



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 5, 2020 – 02:18 PM EST

PDB ID : 7JOQ
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
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)	:	2.14.6

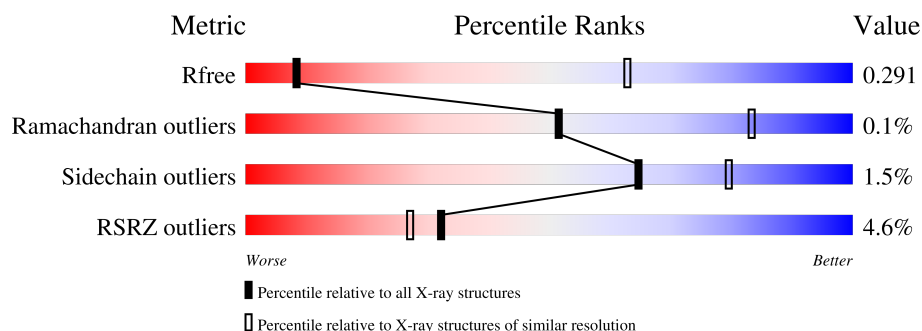
1 Overall quality at a glance

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}	130704	1025 (4.22-3.70)
Ramachandran outliers	138981	1047 (4.22-3.70)
Sidechain outliers	138945	1039 (4.22-3.70)
RSRZ outliers	127900	1013 (4.28-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	<div> <div>3%</div> <div>67%</div> <div>32%</div> </div>
1	1	157	<div> <div>3%</div> <div>65%</div> <div>34%</div> </div>
1	2	157	<div> <div>2%</div> <div>68%</div> <div>32%</div> </div>
1	3	157	<div> <div>2%</div> <div>67%</div> <div>32%</div> </div>
1	4	157	<div> <div>2%</div> <div>64%</div> <div>34%</div> </div>
1	5	157	<div> <div>67%</div> <div>32%</div> </div>

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Mol	Chain	Length	Quality of chain
1	6	157	<div> <div>4%</div> <div>67%</div> <div>32%</div> </div>
1	7	157	<div> <div>2%</div> <div>65%</div> <div>34%</div> </div>
1	8	157	<div> <div>2%</div> <div>67%</div> <div>32%</div> </div>
1	9	157	<div> <div>4%</div> <div>66%</div> <div>32%</div> </div>
1	A	157	<div> <div>2%</div> <div>67%</div> <div>32%</div> </div>
1	AA	157	<div> <div>3%</div> <div>64%</div> <div>34%</div> </div>
1	AB	157	<div> <div></div> <div>68%</div> <div>32%</div> </div>
1	AC	157	<div> <div>%</div> <div>67%</div> <div>32%</div> </div>
1	AD	157	<div> <div>3%</div> <div>64%</div> <div>34%</div> </div>
1	AE	157	<div> <div>%</div> <div>67%</div> <div>32%</div> </div>
1	AF	157	<div> <div>4%</div> <div>68%</div> <div>32%</div> </div>
1	AG	157	<div> <div>2%</div> <div>66%</div> <div>34%</div> </div>
1	AH	157	<div> <div>2%</div> <div>66%</div> <div>32%</div> </div>
1	AI	157	<div> <div></div> <div>67%</div> <div>32%</div> </div>
1	AJ	157	<div> <div>4%</div> <div>64%</div> <div>34%</div> </div>
1	B	157	<div> <div>%</div> <div>65%</div> <div>34%</div> </div>
1	C	157	<div> <div></div> <div>68%</div> <div>32%</div> </div>
1	D	157	<div> <div>%</div> <div>67%</div> <div>32%</div> </div>
1	E	157	<div> <div>3%</div> <div>66%</div> <div>34%</div> </div>
1	F	157	<div> <div>3%</div> <div>67%</div> <div>32%</div> </div>
1	G	157	<div> <div>3%</div> <div>66%</div> <div>33%</div> </div>
1	H	157	<div> <div>%</div> <div>66%</div> <div>34%</div> </div>
1	I	157	<div> <div></div> <div>68%</div> <div>32%</div> </div>
1	J	157	<div> <div>%</div> <div>68%</div> <div>32%</div> </div>
1	K	157	<div> <div>%</div> <div>67%</div> <div>32%</div> </div>

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Mol	Chain	Length	Quality of chain
1	L	157	
1	M	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	
1	Z	157	
1	a	157	
1	b	157	
1	c	157	
1	d	157	
1	e	157	
1	ee	157	
1	f	157	
1	ff	157	
1	g	157	
1	gg	157	

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Mol	Chain	Length	Quality of chain
1	h	157	% 68% 32%
1	hh	157	15% 67% 32%
1	i	157	4% 66% 32%
1	ii	157	11% 67% 32%
1	j	157	3% 64% 34%
1	jj	157	12% 65% 34%
1	k	157	68% 32%
1	kk	157	6% 67% 32%
1	l	157	3% 66% 32%
1	ll	157	15% 66% 32%
1	m	157	3% 65% 34%
1	mm	157	13% 64% 34%
1	n	157	% 68% 32%
1	o	157	2% 67% 32%
1	p	157	3% 67% 33%
1	q	157	2% 67% 32%
1	r	157	3% 66% 32%
1	s	157	3% 64% 34%
1	t	157	2% 68% 32%
1	u	157	2% 68% 32%
1	v	157	% 65% 34%
1	w	157	% 68% 32%
1	x	157	2% 67% 32%
1	y	157	% 66% 34%
1	z	157	2% 68% 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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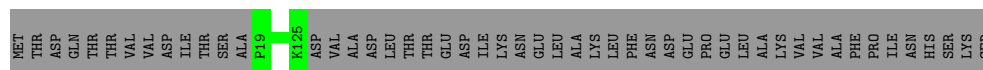
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	ll	106	Total	C	N	O	S	0	0	0
			779	492	141	145	1			
1	mm	103	Total	C	N	O	S	0	0	0
			755	475	137	142	1			

3 Residue-property plots

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.

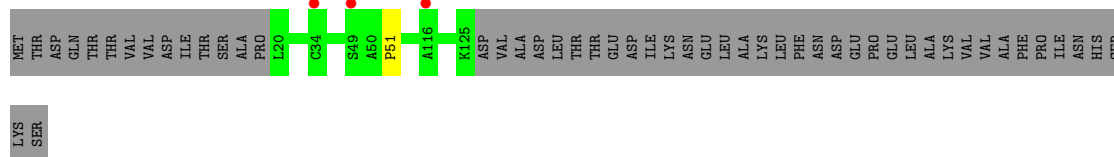
- Molecule 1: Small Terminase subunit

Chain I: 



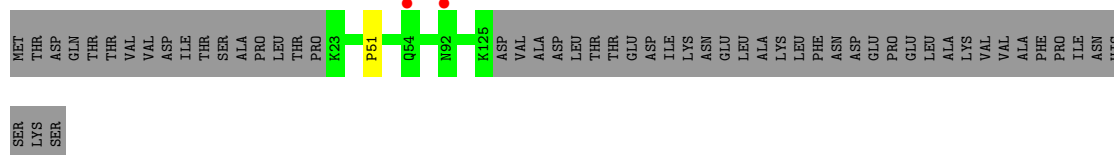
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Chain A: 



