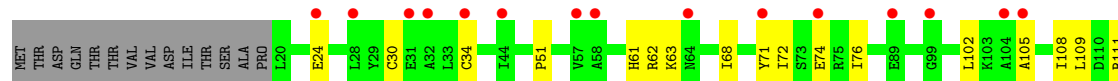


- Molecule 1: Small Terminase subunit





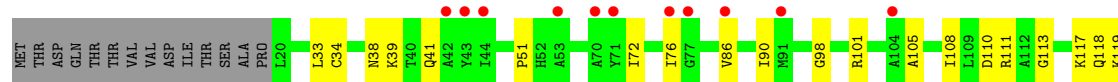
- Molecule 1: Small Terminase subunit



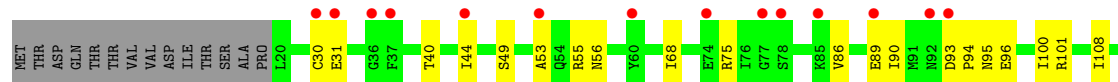
- Molecule 1: Small Terminase subunit



- Molecule 1: Small Terminase subunit

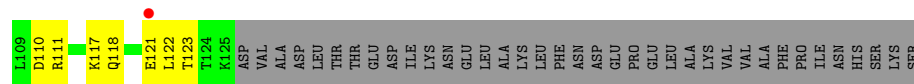


- Molecule 1: Small Terminase subunit

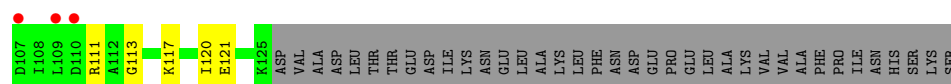


- Molecule 1: Small Terminase subunit

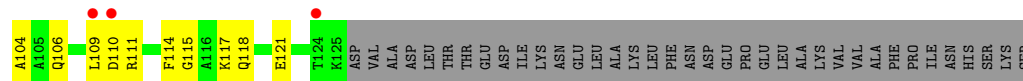
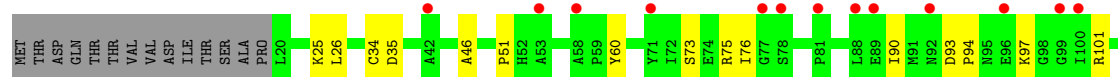




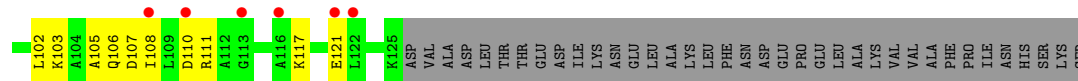
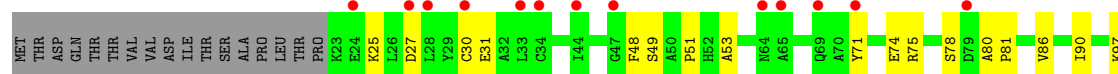
• Molecule 1: Small Terminase subunit



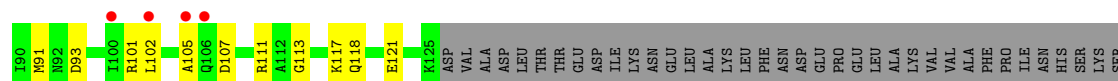
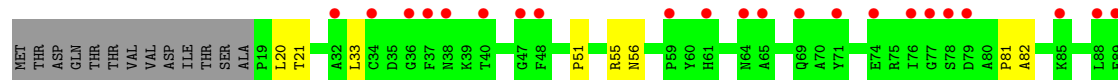
• Molecule 1: Small Terminase subunit



