Full wwPDB X-ray Structure Validation Report (i)

Oct 9, 2023 – 08:37 AM EDT

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 Full wwPDB X-ray Structure Validation 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 (i) 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 (i)) were used in the production of this report:

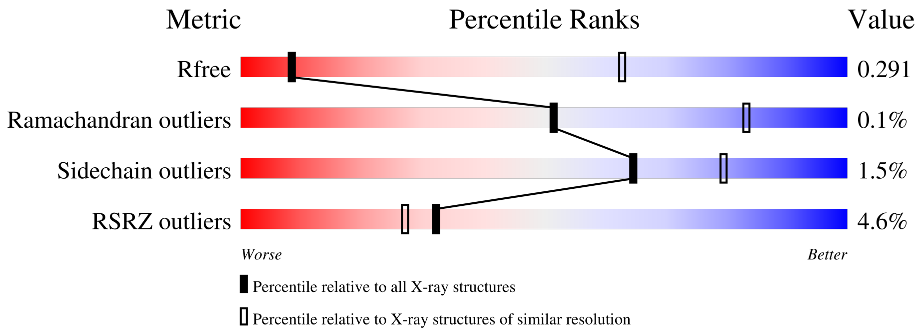
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

Mol	Chain	Length	Quality of chain
1	0	157	3% 67% • 32%
1	1	157	3% 65% • 34%
1	2	157	2% 68% • 32%
1	3	157	2% 67% • 32%
1	4	157	2% 64% • 34%
1	5	157	67% • 32%

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

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Mol	Chain	Length	Quality of chain
1	L	157	4% 64% • 34%
1	M	157	2% 67% • 32%
1	N	157	% 67% • 32%
1	O	157	6% 66% 34%
1	P	157	3% 67% • 32%
1	Q	157	4% 66% • 32%
1	R	157	% 65% • 34%
1	S	157	% 68% • 32%
1	T	157	% 67% • 32%
1	U	157	2% 65% • 34%
1	V	157	% 67% • 32%
1	W	157	3% 67% • 32%
1	X	157	4% 66% • 33%
1	Y	157	66% • 32%
1	Z	157	% 66% • 32%
1	a	157	3% 65% • 34%
1	b	157	3% 68% • 32%
1	c	157	3% 67% • 32%
1	d	157	% 64% • 34%
1	e	157	% 67% • 32%
1	ee	157	15% 68% • 32%
1	f	157	% 67% • 32%
1	ff	157	10% 67% • 32%
1	g	157	4% 65% • 34%
1	gg	157	13% 64% • 34%

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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 (i)

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

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

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

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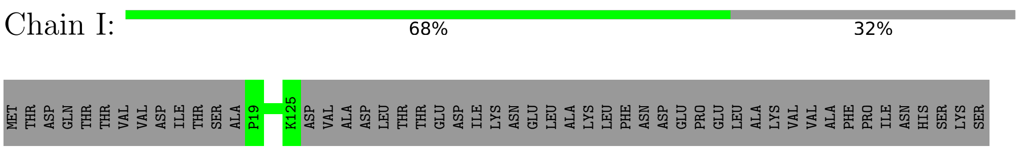
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	ll	106	Total 779	C 492	N 141	O 145	S 1	0	0	0
1	mm	103	Total 755	C 475	N 137	O 142	S 1	0	0	0

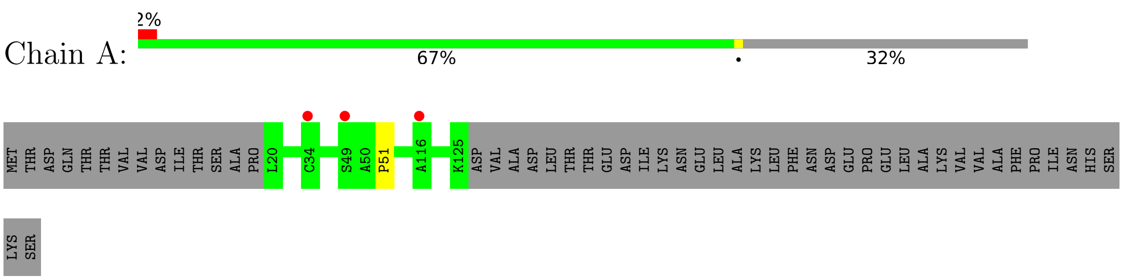
3 Residue-property plots (i)

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.