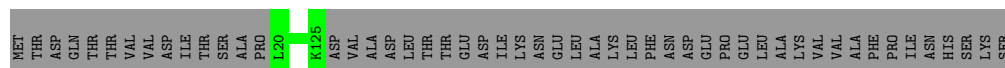
- Molecule 1: Small Terminase subunit

Chain B: 



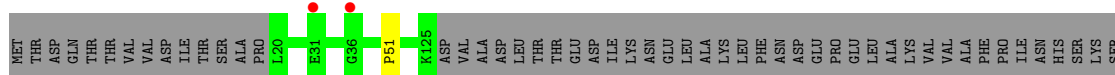
- Molecule 1: Small Terminase subunit

Chain C: 

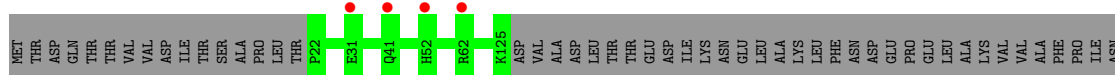


- Molecule 1: Small Terminase subunit

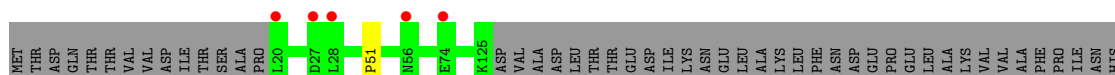
Chain D: 



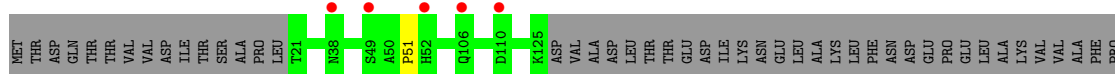
- Molecule 1: Small Terminase subunit



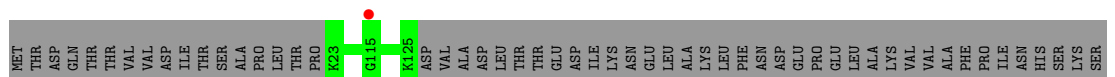
- Molecule 1: Small Terminase subunit



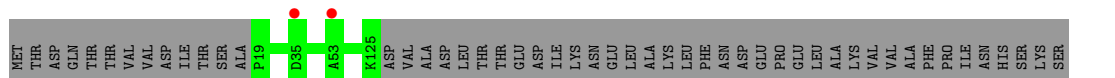
- Molecule 1: Small Terminase subunit



- Molecule 1: Small Terminase subunit

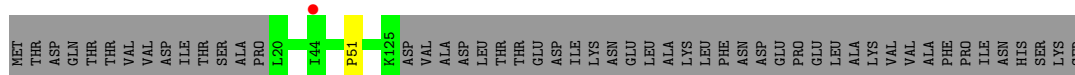


- Molecule 1: Small Terminase subunit

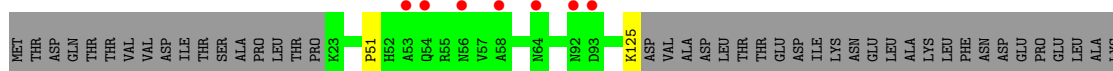


- Molecule 1: Small Terminase subunit

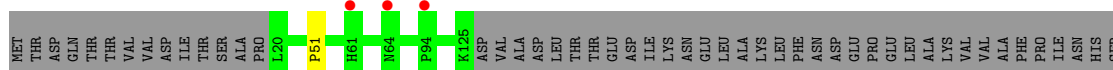




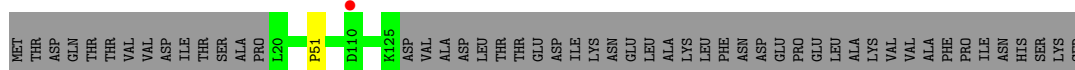
- Molecule 1: Small Terminase subunit



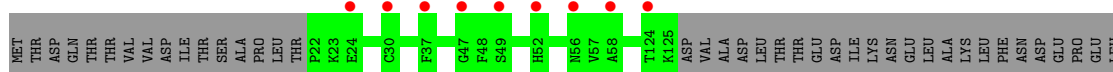
- Molecule 1: Small Terminase subunit



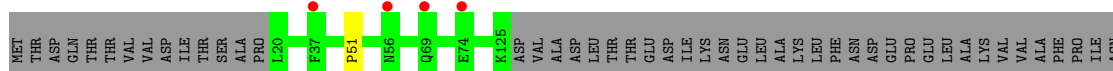
- Molecule 1: Small Terminase subunit



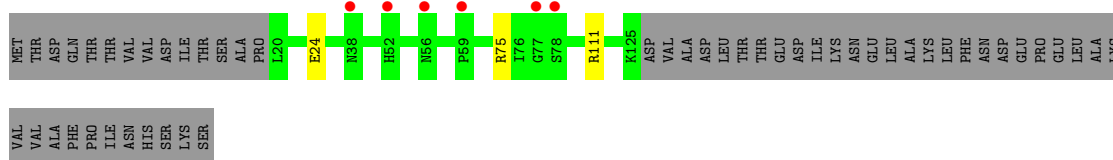
- Molecule 1: Small Terminase subunit



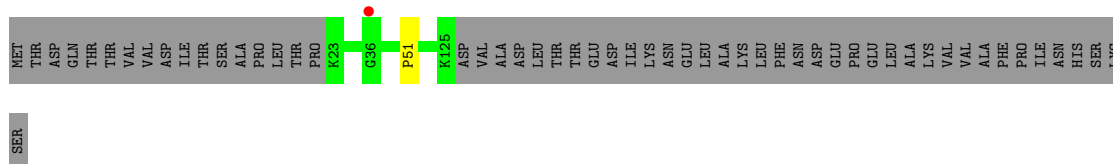
- Molecule 1: Small Terminase subunit



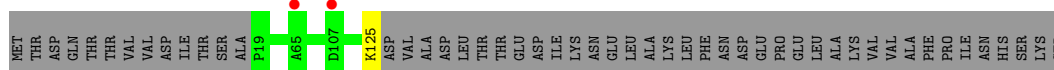
- Molecule 1: Small Terminase subunit



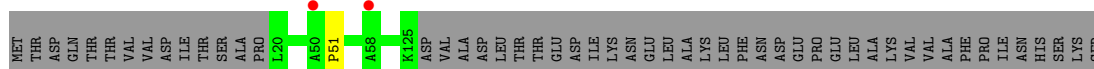
- Molecule 1: Small Terminase subunit



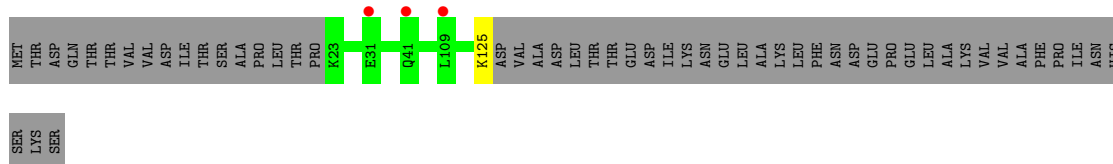
- Molecule 1: Small Terminase subunit



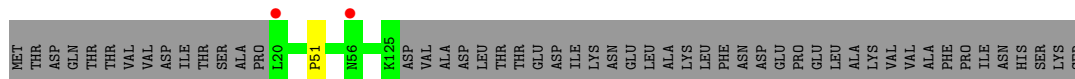
- Molecule 1: Small Terminase subunit



- Molecule 1: Small Terminase subunit



- Molecule 1: Small Terminase subunit

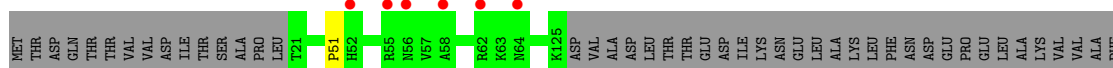


- Molecule 1: Small Terminase subunit



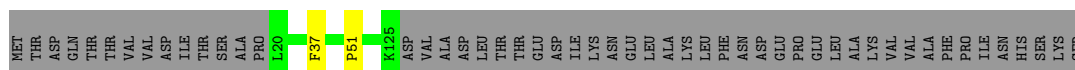
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- Molecule 1: Small Terminase subunit