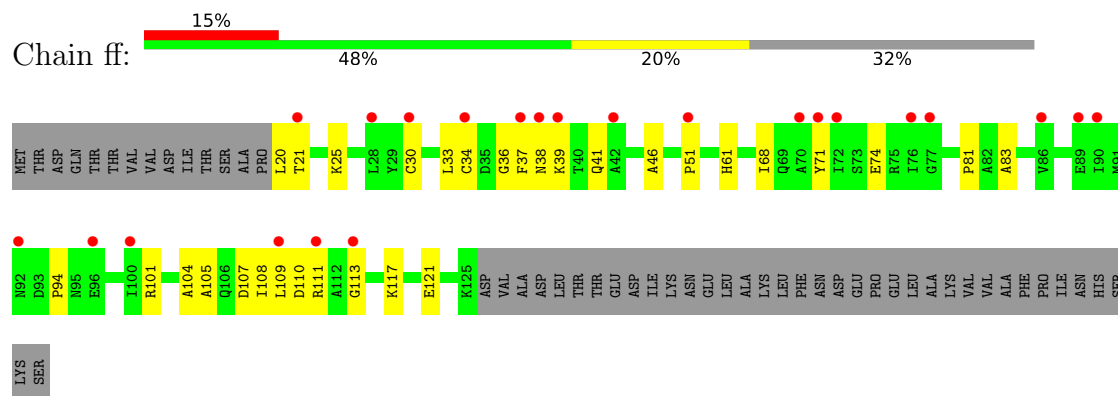
• Molecule 1: Small Terminase subunit



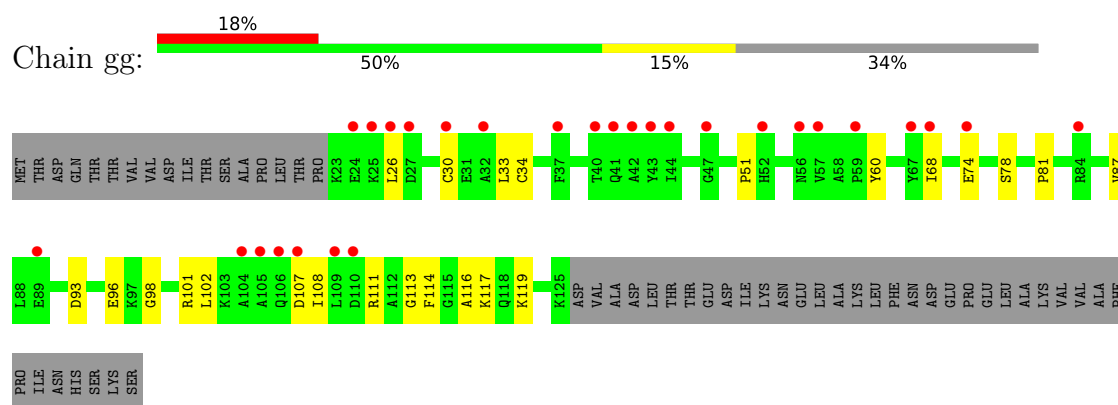
• Molecule 1: Small Terminase subunit



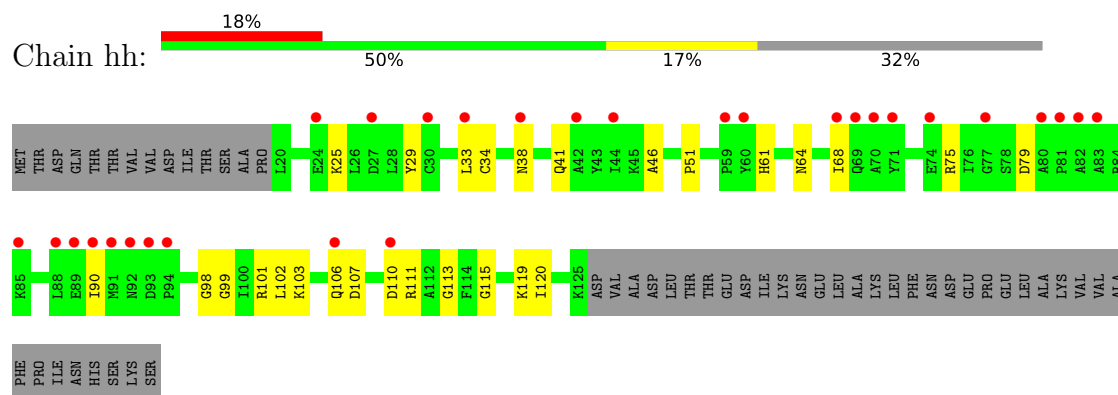
- Molecule 1: Small Terminase subunit



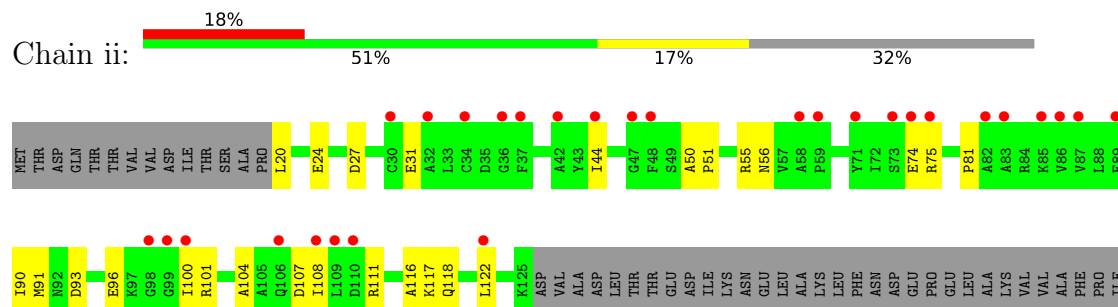
- Molecule 1: Small Terminase subunit



- Molecule 1: Small Terminase subunit

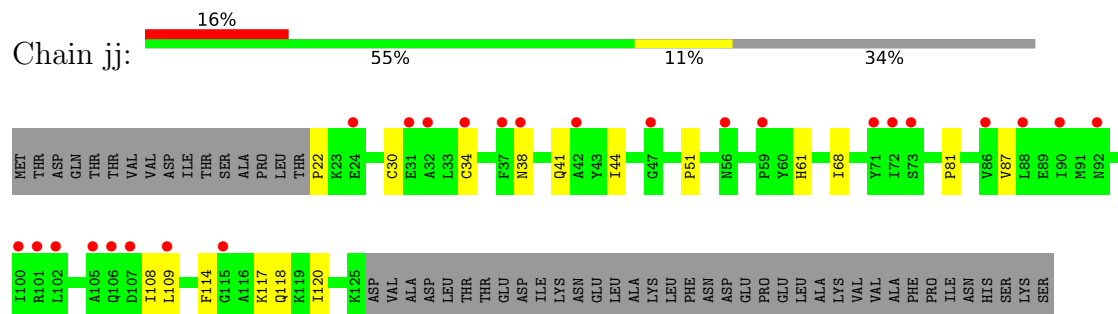


- Molecule 1: Small Terminase subunit

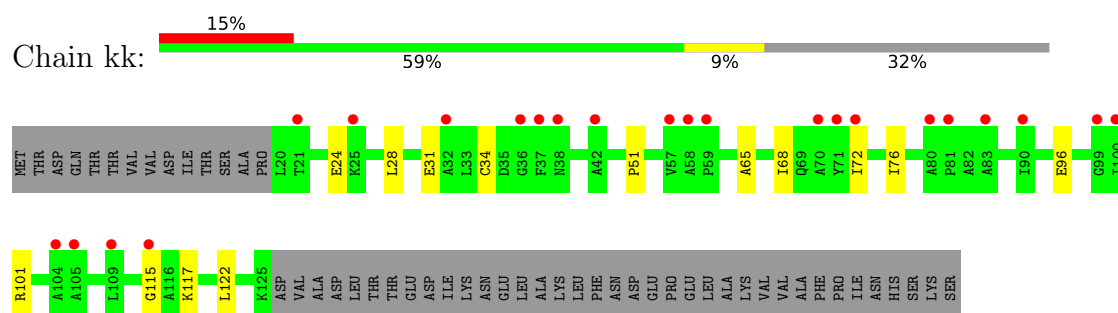


ASN
HIS
SER
LYS
SER

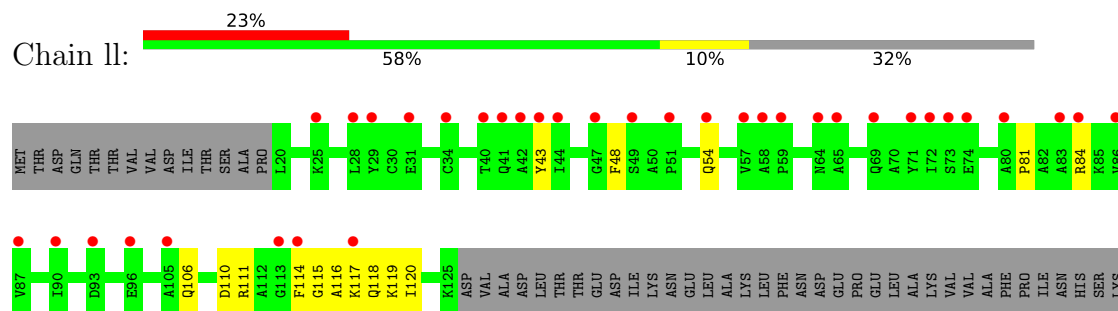
• Molecule 1: Small Terminase subunit



• Molecule 1: Small Terminase subunit

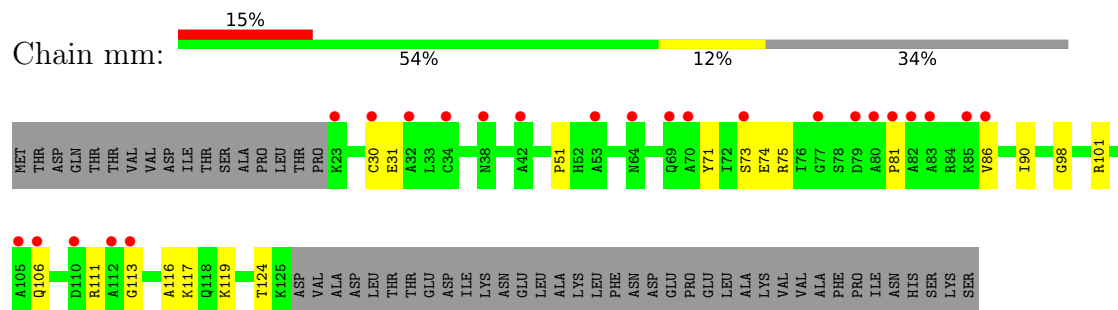


• Molecule 1: Small Terminase subunit



SER

• Molecule 1: Small Terminase subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	119.24Å 119.14Å 382.90Å 89.84° 90.00° 119.96°	Depositor
Resolution (Å)	10.00 – 3.95 10.00 – 3.95	Depositor EDS
% Data completeness (in resolution range)	95.1 (10.00-3.95) 89.7 (10.00-3.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 3.95Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874	Depositor
R, R_{free}	0.259 , 0.291 0.263 , 0.295	Depositor DCC
R_{free} test set	7364 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	168.8	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 6.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.000 for -k,h+k,l 0.000 for h+k,-h,l 0.064 for -h-k,h,l 0.064 for k,-h-k,l 0.100 for -h-k,k,-l 0.065 for h,-h-k,-l 0.000 for -h,-k,l 0.069 for k,h,-l 0.001 for -k,-h,-l 0.000 for h+k,-k,-l 0.001 for -h,h+k,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	62617	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1736e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0	0.19	0/789	0.55	0/1062
1	1	0.17	0/764	0.55	0/1028
1	2	0.17	0/799	0.48	0/1076
1	3	0.15	0/789	0.53	0/1062
1	4	0.16	0/768	0.48	0/1032
1	5	0.15	0/786	0.47	0/1058
1	6	0.13	0/789	0.46	0/1062
1	7	0.15	0/776	0.44	0/1043
1	8	0.14	0/786	0.44	0/1058
1	9	0.16	0/789	0.50	0/1062
1	A	0.15	0/789	0.48	0/1062
1	AA	0.13	0/764	0.42	0/1028
1	AB	0.13	0/799	0.48	0/1076
1	AC	0.14	0/789	0.49	0/1062
1	AD	0.15	0/768	0.44	0/1032
1	AE	0.13	0/786	0.45	0/1058
1	AF	0.14	0/789	0.48	0/1062
1	AG	0.13	0/776	0.45	0/1043
1	AH	0.13	0/786	0.47	0/1058
1	AI	0.15	0/789	0.55	0/1062
1	AJ	0.13	0/764	0.45	0/1028
1	B	0.18	0/768	0.48	0/1032
1	C	0.14	0/786	0.49	0/1058
1	D	0.17	0/789	0.49	0/1062
1	E	0.17	0/776	0.50	0/1043
1	F	0.17	0/786	0.47	0/1058
1	G	0.16	0/783	0.50	0/1054
1	H	0.17	0/764	0.48	0/1028
1	I	0.15	0/799	0.44	0/1076
1	J	0.15	0/799	0.48	0/1076
1	K	0.18	0/789	0.54	0/1062
1	L	0.16	0/768	0.48	0/1032
1	M	0.15	0/786	0.44	0/1058
1	N	0.16	0/789	0.52	0/1062