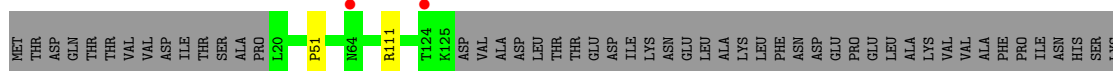


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- Molecule 1: Small Terminase subunit



- Molecule 1: Small Terminase subunit



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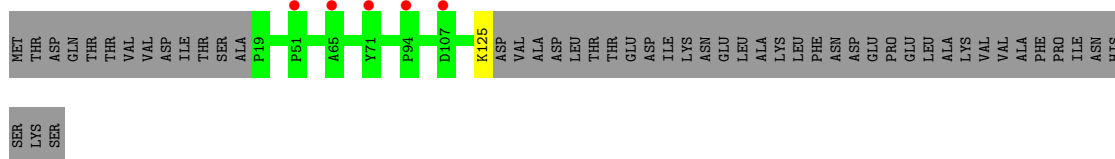
- Molecule 1: Small Terminase subunit



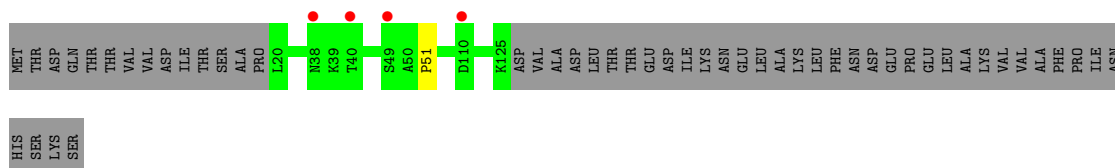
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- Molecule 1: Small Terminase subunit

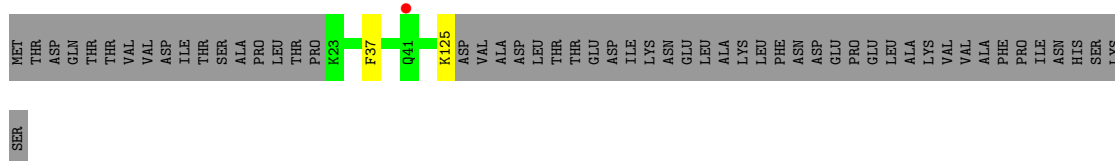




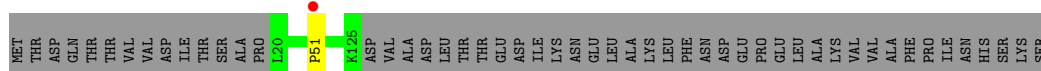
• Molecule 1: Small Terminase subunit



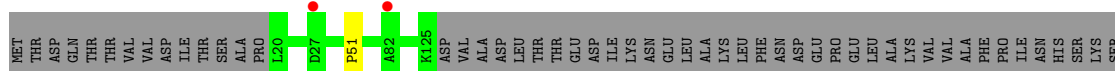
• Molecule 1: Small Terminase subunit



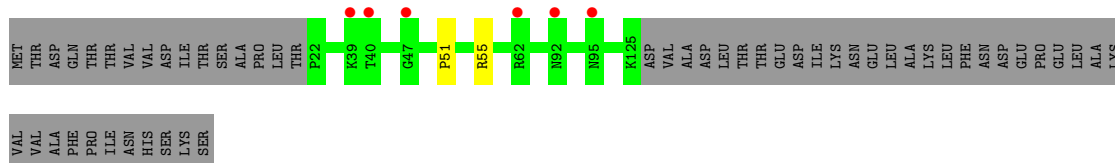
• Molecule 1: Small Terminase subunit



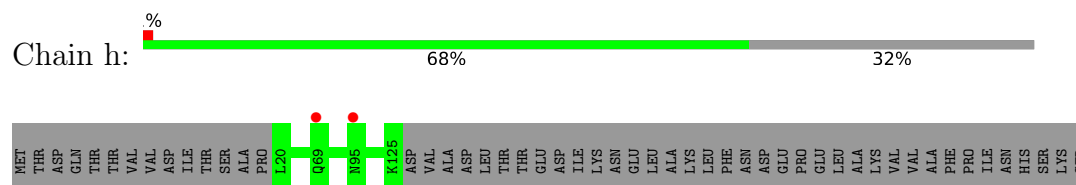
• Molecule 1: Small Terminase subunit



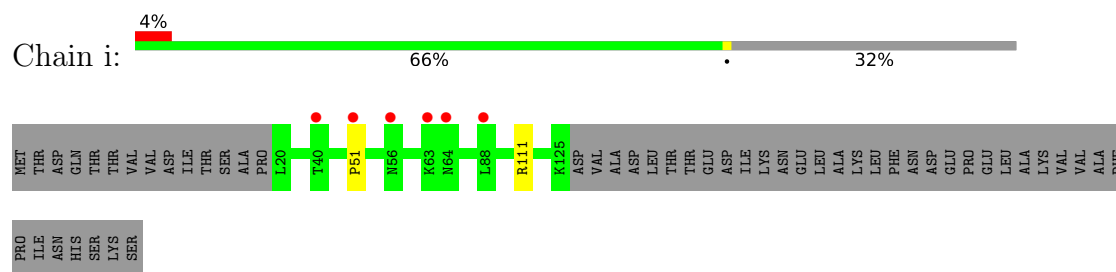
• Molecule 1: Small Terminase subunit



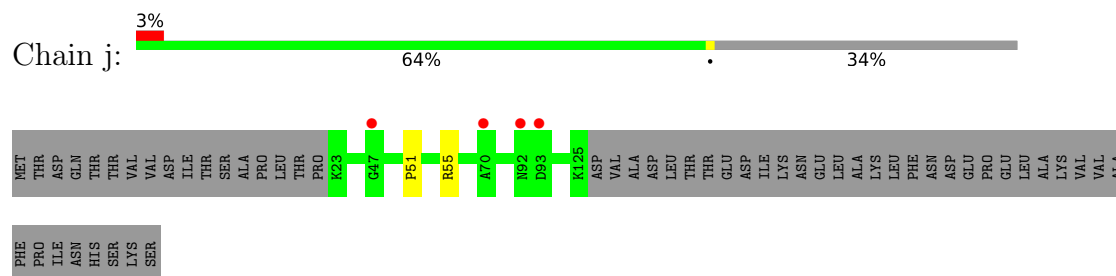
- Molecule 1: Small Terminase subunit



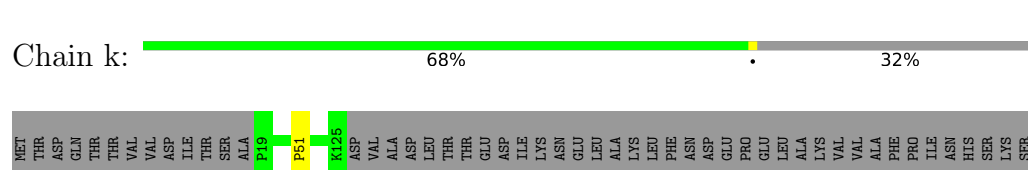
- Molecule 1: Small Terminase subunit



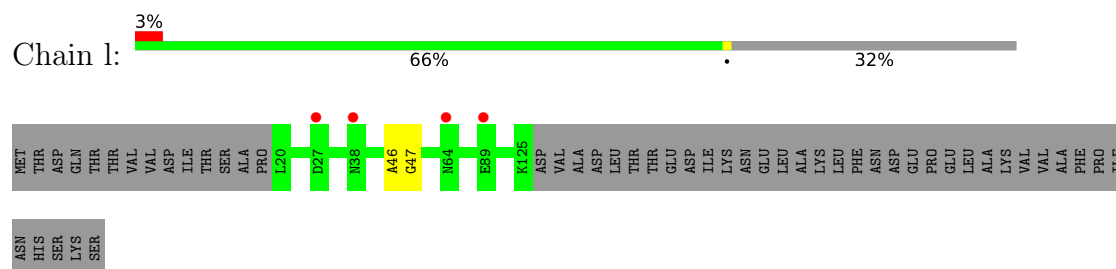
- Molecule 1: Small Terminase subunit



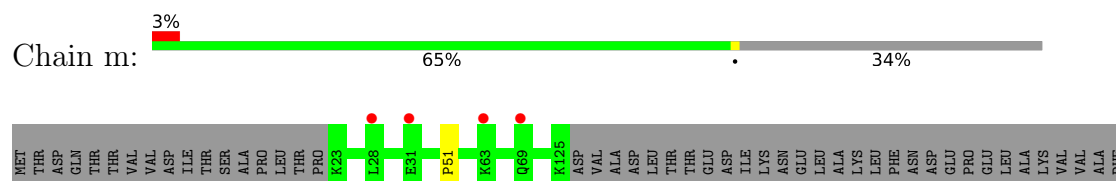
- Molecule 1: Small Terminase subunit



- Molecule 1: Small Terminase subunit



- Molecule 1: Small Terminase subunit



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• Molecule 1: Small Terminase subunit



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• Molecule 1: Small Terminase subunit



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• Molecule 1: Small Terminase subunit



MET THR ASP GLN THR THR VAL VAL ASP ILE THR THR SER SER ALA PRO L20 L95 K125 ASP VAL ALA ASP LEU THR THR THR GLU ASP ILE THR ASN GLU LEU LEU LYS LYS PHE ASN ASP GLU PRO GLU LEU LEU ALA LYS VAL VAL ALA PHE PRO ILE ASN HIS

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• Molecule 1: Small Terminase subunit



MET THR ASP GLN THR THR VAL VAL ASP ILE THR THR SER SER ALA PRO L20 L95 K125 ASP VAL ALA ASP LEU THR THR THR GLU ASP ILE THR ASN GLU LEU LEU LYS LYS PHE ASN ASP GLU PRO GLU LEU LEU ALA LYS VAL VAL ALA PHE PRO ILE ASN HIS

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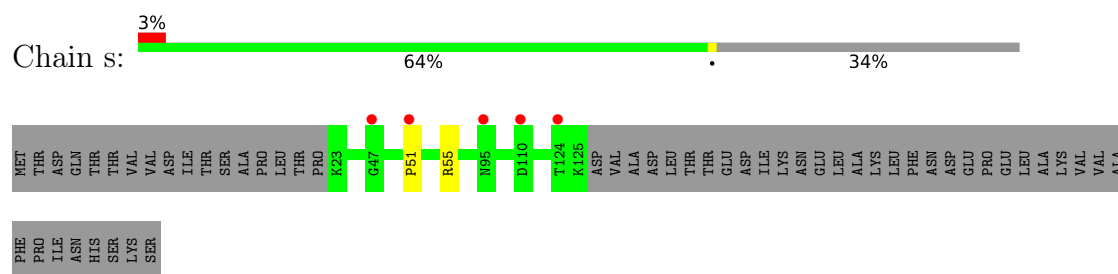
• Molecule 1: Small Terminase subunit



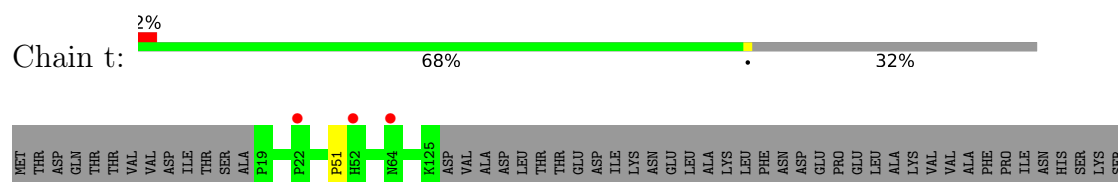
MET THR ASP GLN THR THR VAL VAL ASP ILE THR THR SER SER ALA PRO L20 L95 K125 ASP VAL ALA ASP LEU THR THR THR GLU ASP ILE THR ASN GLU LEU LEU LYS LYS PHE ASN ASP GLU PRO GLU LEU LEU ALA LYS VAL VAL ALA PHE PRO ILE ASN HIS

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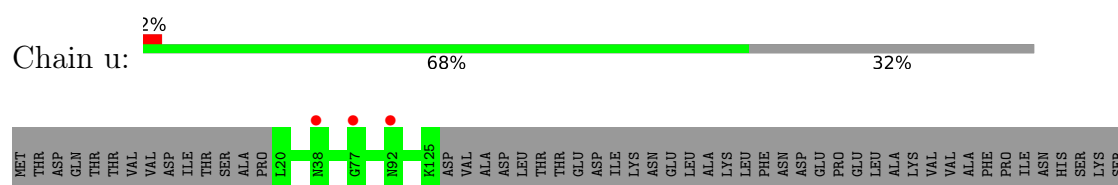
• Molecule 1: Small Terminase subunit