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	O	0.16	0/776	0.46	0/1043
1	P	0.15	0/786	0.54	0/1058
1	Q	0.19	0/791	0.54	0/1065
1	R	0.17	0/764	0.50	0/1028
1	S	0.19	0/799	0.53	0/1076
1	T	0.15	0/789	0.47	0/1062
1	U	0.16	0/768	0.49	0/1032
1	V	0.14	0/786	0.43	0/1058
1	W	0.14	0/789	0.47	0/1062
1	X	0.14	0/781	0.49	0/1051
1	Y	0.14	0/786	0.46	0/1058
1	Z	0.22	0/789	0.48	0/1062
1	a	0.17	0/764	0.47	0/1028
1	b	0.22	0/799	0.48	0/1076
1	c	0.15	0/789	0.49	0/1062
1	d	0.14	0/768	0.47	0/1032
1	e	0.15	0/786	0.47	0/1058
1	ee	0.14	0/799	0.49	0/1076
1	f	0.18	0/789	0.53	0/1062
1	ff	0.13	0/789	0.45	0/1062
1	g	0.15	0/776	0.48	0/1043
1	gg	0.13	0/768	0.44	0/1032
1	h	0.16	0/786	0.49	0/1058
1	hh	0.13	0/786	0.47	0/1058
1	i	0.16	0/789	0.52	0/1062
1	ii	0.14	0/789	0.47	0/1062
1	j	0.17	0/764	0.50	0/1028
1	jj	0.14	0/773	0.56	1/1039 (0.1%)
1	k	0.15	0/799	0.45	0/1076
1	kk	0.13	0/786	0.46	0/1058
1	l	0.17	0/789	0.46	0/1062
1	ll	0.14	0/789	0.47	0/1062
1	m	0.15	0/768	0.44	0/1032
1	mm	0.13	0/764	0.47	0/1028
1	n	0.16	0/786	0.45	0/1058
1	o	0.16	0/789	0.48	0/1062
1	p	0.14	0/781	0.45	0/1051
1	q	0.16	0/786	0.48	0/1058
1	r	0.18	0/789	0.51	0/1062
1	s	0.17	0/764	0.53	0/1028
1	t	0.18	0/799	0.52	0/1076
1	u	0.19	0/789	0.54	0/1062
1	v	0.14	0/768	0.46	0/1032

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	w	0.15	0/786	0.48	0/1058
1	x	0.16	0/789	0.49	0/1062
1	y	0.16	0/776	0.47	0/1043
1	z	0.17	0/786	0.49	0/1058
All	All	0.16	0/63417	0.48	1/85336 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	jj	22	PRO	N-CA-CB	6.81	110.50	103.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	779	0	747	19	0
1	1	755	0	716	17	0
1	2	788	0	760	21	0
1	3	779	0	747	21	0
1	4	759	0	727	25	0
1	5	776	0	738	16	0
1	6	779	0	747	7	0
1	7	766	0	735	18	0
1	8	776	0	738	18	0
1	9	779	0	747	13	0
1	A	779	0	747	9	0
1	AA	755	0	716	12	0
1	AB	788	0	760	27	0
1	AC	779	0	747	19	0
1	AD	759	0	727	25	0
1	AE	776	0	738	24	0
1	AF	779	0	747	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AG	766	0	735	17	0
1	AH	776	0	738	20	0
1	AI	779	0	747	20	0
1	AJ	755	0	716	23	0
1	B	759	0	727	21	0
1	C	776	0	738	27	0
1	D	779	0	747	22	0
1	E	766	0	735	20	0
1	F	776	0	738	17	0
1	G	773	0	741	14	0
1	H	755	0	716	13	0
1	I	788	0	760	18	0
1	J	788	0	760	20	0
1	K	779	0	747	19	0
1	L	759	0	727	20	0
1	M	776	0	738	12	0
1	N	779	0	747	19	0
1	O	766	0	735	16	0
1	P	776	0	738	19	0
1	Q	781	0	752	31	0
1	R	755	0	716	19	0
1	S	788	0	760	33	0
1	T	779	0	747	15	0
1	U	759	0	727	18	0
1	V	776	0	738	15	0
1	W	779	0	747	10	0
1	X	771	0	736	18	0
1	Y	776	0	738	23	0
1	Z	779	0	747	20	0
1	a	755	0	716	24	0
1	b	788	0	760	26	0
1	c	779	0	747	18	0
1	d	759	0	727	14	0
1	e	776	0	738	17	0
1	ee	788	0	760	19	0
1	f	779	0	747	18	0
1	ff	779	0	747	23	0
1	g	766	0	735	20	0
1	gg	759	0	727	20	0
1	h	776	0	738	25	0
1	hh	776	0	738	25	0
1	i	779	0	747	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	ii	779	0	747	23	0
1	j	755	0	716	19	0
1	jj	764	0	729	14	0
1	k	788	0	760	25	0
1	kk	776	0	738	11	0
1	l	779	0	747	24	0
1	ll	779	0	747	15	0
1	m	759	0	727	25	0
1	mm	755	0	716	15	0
1	n	776	0	738	17	0
1	o	779	0	747	12	0
1	p	771	0	736	14	0
1	q	776	0	738	22	0
1	r	779	0	747	21	0
1	s	755	0	716	25	0
1	t	788	0	760	22	0
1	u	779	0	747	15	0
1	v	759	0	727	18	0
1	w	776	0	738	16	0
1	x	779	0	747	21	0
1	y	766	0	735	19	0
1	z	776	0	738	29	0
All	All	62617	0	59890	1076	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 1076 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:S:111:ARG:CZ	1:a:109:LEU:HD23	1.72	1.18
1:S:111:ARG:NH1	1:a:109:LEU:HD23	1.66	1.08
1:S:111:ARG:CZ	1:a:109:LEU:CD2	2.31	1.07
1:b:111:ARG:HG3	1:b:111:ARG:HH11	1.19	1.07
1:r:111:ARG:HH21	1:s:73:SER:HB2	1.25	1.02