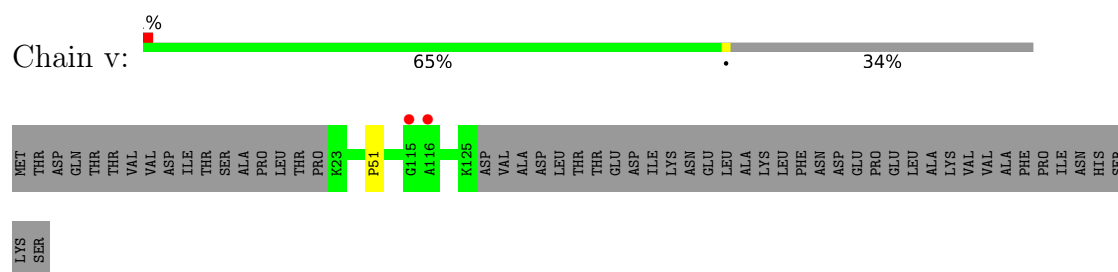
• Molecule 1: Small Terminase subunit



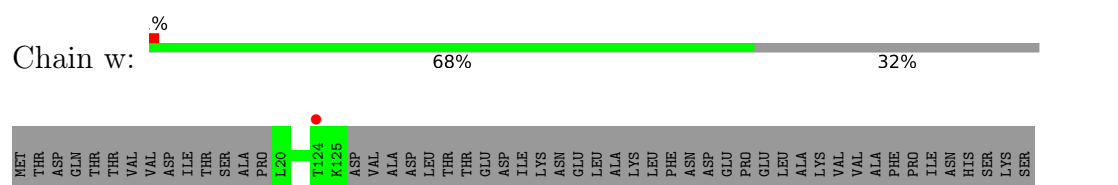
• Molecule 1: Small Terminase subunit



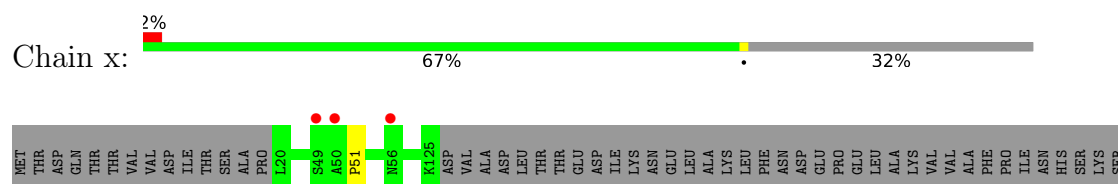
• Molecule 1: Small Terminase subunit



• Molecule 1: Small Terminase subunit

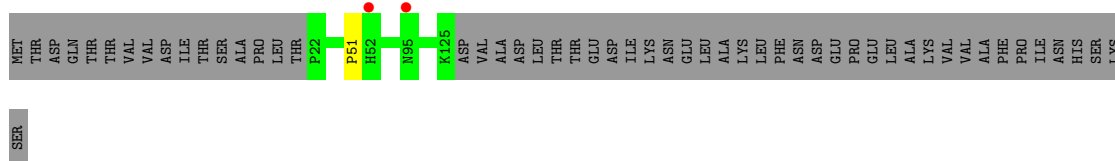


• Molecule 1: Small Terminase subunit

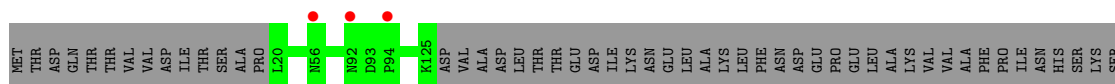


• Molecule 1: Small Terminase subunit

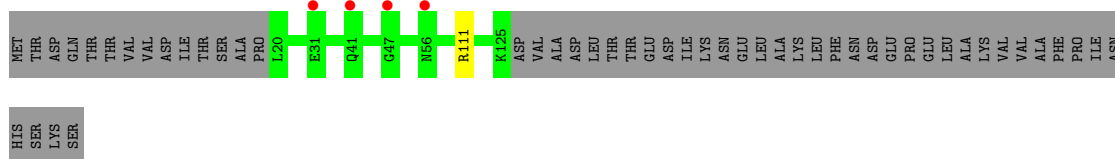




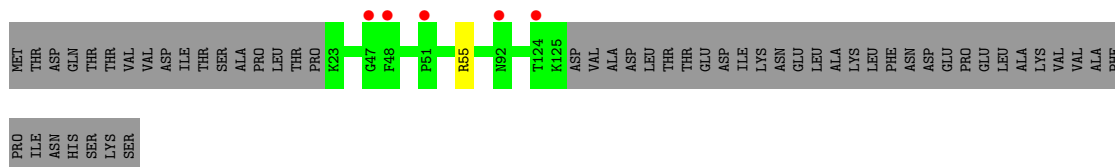
- Molecule 1: Small Terminase subunit



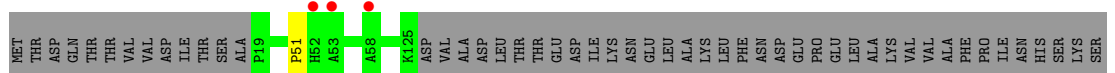
- Molecule 1: Small Terminase subunit



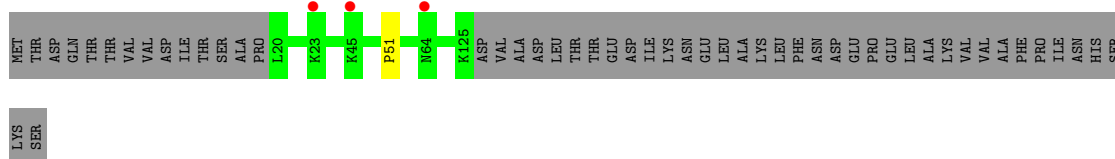
- Molecule 1: Small Terminase subunit



- Molecule 1: Small Terminase subunit



- Molecule 1: Small Terminase subunit

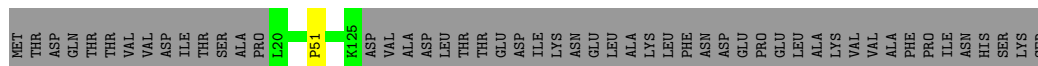


- Molecule 1: Small Terminase subunit

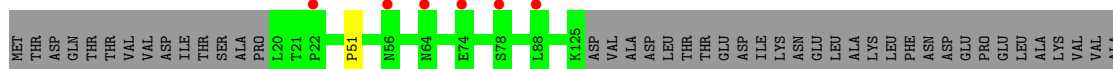


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- Molecule 1: Small Terminase subunit



- Molecule 1: Small Terminase subunit



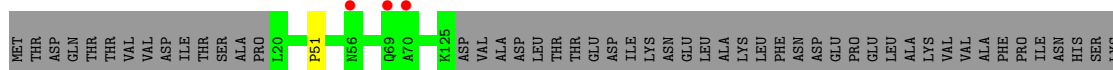
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- Molecule 1: Small Terminase subunit



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- Molecule 1: Small Terminase subunit

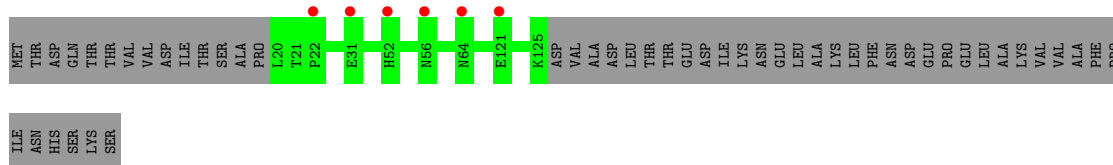


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- Molecule 1: Small Terminase subunit







• 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



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• Molecule 1: Small Terminase subunit



MET THR ASP GLN THR THR VAL VAL ASP ASP ILE THR THR SER ALA PRO L20 C30 C36 F37 N38 K39 T40 A46 G47 A50 P51 H52 I72 S73 N92 G113 K125 ASP VAL ALA ASP LEU THR THR GLU GLU ASP ILE LYS ASN GLU LEU LEU ALA LYS LEU PHE ASN ASP THR GLU

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• Molecule 1: Small Terminase subunit



MET THR THR ASP GLN THR THR VAL VAL ASP ASP ILE THR THR SER ALA PRO L20 C30 C36 F37 N38 K39 T40 A46 G47 F48 S49 A50 P51 H52 I72 S73 N92 G113 K125 ASP VAL ALA ASP LEU THR THR GLU

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• Molecule 1: Small Terminase subunit



MET THR THR ASP GLN THR THR VAL VAL ASP ASP ILE THR THR SER ALA PRO L20 C30 C36 F37 N38 K39 T40 A46 G47 P51 H52 A53 Q54 Y60 K63 N64 S73 E74 A80 P81 A82 A83 R84 L88 E89 D83 P94 G113 K125 ASP VAL ALA ASP LEU

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• Molecule 1: Small Terminase subunit



MET THR THR ASP GLN THR THR VAL VAL ASP ASP ILE THR THR SER ALA PRO L20 T21 P22 D27 C30 C34 D35 G36 F37 N38 S49 A50 P51 H52 A53 Y71 E75 A82 A83 V86 E89 A116 T124 K125 ASP VAL ALA ASP LEU THR THR GLU ASP THR LYS

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• Molecule 1: Small Terminase subunit



MET THR THR ASP GLN THR THR VAL VAL ASP ASP ILE THR THR SER ALA PRO L20 P22 K23 E24 A32 D35 G36 F37 N38 G47 A50 P51 H52 N56 V57 A58 H61 H62 I72 S73 S78 L88 N92 D107 K125 ASP VAL ALA ASP LEU THR THR GLU

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● Molecule 1: Small Terminase subunit



MET THR ASP GLN THR THR VAL VAL ASP ASP THR THR SER SER ALA PRO L20 L21 E24 E25 P51 A58 P59 H64 N92 G99 K103 A104 G115 K125 ASP VAL ALA ASP LEU THR THR GLU ASP ILE LYS ASN GLU LEU ALA LYS LEU PHE ASN ASP GLU PRO GLU

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● Molecule 1: Small Terminase subunit



MET THR ASP GLN THR THR VAL VAL ASP ASP THR THR SER SER ALA PRO L20 L21 T21 P22 K23 E24 L28 T40 Q41 A42 Y43 I44 K45 A46 G47 P51 H52 A53 Q54 A58 P59 E56 A83 R84 N92 D93 G98 G107 R111 A112 G113 F114 K125 ASP VAL ALA

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● Molecule 1: Small Terminase subunit



MET THR ASP GLN THR THR VAL VAL ASP ASP THR THR SER SER ALA PRO L20 L21 K23 P35 N38 F48 S49 A50 P51 Q54 R55 P59 T60 H61 R62 K63 H64 A70 S73 G77 S78 D79 A80 P81 A82 A83 G113 K125 ASP VAL ALA ASP LEU THR THR

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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) 95.6 (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 0.260 , 0.291	Depositor DCC
R_{free} test set	7364 reflections (5.13%)	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 , 5.9	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	0.83	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 [i](#)

5.1 Standard geometry [i](#)

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	0.28	0/789	0.57	0/1062
1	1	0.27	0/764	0.52	0/1028
1	2	0.26	0/799	0.49	0/1076
1	3	0.26	0/789	0.53	0/1062
1	4	0.26	0/768	0.48	0/1032
1	5	0.26	0/786	0.47	0/1058
1	6	0.25	0/789	0.48	0/1062
1	7	0.26	0/776	0.48	0/1043
1	8	0.25	0/786	0.46	0/1058
1	9	0.25	0/789	0.49	0/1062
1	A	0.25	0/789	0.49	0/1062
1	AA	0.25	0/764	0.45	0/1028
1	AB	0.25	0/799	0.47	0/1076
1	AC	0.25	0/789	0.51	0/1062
1	AD	0.25	0/768	0.45	0/1032
1	AE	0.25	0/786	0.45	0/1058
1	AF	0.25	0/789	0.49	0/1062
1	AG	0.25	0/776	0.46	0/1043
1	AH	0.25	0/786	0.48	0/1058
1	AI	0.26	0/789	0.50	0/1062
1	AJ	0.25	0/764	0.46	0/1028
1	B	0.27	0/768	0.47	0/1032
1	C	0.25	0/786	0.48	0/1058
1	D	0.26	0/789	0.51	0/1062
1	E	0.27	0/776	0.52	0/1043
1	F	0.26	0/786	0.51	0/1058
1	G	0.26	0/783	0.50	0/1054
1	H	0.26	0/764	0.49	0/1028
1	I	0.25	0/799	0.48	0/1076
1	J	0.25	0/799	0.48	0/1076
1	K	0.28	0/789	0.53	0/1062
1	L	0.26	0/768	0.49	0/1032
1	M	0.26	0/786	0.48	0/1058
1	N	0.26	0/789	0.51	0/1062

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	O	0.26	0/776	0.49	0/1043
1	P	0.25	0/786	0.51	0/1058
1	Q	0.27	0/791	0.53	0/1065
1	R	0.27	0/764	0.50	0/1028
1	S	0.27	0/799	0.54	0/1076
1	T	0.26	0/789	0.48	0/1062
1	U	0.26	0/768	0.50	0/1032
1	V	0.25	0/786	0.46	0/1058
1	W	0.26	0/789	0.49	0/1062
1	X	0.25	0/781	0.50	0/1051
1	Y	0.26	0/786	0.49	0/1058
1	Z	0.30	0/789	0.48	0/1062
1	a	0.26	0/764	0.46	0/1028
1	b	0.27	0/799	0.49	0/1076
1	c	0.26	0/789	0.49	0/1062
1	d	0.24	0/768	0.46	0/1032
1	e	0.26	0/786	0.48	0/1058
1	ee	0.25	0/799	0.51	0/1076
1	f	0.27	0/789	0.54	0/1062
1	ff	0.25	0/789	0.47	0/1062
1	g	0.26	0/776	0.52	0/1043
1	gg	0.25	0/768	0.45	0/1032
1	h	0.25	0/786	0.52	0/1058
1	hh	0.25	0/786	0.47	0/1058
1	i	0.26	0/789	0.50	0/1062
1	ii	0.25	0/789	0.49	0/1062
1	j	0.26	0/764	0.49	0/1028
1	jj	0.25	0/773	0.54	1/1039 (0.1%)
1	k	0.26	0/799	0.48	0/1076
1	kk	0.25	0/786	0.48	0/1058
1	l	0.27	0/789	0.49	0/1062
1	ll	0.26	0/789	0.48	0/1062
1	m	0.26	0/768	0.46	0/1032
1	mm	0.25	0/764	0.49	0/1028
1	n	0.26	0/786	0.47	0/1058
1	o	0.26	0/789	0.49	0/1062
1	p	0.26	0/781	0.48	0/1051
1	q	0.26	0/786	0.50	0/1058
1	r	0.28	0/789	0.51	0/1062
1	s	0.26	0/764	0.51	0/1028
1	t	0.26	0/799	0.52	0/1076
1	u	0.29	0/789	0.52	0/1062
1	v	0.25	0/768	0.47	0/1032

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	w	0.26	0/786	0.48	0/1058
1	x	0.26	0/789	0.50	0/1062
1	y	0.26	0/776	0.49	0/1043
1	z	0.26	0/786	0.50	0/1058
All	All	0.26	0/63417	0.49	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	6.00	110.50	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	15	52
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
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%)	15	52
1	R	101/157 (64%)	93 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	15	52
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%)	15	52
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
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%)	8	40
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	15	52
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%)	51	83