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	0	104/157 (66%)	97 (93%)	7 (7%)	0	100	100
1	1	101/157 (64%)	92 (91%)	9 (9%)	0	100	100
1	2	105/157 (67%)	95 (90%)	10 (10%)	0	100	100
1	3	104/157 (66%)	97 (93%)	7 (7%)	0	100	100
1	4	101/157 (64%)	94 (93%)	7 (7%)	0	100	100
1	5	104/157 (66%)	98 (94%)	6 (6%)	0	100	100
1	6	104/157 (66%)	98 (94%)	6 (6%)	0	100	100
1	7	102/157 (65%)	95 (93%)	7 (7%)	0	100	100
1	8	104/157 (66%)	100 (96%)	4 (4%)	0	100	100
1	9	104/157 (66%)	97 (93%)	7 (7%)	0	100	100
1	A	104/157 (66%)	95 (91%)	9 (9%)	0	100	100
1	AA	101/157 (64%)	92 (91%)	9 (9%)	0	100	100
1	AB	105/157 (67%)	95 (90%)	10 (10%)	0	100	100
1	AC	104/157 (66%)	95 (91%)	9 (9%)	0	100	100
1	AD	101/157 (64%)	94 (93%)	7 (7%)	0	100	100
1	AE	104/157 (66%)	98 (94%)	6 (6%)	0	100	100
1	AF	104/157 (66%)	99 (95%)	5 (5%)	0	100	100
1	AG	102/157 (65%)	94 (92%)	8 (8%)	0	100	100
1	AH	104/157 (66%)	99 (95%)	4 (4%)	1 (1%)	12	45
1	AI	104/157 (66%)	97 (93%)	7 (7%)	0	100	100
1	AJ	101/157 (64%)	94 (93%)	7 (7%)	0	100	100
1	B	101/157 (64%)	96 (95%)	5 (5%)	0	100	100
1	C	104/157 (66%)	99 (95%)	5 (5%)	0	100	100
1	D	104/157 (66%)	101 (97%)	3 (3%)	0	100	100
1	E	102/157 (65%)	96 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	104/157 (66%)	99 (95%)	5 (5%)	0	100	100
1	G	103/157 (66%)	97 (94%)	6 (6%)	0	100	100
1	H	101/157 (64%)	92 (91%)	9 (9%)	0	100	100
1	I	105/157 (67%)	96 (91%)	9 (9%)	0	100	100
1	J	105/157 (67%)	95 (90%)	10 (10%)	0	100	100
1	K	104/157 (66%)	95 (91%)	9 (9%)	0	100	100
1	L	101/157 (64%)	95 (94%)	6 (6%)	0	100	100
1	M	104/157 (66%)	100 (96%)	4 (4%)	0	100	100
1	N	104/157 (66%)	97 (93%)	7 (7%)	0	100	100
1	O	102/157 (65%)	98 (96%)	4 (4%)	0	100	100
1	P	104/157 (66%)	98 (94%)	6 (6%)	0	100	100
1	Q	104/157 (66%)	94 (90%)	9 (9%)	1 (1%)	12	45
1	R	101/157 (64%)	93 (92%)	8 (8%)	0	100	100
1	S	105/157 (67%)	96 (91%)	9 (9%)	0	100	100
1	T	104/157 (66%)	96 (92%)	8 (8%)	0	100	100
1	U	101/157 (64%)	95 (94%)	6 (6%)	0	100	100
1	V	104/157 (66%)	97 (93%)	7 (7%)	0	100	100
1	W	104/157 (66%)	97 (93%)	7 (7%)	0	100	100
1	X	103/157 (66%)	97 (94%)	6 (6%)	0	100	100
1	Y	104/157 (66%)	98 (94%)	5 (5%)	1 (1%)	12	45
1	Z	104/157 (66%)	96 (92%)	8 (8%)	0	100	100
1	a	101/157 (64%)	91 (90%)	10 (10%)	0	100	100
1	b	105/157 (67%)	96 (91%)	9 (9%)	0	100	100
1	c	104/157 (66%)	95 (91%)	9 (9%)	0	100	100
1	d	101/157 (64%)	96 (95%)	4 (4%)	1 (1%)	12	45
1	e	104/157 (66%)	98 (94%)	6 (6%)	0	100	100
1	ee	105/157 (67%)	95 (90%)	10 (10%)	0	100	100
1	f	104/157 (66%)	97 (93%)	7 (7%)	0	100	100
1	ff	104/157 (66%)	96 (92%)	8 (8%)	0	100	100
1	g	102/157 (65%)	97 (95%)	5 (5%)	0	100	100
1	gg	101/157 (64%)	95 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	h	104/157 (66%)	96 (92%)	8 (8%)	0	100	100
1	hh	104/157 (66%)	98 (94%)	6 (6%)	0	100	100
1	i	104/157 (66%)	96 (92%)	8 (8%)	0	100	100
1	ii	104/157 (66%)	97 (93%)	7 (7%)	0	100	100
1	j	101/157 (64%)	90 (89%)	11 (11%)	0	100	100
1	jj	102/157 (65%)	96 (94%)	6 (6%)	0	100	100
1	k	105/157 (67%)	97 (92%)	8 (8%)	0	100	100
1	kk	104/157 (66%)	99 (95%)	5 (5%)	0	100	100
1	l	104/157 (66%)	96 (92%)	6 (6%)	2 (2%)	6	33
1	ll	104/157 (66%)	98 (94%)	6 (6%)	0	100	100
1	m	101/157 (64%)	95 (94%)	6 (6%)	0	100	100
1	mm	101/157 (64%)	93 (92%)	8 (8%)	0	100	100
1	n	104/157 (66%)	100 (96%)	4 (4%)	0	100	100
1	o	104/157 (66%)	99 (95%)	5 (5%)	0	100	100
1	p	103/157 (66%)	98 (95%)	5 (5%)	0	100	100
1	q	104/157 (66%)	100 (96%)	4 (4%)	0	100	100
1	r	104/157 (66%)	96 (92%)	7 (7%)	1 (1%)	12	45
1	s	101/157 (64%)	93 (92%)	8 (8%)	0	100	100
1	t	105/157 (67%)	97 (92%)	8 (8%)	0	100	100
1	u	104/157 (66%)	96 (92%)	8 (8%)	0	100	100
1	v	101/157 (64%)	95 (94%)	6 (6%)	0	100	100
1	w	104/157 (66%)	99 (95%)	5 (5%)	0	100	100
1	x	104/157 (66%)	98 (94%)	6 (6%)	0	100	100
1	y	102/157 (65%)	96 (94%)	6 (6%)	0	100	100
1	z	104/157 (66%)	100 (96%)	4 (4%)	0	100	100
All	All	8362/12717 (66%)	7802 (93%)	553 (7%)	7 (0%)	48	81