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	24	GLU
1	AH	56	ASN
1	Y	37	PHE
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%)	66 (98%)	1 (2%)	65	79
1	1	64/130 (49%)	63 (98%)	1 (2%)	62	79
1	2	69/130 (53%)	68 (99%)	1 (1%)	67	80
1	3	67/130 (52%)	66 (98%)	1 (2%)	65	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4	65/130 (50%)	63 (97%)	2 (3%)	40	63
1	5	66/130 (51%)	65 (98%)	1 (2%)	65	79
1	6	67/130 (52%)	66 (98%)	1 (2%)	65	79
1	7	66/130 (51%)	64 (97%)	2 (3%)	41	64
1	8	66/130 (51%)	65 (98%)	1 (2%)	65	79
1	9	67/130 (52%)	65 (97%)	2 (3%)	41	64
1	A	67/130 (52%)	66 (98%)	1 (2%)	65	79
1	AA	64/130 (49%)	62 (97%)	2 (3%)	40	63
1	AB	69/130 (53%)	69 (100%)	0	100	100
1	AC	67/130 (52%)	66 (98%)	1 (2%)	65	79
1	AD	65/130 (50%)	63 (97%)	2 (3%)	40	63
1	AE	66/130 (51%)	65 (98%)	1 (2%)	65	79
1	AF	67/130 (52%)	67 (100%)	0	100	100
1	AG	66/130 (51%)	65 (98%)	1 (2%)	65	79
1	AH	66/130 (51%)	65 (98%)	1 (2%)	65	79
1	AI	67/130 (52%)	66 (98%)	1 (2%)	65	79
1	AJ	64/130 (49%)	62 (97%)	2 (3%)	40	63
1	B	65/130 (50%)	64 (98%)	1 (2%)	65	79
1	C	66/130 (51%)	66 (100%)	0	100	100
1	D	67/130 (52%)	66 (98%)	1 (2%)	65	79
1	E	66/130 (51%)	66 (100%)	0	100	100
1	F	66/130 (51%)	65 (98%)	1 (2%)	65	79
1	G	67/130 (52%)	66 (98%)	1 (2%)	65	79
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%)	65	79
1	L	65/130 (50%)	63 (97%)	2 (3%)	40	63
1	M	66/130 (51%)	65 (98%)	1 (2%)	65	79
1	N	67/130 (52%)	66 (98%)	1 (2%)	65	79
1	O	66/130 (51%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	66/130 (51%)	65 (98%)	1 (2%)	65	79
1	Q	68/130 (52%)	66 (97%)	2 (3%)	42	64
1	R	64/130 (49%)	63 (98%)	1 (2%)	62	79
1	S	69/130 (53%)	68 (99%)	1 (1%)	67	80
1	T	67/130 (52%)	66 (98%)	1 (2%)	65	79
1	U	65/130 (50%)	64 (98%)	1 (2%)	65	79
1	V	66/130 (51%)	65 (98%)	1 (2%)	65	79
1	W	67/130 (52%)	66 (98%)	1 (2%)	65	79
1	X	66/130 (51%)	65 (98%)	1 (2%)	65	79
1	Y	66/130 (51%)	65 (98%)	1 (2%)	65	79
1	Z	67/130 (52%)	65 (97%)	2 (3%)	41	64
1	a	64/130 (49%)	63 (98%)	1 (2%)	62	79
1	b	69/130 (53%)	68 (99%)	1 (1%)	67	80
1	c	67/130 (52%)	66 (98%)	1 (2%)	65	79
1	d	65/130 (50%)	64 (98%)	1 (2%)	65	79
1	e	66/130 (51%)	65 (98%)	1 (2%)	65	79
1	ee	69/130 (53%)	68 (99%)	1 (1%)	67	80
1	f	67/130 (52%)	66 (98%)	1 (2%)	65	79
1	ff	67/130 (52%)	66 (98%)	1 (2%)	65	79
1	g	66/130 (51%)	64 (97%)	2 (3%)	41	64
1	gg	65/130 (50%)	63 (97%)	2 (3%)	40	63
1	h	66/130 (51%)	66 (100%)	0	100	100
1	hh	66/130 (51%)	65 (98%)	1 (2%)	65	79
1	i	67/130 (52%)	65 (97%)	2 (3%)	41	64
1	ii	67/130 (52%)	66 (98%)	1 (2%)	65	79
1	j	64/130 (49%)	62 (97%)	2 (3%)	40	63
1	jj	65/130 (50%)	64 (98%)	1 (2%)	65	79
1	k	69/130 (53%)	68 (99%)	1 (1%)	67	80
1	kk	66/130 (51%)	65 (98%)	1 (2%)	65	79
1	l	67/130 (52%)	67 (100%)	0	100	100
1	ll	67/130 (52%)	65 (97%)	2 (3%)	41	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	m	65/130 (50%)	64 (98%)	1 (2%)	65	79
1	mm	64/130 (49%)	62 (97%)	2 (3%)	40	63
1	n	66/130 (51%)	66 (100%)	0	100	100
1	o	67/130 (52%)	66 (98%)	1 (2%)	65	79
1	p	66/130 (51%)	66 (100%)	0	100	100
1	q	66/130 (51%)	65 (98%)	1 (2%)	65	79
1	r	67/130 (52%)	66 (98%)	1 (2%)	65	79
1	s	64/130 (49%)	62 (97%)	2 (3%)	40	63
1	t	69/130 (53%)	68 (99%)	1 (1%)	67	80
1	u	67/130 (52%)	67 (100%)	0	100	100
1	v	65/130 (50%)	64 (98%)	1 (2%)	65	79
1	w	66/130 (51%)	66 (100%)	0	100	100
1	x	67/130 (52%)	66 (98%)	1 (2%)	65	79
1	y	66/130 (51%)	65 (98%)	1 (2%)	65	79
1	z	66/130 (51%)	66 (100%)	0	100	100
All	All	5373/10530 (51%)	5291 (98%)	82 (2%)	65	79