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	24	GLU
1	AH	56	ASN
1	Y	37	PHE

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Mol	Chain	Res	Type
1	d	37	PHE
1	l	46	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	0	67/130 (52%)	67 (100%)	0	100	100
1	1	64/130 (49%)	64 (100%)	0	100	100
1	2	69/130 (53%)	68 (99%)	1 (1%)	59	71
1	3	67/130 (52%)	66 (98%)	1 (2%)	57	70
1	4	65/130 (50%)	64 (98%)	1 (2%)	57	70
1	5	66/130 (51%)	65 (98%)	1 (2%)	57	70
1	6	67/130 (52%)	66 (98%)	1 (2%)	57	70
1	7	66/130 (51%)	65 (98%)	1 (2%)	57	70
1	8	66/130 (51%)	65 (98%)	1 (2%)	57	70
1	9	67/130 (52%)	66 (98%)	1 (2%)	57	70
1	A	67/130 (52%)	66 (98%)	1 (2%)	57	70
1	AA	64/130 (49%)	63 (98%)	1 (2%)	55	69
1	AB	69/130 (53%)	69 (100%)	0	100	100
1	AC	67/130 (52%)	66 (98%)	1 (2%)	57	70
1	AD	65/130 (50%)	64 (98%)	1 (2%)	57	70
1	AE	66/130 (51%)	65 (98%)	1 (2%)	57	70
1	AF	67/130 (52%)	67 (100%)	0	100	100
1	AG	66/130 (51%)	65 (98%)	1 (2%)	57	70
1	AH	66/130 (51%)	65 (98%)	1 (2%)	57	70
1	AI	67/130 (52%)	66 (98%)	1 (2%)	57	70
1	AJ	64/130 (49%)	63 (98%)	1 (2%)	55	69
1	B	65/130 (50%)	64 (98%)	1 (2%)	57	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	66/130 (51%)	66 (100%)	0	100	100
1	D	67/130 (52%)	66 (98%)	1 (2%)	57	70
1	E	66/130 (51%)	66 (100%)	0	100	100
1	F	66/130 (51%)	65 (98%)	1 (2%)	57	70
1	G	67/130 (52%)	66 (98%)	1 (2%)	57	70
1	H	64/130 (49%)	64 (100%)	0	100	100
1	I	69/130 (53%)	69 (100%)	0	100	100
1	J	69/130 (53%)	69 (100%)	0	100	100
1	K	67/130 (52%)	66 (98%)	1 (2%)	57	70
1	L	65/130 (50%)	64 (98%)	1 (2%)	57	70
1	M	66/130 (51%)	65 (98%)	1 (2%)	57	70
1	N	67/130 (52%)	66 (98%)	1 (2%)	57	70
1	O	66/130 (51%)	66 (100%)	0	100	100
1	P	66/130 (51%)	65 (98%)	1 (2%)	57	70
1	Q	68/130 (52%)	68 (100%)	0	100	100
1	R	64/130 (49%)	63 (98%)	1 (2%)	55	69
1	S	69/130 (53%)	69 (100%)	0	100	100
1	T	67/130 (52%)	66 (98%)	1 (2%)	57	70
1	U	65/130 (50%)	65 (100%)	0	100	100
1	V	66/130 (51%)	65 (98%)	1 (2%)	57	70
1	W	67/130 (52%)	66 (98%)	1 (2%)	57	70
1	X	66/130 (51%)	65 (98%)	1 (2%)	57	70
1	Y	66/130 (51%)	65 (98%)	1 (2%)	57	70
1	Z	67/130 (52%)	66 (98%)	1 (2%)	57	70
1	a	64/130 (49%)	64 (100%)	0	100	100
1	b	69/130 (53%)	69 (100%)	0	100	100
1	c	67/130 (52%)	66 (98%)	1 (2%)	57	70
1	d	65/130 (50%)	65 (100%)	0	100	100
1	e	66/130 (51%)	65 (98%)	1 (2%)	57	70
1	ee	69/130 (53%)	68 (99%)	1 (1%)	59	71
1	f	67/130 (52%)	66 (98%)	1 (2%)	57	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	ff	67/130 (52%)	66 (98%)	1 (2%)	57	70
1	g	66/130 (51%)	65 (98%)	1 (2%)	57	70
1	gg	65/130 (50%)	64 (98%)	1 (2%)	57	70
1	h	66/130 (51%)	66 (100%)	0	100	100
1	hh	66/130 (51%)	65 (98%)	1 (2%)	57	70
1	i	67/130 (52%)	66 (98%)	1 (2%)	57	70
1	ii	67/130 (52%)	66 (98%)	1 (2%)	57	70
1	j	64/130 (49%)	63 (98%)	1 (2%)	55	69
1	jj	65/130 (50%)	64 (98%)	1 (2%)	57	70
1	k	69/130 (53%)	68 (99%)	1 (1%)	59	71
1	kk	66/130 (51%)	65 (98%)	1 (2%)	57	70
1	l	67/130 (52%)	67 (100%)	0	100	100
1	ll	67/130 (52%)	67 (100%)	0	100	100
1	m	65/130 (50%)	64 (98%)	1 (2%)	57	70
1	mm	64/130 (49%)	63 (98%)	1 (2%)	55	69
1	n	66/130 (51%)	66 (100%)	0	100	100
1	o	67/130 (52%)	66 (98%)	1 (2%)	57	70
1	p	66/130 (51%)	66 (100%)	0	100	100
1	q	66/130 (51%)	65 (98%)	1 (2%)	57	70
1	r	67/130 (52%)	67 (100%)	0	100	100
1	s	64/130 (49%)	63 (98%)	1 (2%)	55	69
1	t	69/130 (53%)	68 (99%)	1 (1%)	59	71
1	u	67/130 (52%)	67 (100%)	0	100	100
1	v	65/130 (50%)	64 (98%)	1 (2%)	57	70
1	w	66/130 (51%)	66 (100%)	0	100	100
1	x	67/130 (52%)	66 (98%)	1 (2%)	57	70
1	y	66/130 (51%)	65 (98%)	1 (2%)	57	70
1	z	66/130 (51%)	66 (100%)	0	100	100
All	All	5373/10530 (51%)	5317 (99%)	56 (1%)	68	76

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	t	51	PRO
1	mm	51	PRO
1	5	51	PRO
1	kk	51	PRO
1	ff	51	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	AH	41	GLN
1	AJ	61	HIS
1	jj	38	ASN
1	a	52	HIS
1	Z	61	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	0	106/157 (67%)	0.92	18 (16%)	4 7	84, 128, 146, 158	0
1	1	103/157 (65%)	0.90	14 (13%)	7 10	82, 133, 170, 199	0
1	2	107/157 (68%)	0.63	13 (12%)	8 12	94, 114, 139, 150	0
1	3	106/157 (67%)	1.10	23 (21%)	2 4	95, 122, 140, 158	0
1	4	103/157 (65%)	0.97	17 (16%)	4 7	95, 121, 140, 150	0
1	5	106/157 (67%)	0.82	8 (7%)	20 19	95, 118, 140, 154	0
1	6	106/157 (67%)	0.91	11 (10%)	11 13	91, 123, 143, 151	0
1	7	104/157 (66%)	0.72	13 (12%)	8 11	97, 124, 156, 175	0
1	8	106/157 (67%)	0.96	14 (13%)	7 10	91, 120, 138, 147	0
1	9	106/157 (67%)	1.10	21 (19%)	3 5	85, 126, 148, 161	0
1	A	106/157 (67%)	1.09	17 (16%)	5 8	98, 124, 146, 157	0
1	AA	103/157 (65%)	1.03	14 (13%)	7 10	92, 132, 170, 189	0
1	AB	107/157 (68%)	0.91	15 (14%)	6 9	90, 117, 142, 155	0
1	AC	106/157 (67%)	1.00	15 (14%)	6 9	91, 122, 140, 148	0
1	AD	103/157 (65%)	1.01	17 (16%)	4 7	86, 119, 141, 159	0
1	AE	106/157 (67%)	0.81	12 (11%)	10 13	90, 114, 140, 159	0
1	AF	106/157 (67%)	0.89	17 (16%)	5 8	90, 116, 140, 151	0
1	AG	104/157 (66%)	0.75	15 (14%)	6 9	92, 118, 142, 164	0
1	AH	106/157 (67%)	0.93	14 (13%)	7 10	88, 110, 127, 137	0
1	AI	106/157 (67%)	1.01	16 (15%)	5 8	93, 119, 144, 150	0
1	AJ	103/157 (65%)	0.94	19 (18%)	3 6	92, 126, 156, 173	0
1	B	103/157 (65%)	0.82	14 (13%)	7 10	95, 134, 152, 159	0
1	C	106/157 (67%)	1.00	19 (17%)	3 6	97, 124, 138, 150	0
1	D	106/157 (67%)	0.88	14 (13%)	7 10	89, 119, 137, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	104/157 (66%)	0.85	12 (11%) 9 12	92, 118, 150, 163	0
1	F	106/157 (67%)	0.84	15 (14%) 6 9	88, 113, 130, 141	0
1	G	105/157 (66%)	0.84	12 (11%) 10 12	97, 125, 154, 164	0
1	H	103/157 (65%)	1.04	19 (18%) 3 6	95, 128, 162, 175	0
1	I	107/157 (68%)	1.17	24 (22%) 2 4	90, 118, 141, 148	0
1	J	107/157 (68%)	1.04	15 (14%) 6 9	94, 117, 138, 143	0
1	K	106/157 (67%)	0.96	18 (16%) 4 7	98, 125, 147, 163	0
1	L	103/157 (65%)	1.00	18 (17%) 4 6	98, 130, 158, 169	0
1	M	106/157 (67%)	1.18	24 (22%) 2 4	93, 119, 138, 151	0
1	N	106/157 (67%)	0.90	17 (16%) 5 8	94, 119, 134, 149	0
1	O	104/157 (66%)	0.99	17 (16%) 4 8	91, 123, 155, 170	0
1	P	106/157 (67%)	1.18	25 (23%) 2 4	92, 114, 132, 148	0
1	Q	106/157 (67%)	1.29	24 (22%) 2 4	95, 124, 148, 161	0
1	R	103/157 (65%)	0.96	13 (12%) 8 11	92, 123, 153, 171	0
1	S	107/157 (68%)	0.86	16 (14%) 5 9	89, 116, 138, 151	0
1	T	106/157 (67%)	0.87	14 (13%) 7 10	90, 126, 150, 160	0
1	U	103/157 (65%)	1.31	32 (31%) 1 3	94, 122, 142, 156	0
1	V	106/157 (67%)	0.84	18 (16%) 4 7	91, 118, 140, 155	0