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	o	51	PRO
1	y	51	PRO
1	ii	51	PRO
1	q	51	PRO
1	s	55	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	i	61	HIS
1	j	118	GLN
1	ff	41	GLN
1	f	52	HIS
1	gg	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 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, 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%)	0.25	4 (3%) 40 32	84, 128, 146, 158	0
1	1	103/157 (65%)	0.29	5 (4%) 29 25	82, 133, 170, 199	0
1	2	107/157 (68%)	0.06	3 (2%) 53 42	94, 114, 139, 150	0
1	3	106/157 (67%)	0.29	3 (2%) 53 42	95, 122, 140, 158	0
1	4	103/157 (65%)	0.36	3 (2%) 51 41	95, 121, 140, 150	0
1	5	106/157 (67%)	0.12	0 100 100	95, 118, 140, 154	0
1	6	106/157 (67%)	0.34	6 (5%) 23 20	91, 123, 143, 151	0
1	7	104/157 (66%)	0.12	3 (2%) 51 41	97, 124, 156, 175	0
1	8	106/157 (67%)	0.25	3 (2%) 53 42	91, 120, 138, 147	0
1	9	106/157 (67%)	0.50	7 (6%) 18 14	85, 126, 148, 161	0
1	A	106/157 (67%)	0.13	3 (2%) 53 42	98, 124, 146, 157	0
1	AA	103/157 (65%)	0.41	5 (4%) 29 25	92, 132, 170, 189	0
1	AB	107/157 (68%)	0.11	0 100 100	90, 117, 142, 155	0
1	AC	106/157 (67%)	0.19	2 (1%) 66 58	91, 122, 140, 148	0
1	AD	103/157 (65%)	0.25	4 (3%) 39 31	86, 119, 141, 159	0
1	AE	106/157 (67%)	-0.02	1 (0%) 84 77	90, 114, 140, 159	0
1	AF	106/157 (67%)	0.13	6 (5%) 23 20	90, 116, 140, 151	0
1	AG	104/157 (66%)	0.09	3 (2%) 51 41	92, 118, 143, 164	0
1	AH	106/157 (67%)	0.10	3 (2%) 53 42	88, 110, 127, 137	0
1	AI	106/157 (67%)	0.28	0 100 100	93, 119, 144, 150	0
1	AJ	103/157 (65%)	0.33	6 (5%) 23 19	92, 126, 156, 173	0
1	B	103/157 (65%)	0.11	2 (1%) 66 58	95, 134, 152, 159	0
1	C	106/157 (67%)	0.22	0 100 100	97, 124, 138, 150	0
1	D	106/157 (67%)	0.16	2 (1%) 66 58	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%)	0.23	4 (3%)	40	32	92, 118, 150, 163	0
1	F	106/157 (67%)	0.15	5 (4%)	31	26	88, 113, 130, 141	0
1	G	105/157 (66%)	0.33	5 (4%)	30	26	97, 125, 154, 164	0
1	H	103/157 (65%)	0.20	1 (0%)	82	74	95, 128, 162, 175	0
1	I	107/157 (68%)	0.27	0	100	100	90, 118, 141, 148	0
1	J	107/157 (68%)	0.23	2 (1%)	66	58	94, 117, 138, 143	0
1	K	106/157 (67%)	0.21	1 (0%)	84	77	98, 125, 147, 163	0
1	L	103/157 (65%)	0.30	7 (6%)	17	14	98, 130, 158, 169	0
1	M	106/157 (67%)	0.25	3 (2%)	53	42	93, 119, 138, 151	0
1	N	106/157 (67%)	0.26	1 (0%)	84	77	94, 119, 134, 149	0
1	O	104/157 (66%)	0.49	9 (8%)	10	9	91, 123, 155, 170	0
1	P	106/157 (67%)	0.23	4 (3%)	40	32	92, 114, 132, 148	0
1	Q	106/157 (67%)	0.42	6 (5%)	23	20	95, 124, 148, 161	0
1	R	103/157 (65%)	0.17	1 (0%)	82	74	92, 123, 153, 171	0
1	S	107/157 (68%)	0.26	2 (1%)	66	58	89, 116, 138, 151	0
1	T	106/157 (67%)	0.34	2 (1%)	66	58	90, 126, 150, 160	0
1	U	103/157 (65%)	0.38	3 (2%)	51	41	94, 122, 142, 156	0
1	V	106/157 (67%)	0.09	2 (1%)	66	58	91, 118, 140, 155	0
1	W	106/157 (67%)	0.25	4 (3%)	40	32	94, 125, 142, 159	0
1	X	105/157 (66%)	0.38	6 (5%)	23	20	94, 120, 153, 161	0
1	Y	106/157 (67%)	0.08	0	100	100	89, 114, 135, 146	0
1	Z	106/157 (67%)	0.14	2 (1%)	66	58	103, 122, 142, 156	0
1	a	103/157 (65%)	0.29	4 (3%)	39	31	89, 135, 166, 179	0
1	b	107/157 (68%)	0.33	5 (4%)	31	26	92, 116, 136, 146	0
1	c	106/157 (67%)	0.40	4 (3%)	40	32	89, 127, 154, 163	0
1	d	103/157 (65%)	0.35	1 (0%)	82	74	92, 122, 146, 160	0
1	e	106/157 (67%)	0.06	1 (0%)	84	77	82, 115, 140, 157	0
1	ee	107/157 (68%)	1.05	23 (21%)	0	1	100, 130, 144, 151	0
1	f	106/157 (67%)	0.17	2 (1%)	66	58	96, 120, 137, 147	0
1	ff	106/157 (67%)	0.85	15 (14%)	2	3	99, 134, 157, 167	0
1	g	104/157 (66%)	0.43	6 (5%)	23	19	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%)	1.07	20 (19%) 1 1	101, 140, 157, 167	0
1	h	106/157 (67%)	0.18	2 (1%) 66 58	99, 117, 137, 145	0
1	hh	106/157 (67%)	1.30	23 (21%) 0 1	109, 136, 156, 183	0
1	i	106/157 (67%)	0.34	6 (5%) 23 20	93, 122, 141, 156	0
1	ii	106/157 (67%)	1.13	18 (16%) 1 2	102, 131, 157, 167	0
1	j	103/157 (65%)	0.35	4 (3%) 39 31	90, 129, 155, 168	0
1	jj	104/157 (66%)	0.98	19 (18%) 1 1	107, 136, 164, 186	0
1	k	107/157 (68%)	-0.00	0 100 100	90, 120, 137, 153	0
1	kk	106/157 (67%)	0.84	10 (9%) 8 8	107, 129, 140, 151	0
1	l	106/157 (67%)	0.37	4 (3%) 40 32	87, 133, 155, 175	0
1	ll	106/157 (67%)	1.24	23 (21%) 0 1	106, 138, 160, 175	0
1	m	103/157 (65%)	0.28	4 (3%) 39 31	105, 129, 155, 171	0
1	mm	103/157 (65%)	1.04	20 (19%) 1 1	101, 143, 174, 183	0
1	n	106/157 (67%)	0.26	1 (0%) 84 77	92, 123, 144, 156	0
1	o	106/157 (67%)	0.33	3 (2%) 53 42	87, 121, 146, 165	0
1	p	105/157 (66%)	0.22	4 (3%) 40 32	90, 129, 168, 187	0
1	q	106/157 (67%)	0.16	3 (2%) 53 42	94, 118, 137, 147	0
1	r	106/157 (67%)	0.22	5 (4%) 31 26	95, 126, 147, 159	0
1	s	103/157 (65%)	0.35	5 (4%) 29 25	102, 134, 162, 176	0
1	t	107/157 (68%)	0.08	3 (2%) 53 42	87, 118, 136, 144	0
1	u	106/157 (67%)	0.25	3 (2%) 53 42	90, 126, 149, 167	0
1	v	103/157 (65%)	0.08	2 (1%) 66 58	95, 119, 135, 148	0
1	w	106/157 (67%)	0.26	1 (0%) 84 77	79, 115, 132, 157	0
1	x	106/157 (67%)	0.18	3 (2%) 53 42	82, 120, 142, 160	0
1	y	104/157 (66%)	0.05	2 (1%) 66 58	83, 123, 157, 164	0
1	z	106/157 (67%)	0.15	3 (2%) 53 42	83, 113, 133, 151	0
All	All	8524/12717 (67%)	0.33	396 (4%) 32 27	79, 122, 153, 199	0

The worst 5 of 396 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	ff	38	ASN	8.2
1	ll	54	GLN	6.9

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Mol	Chain	Res	Type	RSRZ
1	gg	40	THR	6.5
1	hh	54	GLN	6.1
1	jj	92	ASN	6.1

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.