1	W	106/157 (67%)	0.95	19 (17%) 3 6	94, 125, 142, 159	0
1	X	105/157 (66%)	1.09	20 (19%) 3 6	94, 120, 153, 161	0
1	Y	106/157 (67%)	0.83	11 (10%) 11 13	89, 114, 135, 146	0
1	Z	106/157 (67%)	0.88	10 (9%) 14 16	103, 122, 142, 156	0
1	a	103/157 (65%)	0.81	9 (8%) 16 16	89, 135, 166, 179	0
1	b	107/157 (68%)	0.99	20 (18%) 3 6	92, 116, 136, 146	0
1	c	106/157 (67%)	1.06	16 (15%) 5 8	89, 127, 154, 163	0
1	d	103/157 (65%)	1.32	23 (22%) 2 4	92, 122, 146, 160	0
1	e	106/157 (67%)	0.89	17 (16%) 5 8	82, 115, 140, 157	0
1	ee	107/157 (68%)	1.31	26 (24%) 2 4	100, 130, 144, 151	0
1	f	106/157 (67%)	0.94	18 (16%) 4 7	96, 120, 137, 147	0
1	ff	106/157 (67%)	1.28	23 (21%) 2 4	99, 134, 157, 167	0
1	g	104/157 (66%)	1.30	22 (21%) 2 4	91, 121, 157, 165	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	gg	103/157 (65%)	1.55	28 (27%) 1 3	101, 140, 157, 167	0
1	h	106/157 (67%)	0.96	17 (16%) 5 8	99, 117, 137, 145	0
1	hh	106/157 (67%)	1.58	29 (27%) 1 3	109, 136, 156, 183	0
1	i	106/157 (67%)	1.06	23 (21%) 2 4	93, 122, 141, 156	0
1	ii	106/157 (67%)	1.46	29 (27%) 1 3	102, 131, 157, 167	0
1	j	103/157 (65%)	0.91	14 (13%) 7 10	90, 129, 154, 168	0
1	jj	104/157 (66%)	1.31	25 (24%) 2 4	107, 136, 164, 186	0
1	k	107/157 (68%)	0.76	12 (11%) 10 13	90, 120, 137, 153	0
1	kk	106/157 (67%)	1.20	23 (21%) 2 4	107, 129, 140, 151	0
1	l	106/157 (67%)	1.15	22 (20%) 2 4	87, 133, 155, 175	0
1	ll	106/157 (67%)	1.74	36 (33%) 1 2	106, 138, 160, 175	0
1	m	103/157 (65%)	0.95	20 (19%) 3 5	105, 129, 155, 171	0
1	mm	103/157 (65%)	1.32	24 (23%) 2 4	101, 143, 174, 183	0
1	n	106/157 (67%)	1.03	14 (13%) 7 10	92, 123, 144, 156	0
1	o	106/157 (67%)	1.01	14 (13%) 7 10	87, 121, 146, 165	0
1	p	105/157 (66%)	0.66	9 (8%) 16 17	90, 129, 168, 187	0
1	q	106/157 (67%)	0.92	15 (14%) 6 9	94, 118, 137, 147	0
1	r	106/157 (67%)	0.73	11 (10%) 11 13	95, 126, 147, 159	0
1	s	103/157 (65%)	1.04	17 (16%) 4 7	102, 134, 162, 176	0
1	t	107/157 (68%)	0.69	11 (10%) 12 13	87, 118, 136, 144	0
1	u	106/157 (67%)	0.88	13 (12%) 8 11	90, 126, 149, 167	0
1	v	103/157 (65%)	0.92	16 (15%) 5 8	95, 119, 135, 148	0
1	w	106/157 (67%)	1.35	27 (25%) 1 4	79, 115, 132, 157	0
1	x	106/157 (67%)	0.86	12 (11%) 10 13	82, 120, 142, 160	0
1	y	104/157 (66%)	0.70	10 (9%) 13 15	83, 123, 157, 164	0
1	z	106/157 (67%)	0.93	16 (15%) 5 8	83, 113, 133, 151	0
All	All	8524/12717 (67%)	1.01	1424 (16%) 4 7	79, 122, 153, 199	0

The worst 5 of 1424 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	CYS	12.5
1	gg	104	ALA	9.9

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Mol	Chain	Res	Type	RSRZ
1	hh	82	ALA	9.8
1	1	47	GLY	9.7
1	K	34	CYS	8.8

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 oligosaccharides 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.