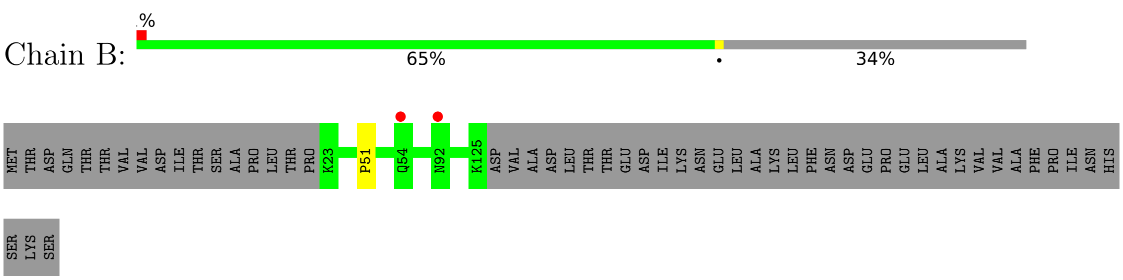
- Molecule 1: Small Terminase subunit



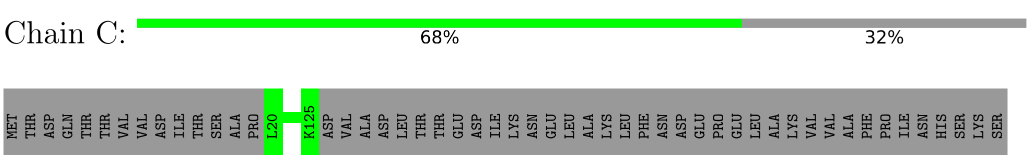
- Molecule 1: Small Terminase subunit



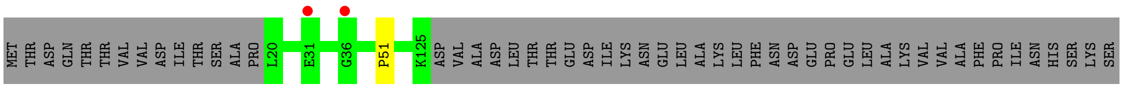
- Molecule 1: Small Terminase subunit



- Molecule 1: Small Terminase subunit

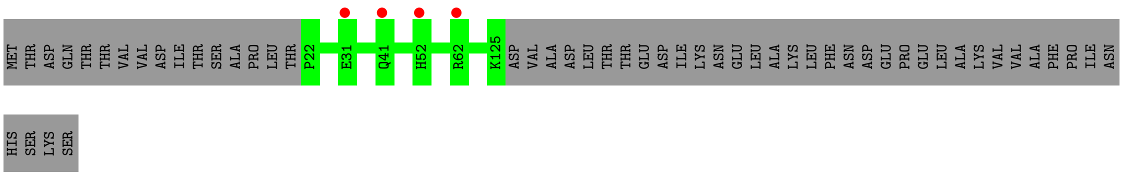


- Molecule 1: Small Terminase subunit



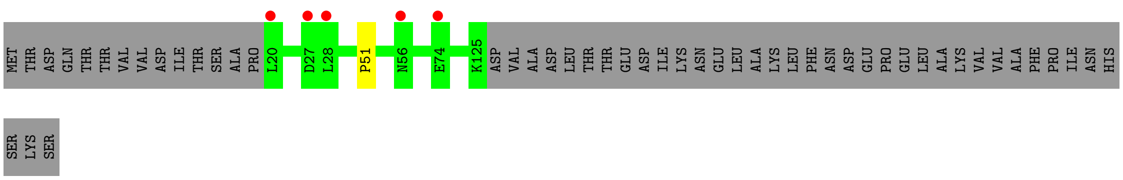
• Molecule 1: Small Terminase subunit

Chain E:



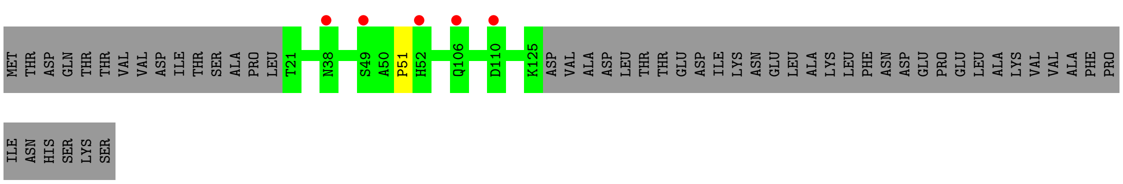
• Molecule 1: Small Terminase subunit

Chain F:



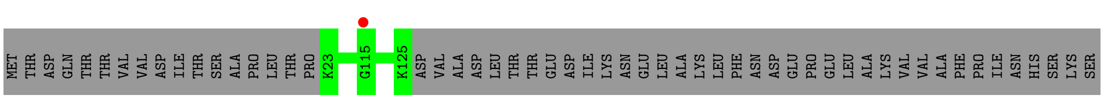
• Molecule 1: Small Terminase subunit

Chain G:



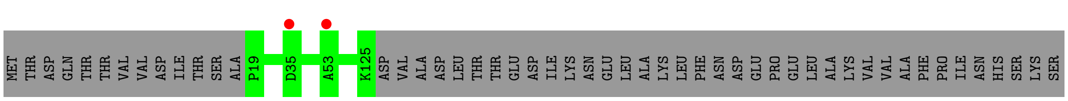
• Molecule 1: Small Terminase subunit

Chain H:



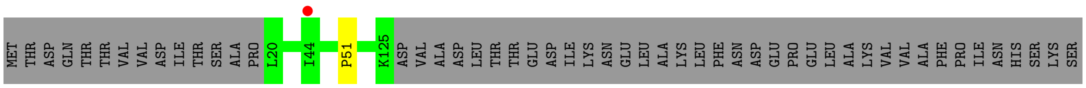
• Molecule 1: Small Terminase subunit

Chain J:



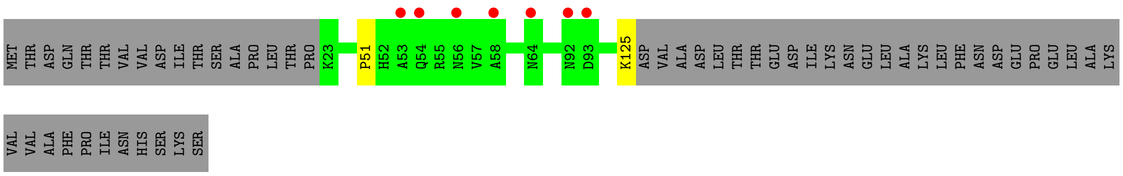
• Molecule 1: Small Terminase subunit

Chain K:



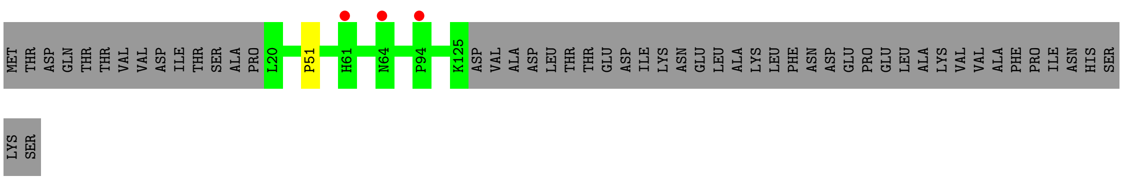
• Molecule 1: Small Terminase subunit

Chain L:



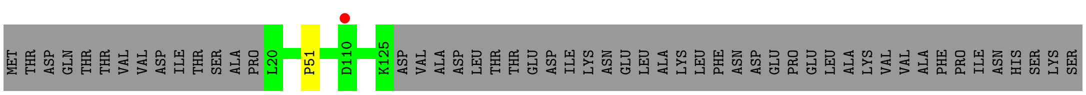
• Molecule 1: Small Terminase subunit

Chain M:



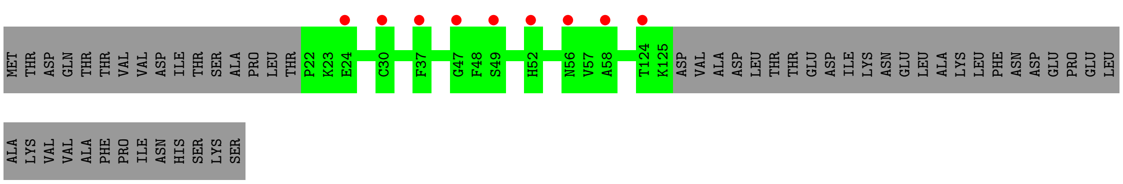
• Molecule 1: Small Terminase subunit

Chain N:



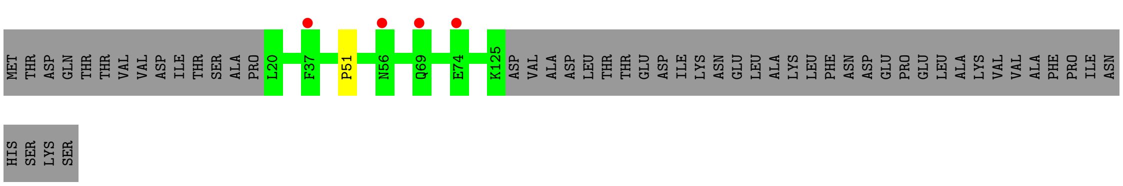
• Molecule 1: Small Terminase subunit

Chain O:



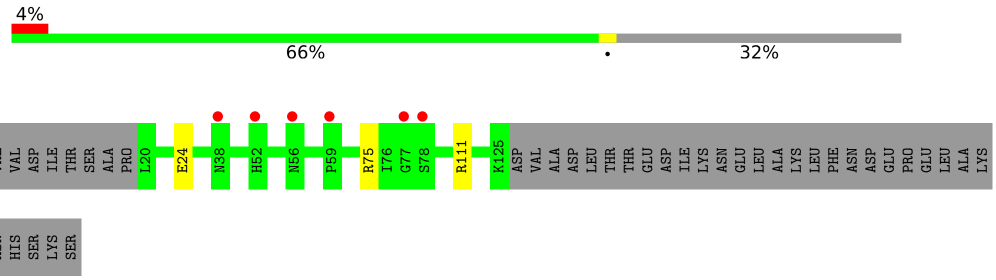
• Molecule 1: Small Terminase subunit

Chain P:



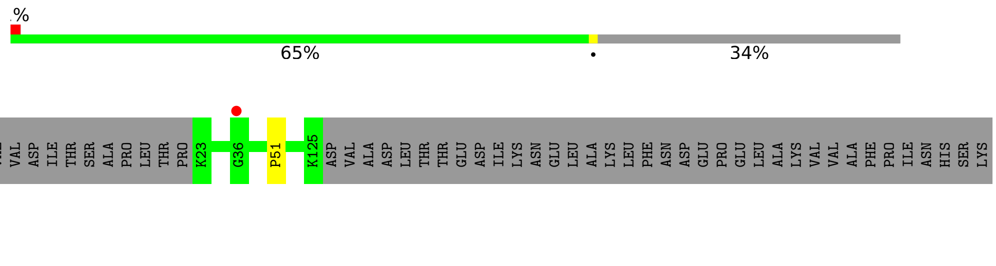
• Molecule 1: Small Terminase subunit

Chain Q:



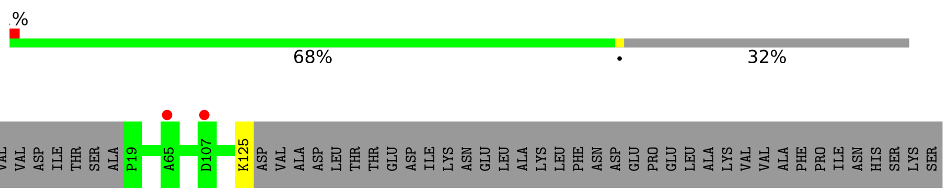
• Molecule 1: Small Terminase subunit

Chain R:



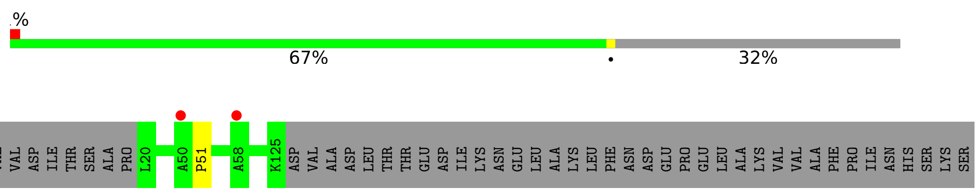
• Molecule 1: Small Terminase subunit

Chain S:



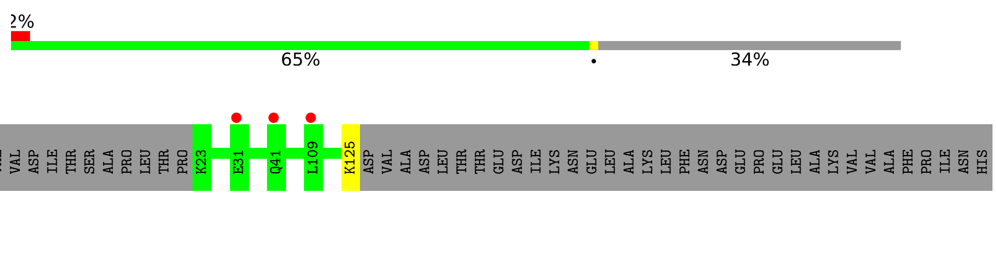
• Molecule 1: Small Terminase subunit

Chain T:



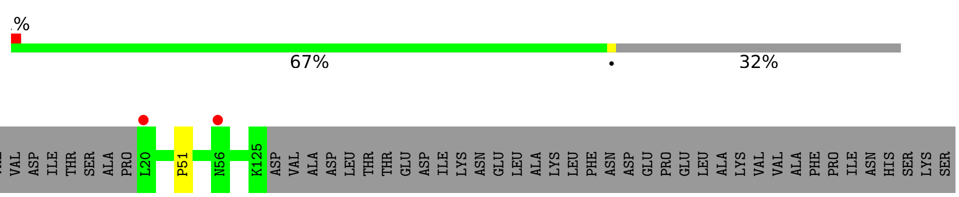
• Molecule 1: Small Terminase subunit

Chain U:

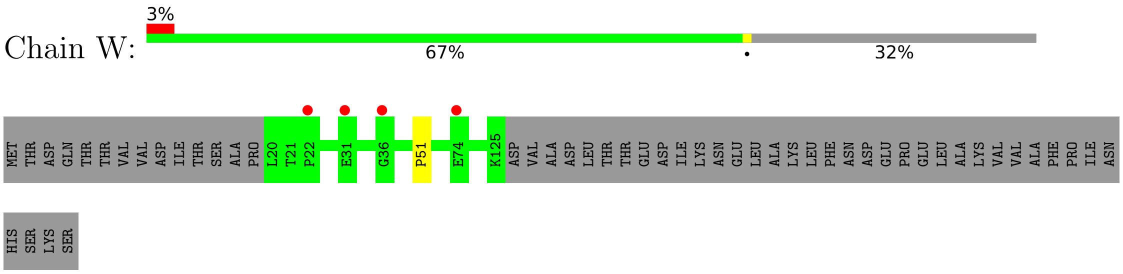


• Molecule 1: Small Terminase subunit

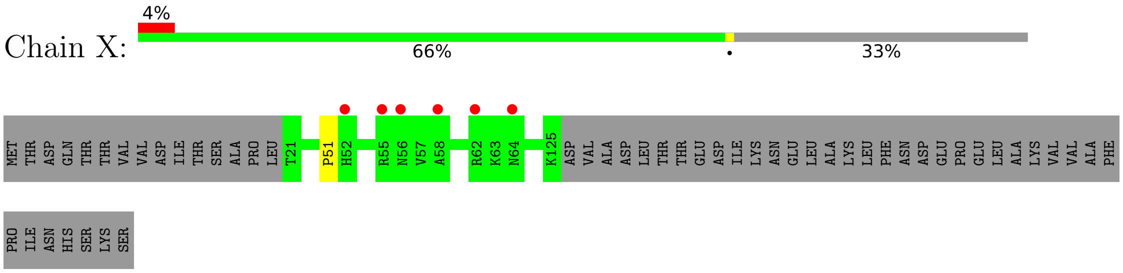
Chain V:



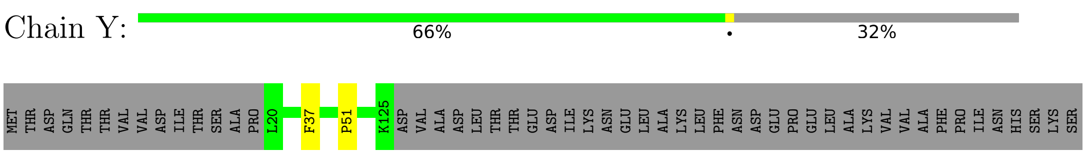
• Molecule 1: Small Terminase subunit



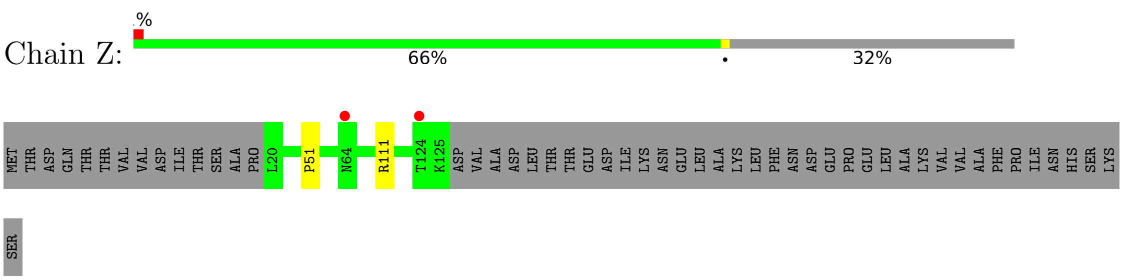
• Molecule 1: Small Terminase subunit



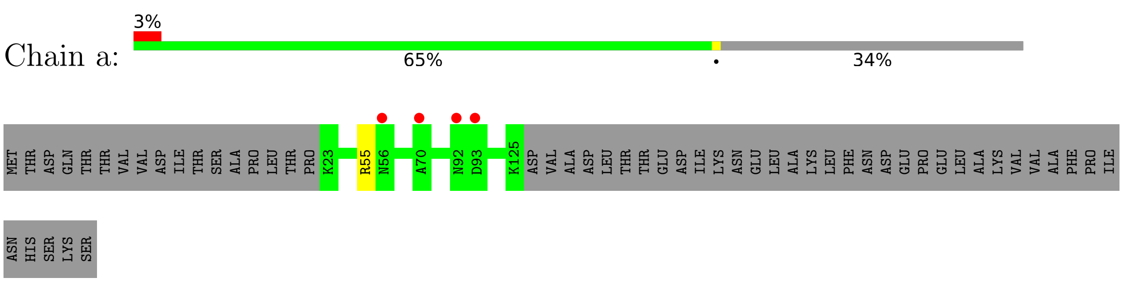
• Molecule 1: Small Terminase subunit



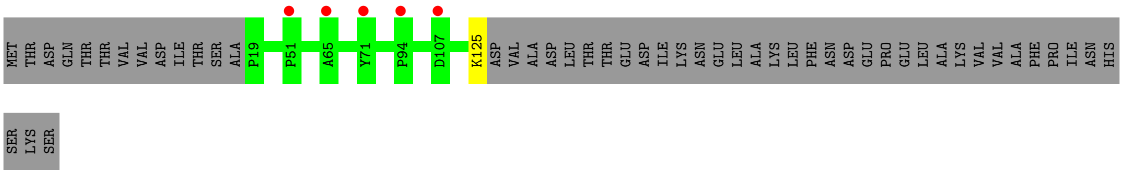
• Molecule 1: Small Terminase subunit



• Molecule 1: Small Terminase subunit

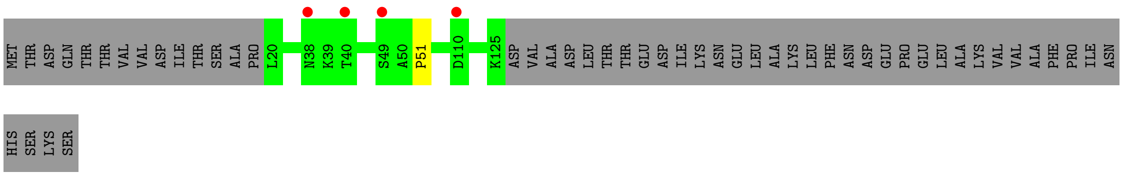


• Molecule 1: Small Terminase subunit



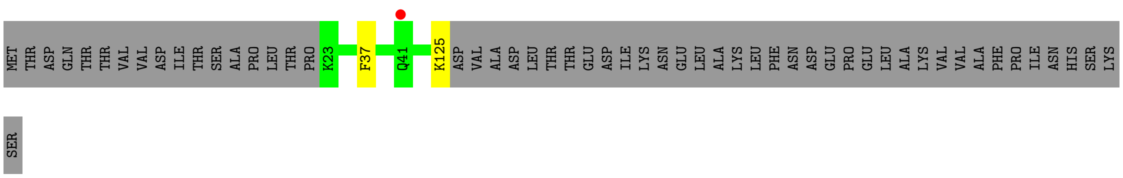
• Molecule 1: Small Terminase subunit

Chain c:



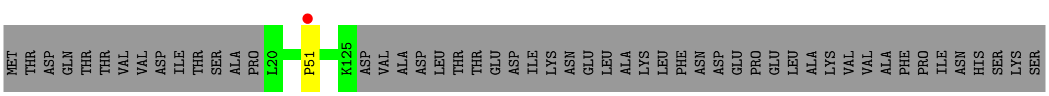
• Molecule 1: Small Terminase subunit

Chain d:



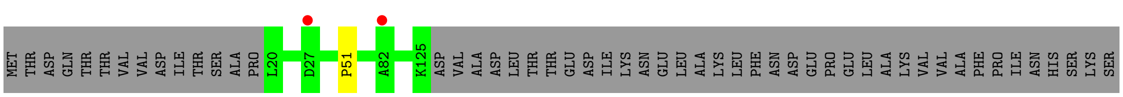
• Molecule 1: Small Terminase subunit

Chain e:



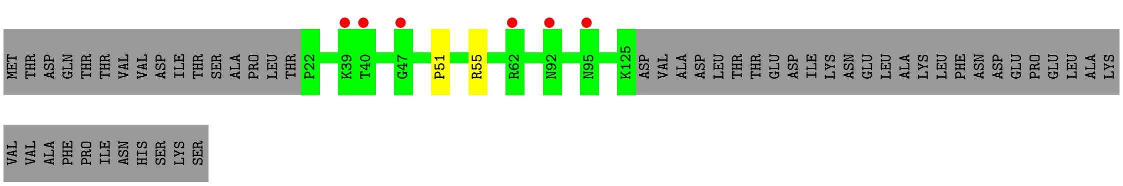
• Molecule 1: Small Terminase subunit

Chain f:

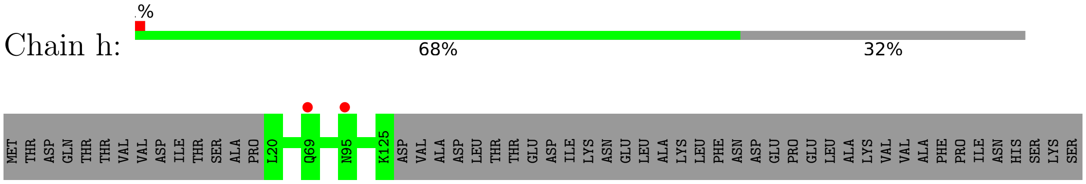


• Molecule 1: Small Terminase subunit

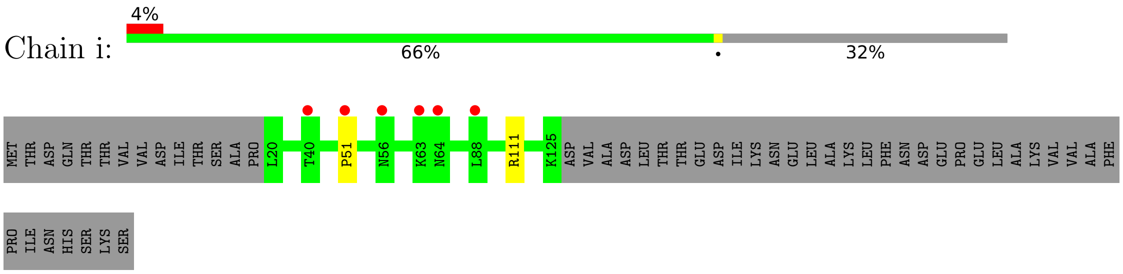
Chain g:



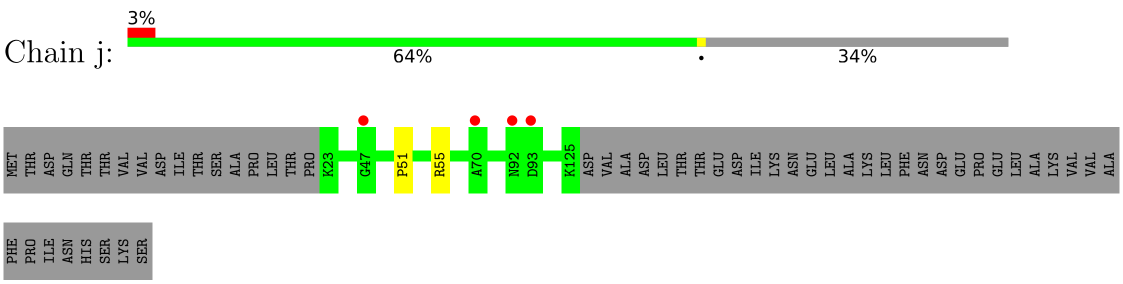
• Molecule 1: Small Terminase subunit



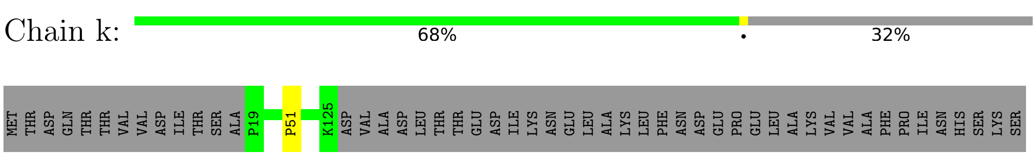
• Molecule 1: Small Terminase subunit



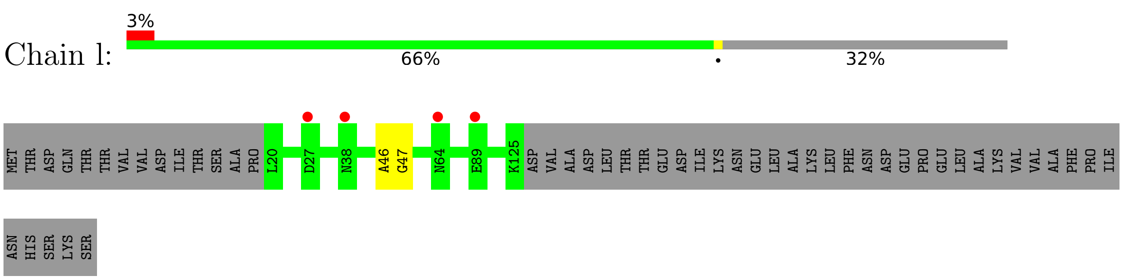
• Molecule 1: Small Terminase subunit



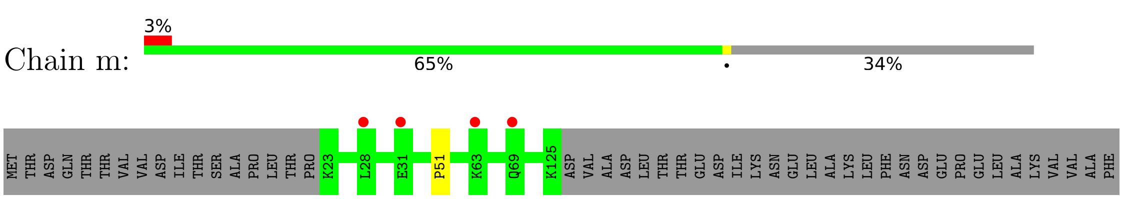
• Molecule 1: Small Terminase subunit



• Molecule 1: Small Terminase subunit



• Molecule 1: Small Terminase subunit



PRO ILE ASN HIS SER LYS SER

• Molecule 1: Small Terminase subunit

Chain n: %, 68%, 32%

MET THR ASP GLN THR THR VAL VAL ASP ILE THR SER ALA PRO L20 N95 K125 ASP VAL ALA ASP LEU THR THR GLU ASP ILE LYS ASN GLU LEU ALA LYS LEU PHE ASN ASP GLU PRO GLU LEU ALA LYS VAL VAL ALA PHE PRO ILE ASN HIS SER LYS SER

• Molecule 1: Small Terminase subunit

Chain o: 2%, 67%, 32%

MET THR ASP GLN THR THR VAL VAL ASP ILE THR SER ALA PRO L20 S49 A50 P51 E74 D79 K125 ASP VAL ALA ASP LEU THR THR GLU ASP ILE LYS ASN GLU LEU ALA LYS LEU PHE ASN ASP GLU PRO GLU LEU ALA LYS VAL VAL ALA PHE PRO ILE ASN HIS SER

LYS SER

• Molecule 1: Small Terminase subunit

Chain p: 3%, 67%, 33%

MET THR ASP GLN THR THR VAL VAL ASP ILE THR SER ALA PRO LEU T21 E24 Q54 A58 K63 K125 ASP VAL ALA ASP LEU THR THR GLU ASP ILE LYS ASN GLU LEU ALA LYS LEU PHE ASN ASP GLU PRO GLU LEU ALA LYS VAL VAL ALA PHE PRO ILE ASN HIS

SER LYS SER

• Molecule 1: Small Terminase subunit

Chain q: 2%, 67%, 32%

MET THR ASP GLN THR THR VAL VAL ASP ILE THR SER ALA PRO L20 P51 N56 N92 D93 P94 K125 ASP VAL ALA ASP LEU THR THR GLU ASP ILE LYS ASN GLU LEU ALA LYS LEU PHE ASN ASP GLU PRO GLU LEU ALA LYS VAL VAL ALA PHE PRO ILE ASN HIS SER

LYS SER

• Molecule 1: Small Terminase subunit

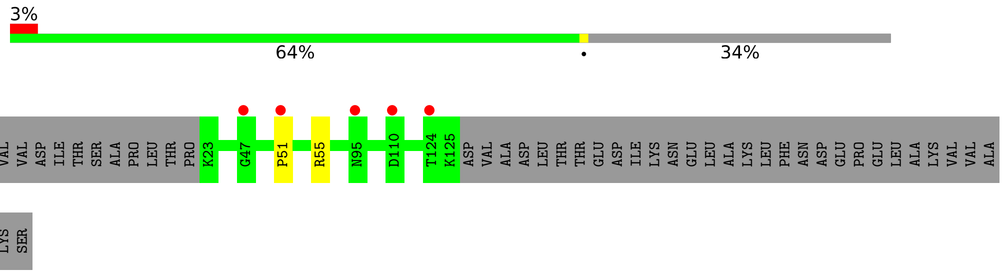
Chain r: 3%, 66%, 32%

MET THR ASP GLN THR THR VAL VAL ASP ILE THR SER ALA PRO L20 T21 P22 L26 D27 Q41 G47 Q54 R111 K125 ASP VAL ALA ASP LEU THR THR GLU ASP ILE LYS ASN GLU LEU ALA LYS LEU PHE ASN ASP GLU PRO GLU LEU ALA LYS VAL VAL ALA PHE

PRO ILE ASN HIS SER LYS SER

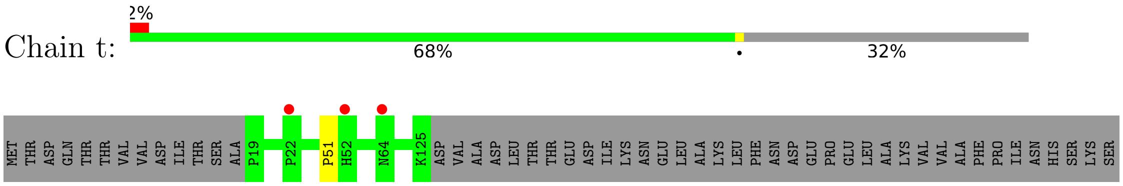
• Molecule 1: Small Terminase subunit

Chain s:



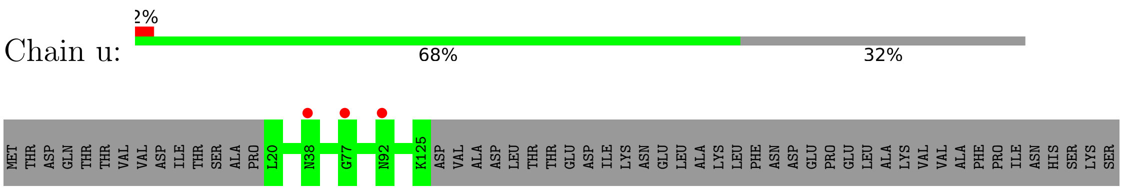
• Molecule 1: Small Terminase subunit

Chain t:



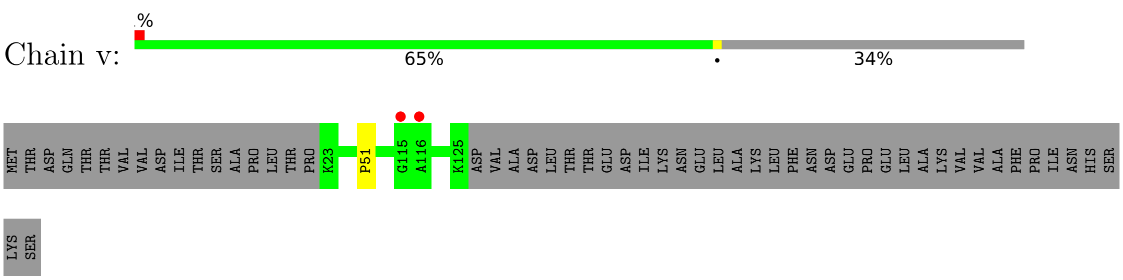
• Molecule 1: Small Terminase subunit

Chain u:



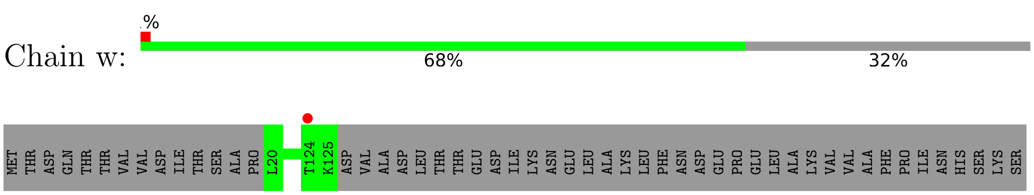
• Molecule 1: Small Terminase subunit

Chain v:



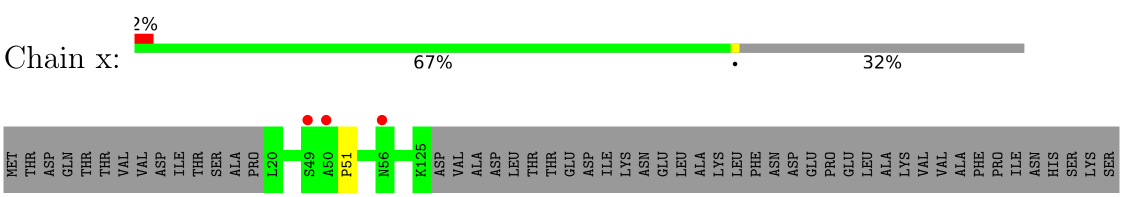
• Molecule 1: Small Terminase subunit

Chain w:



• Molecule 1: Small Terminase subunit

Chain x:

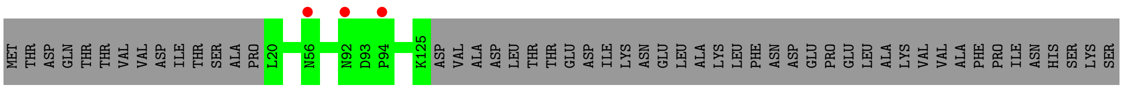


• Molecule 1: Small Terminase subunit

Chain y:

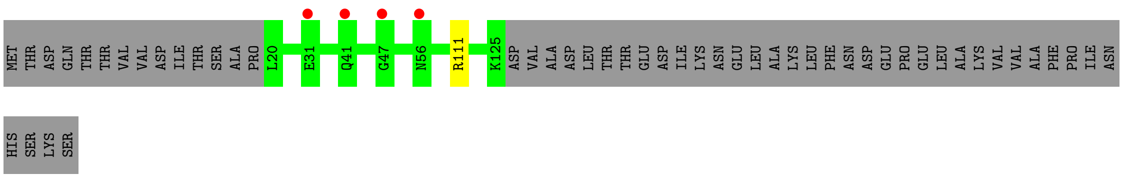
• Molecule 1: Small Terminase subunit

Chain z:



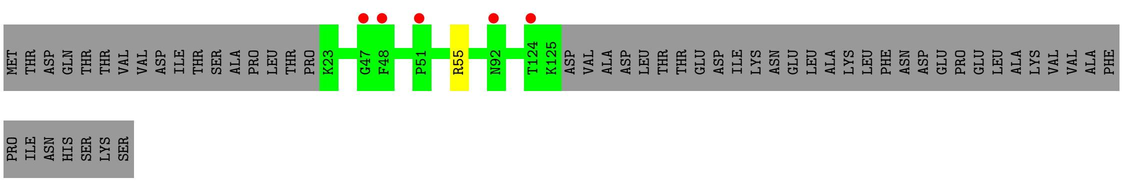
• Molecule 1: Small Terminase subunit

Chain 0:



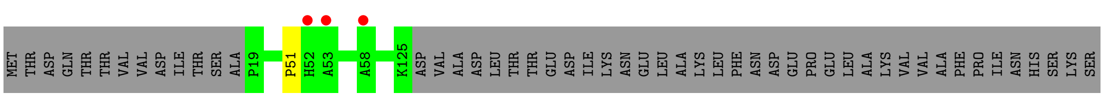
• Molecule 1: Small Terminase subunit

Chain 1:



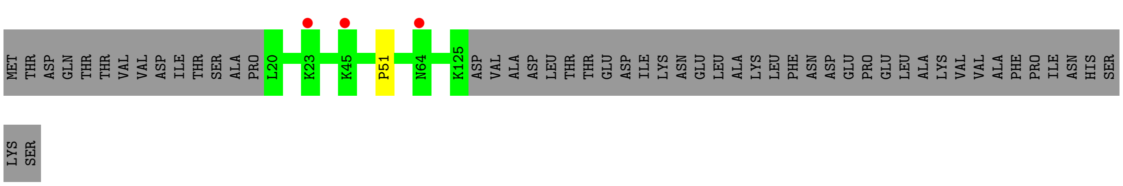
• Molecule 1: Small Terminase subunit

Chain 2:



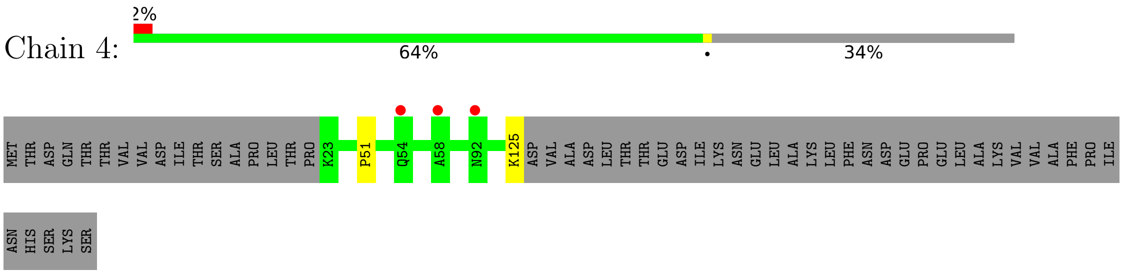
• Molecule 1: Small Terminase subunit

Chain 3:



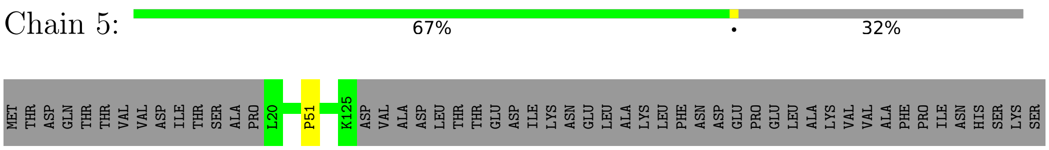
• Molecule 1: Small Terminase subunit

Chain 4:



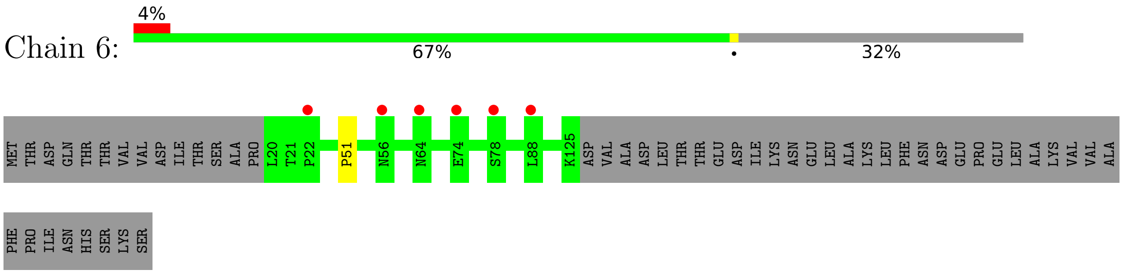
- Molecule 1: Small Terminase subunit

Chain 5:



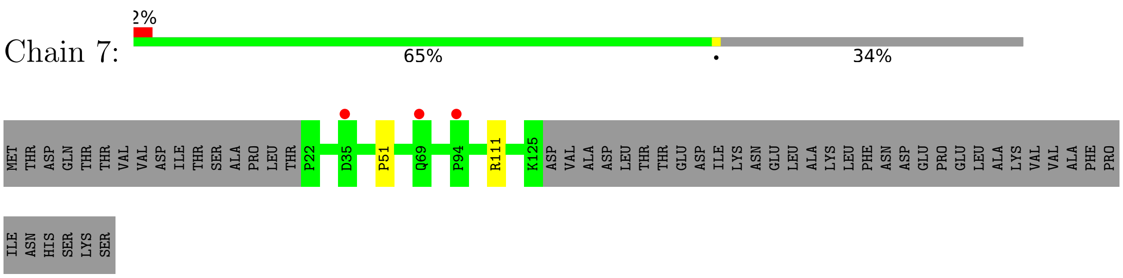
- Molecule 1: Small Terminase subunit

Chain 6:



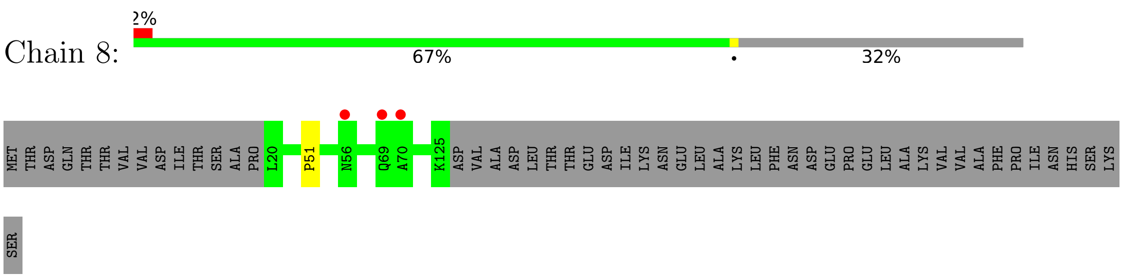
- Molecule 1: Small Terminase subunit

Chain 7:



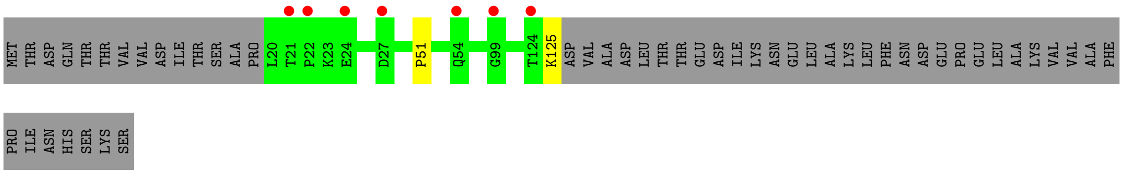
- Molecule 1: Small Terminase subunit

Chain 8:



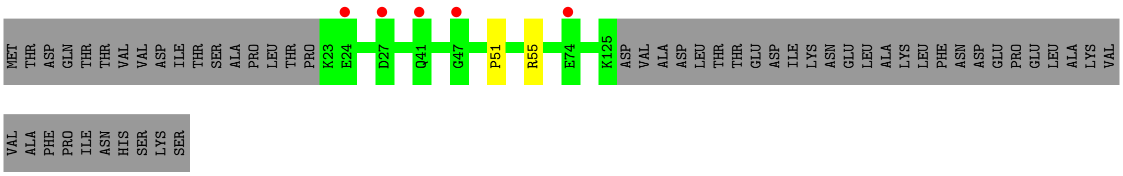
- Molecule 1: Small Terminase subunit

Chain 9:



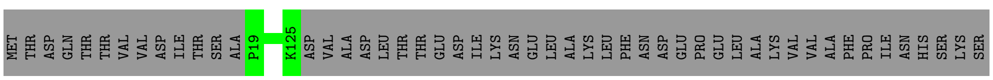
• Molecule 1: Small Terminase subunit

Chain AA:



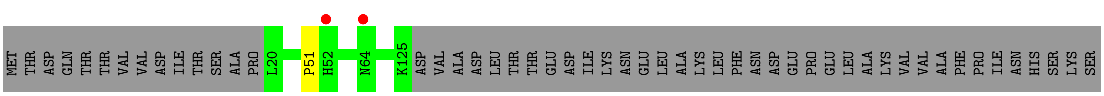
• Molecule 1: Small Terminase subunit

Chain AB:



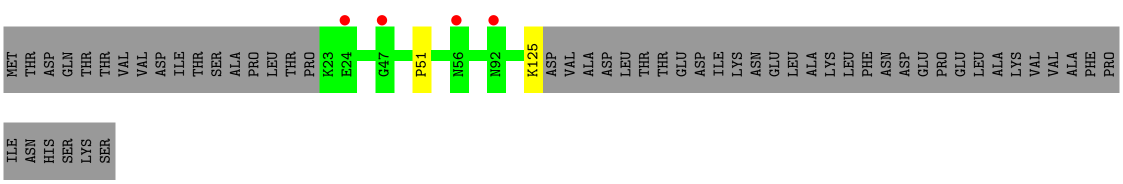
• Molecule 1: Small Terminase subunit

Chain AC:



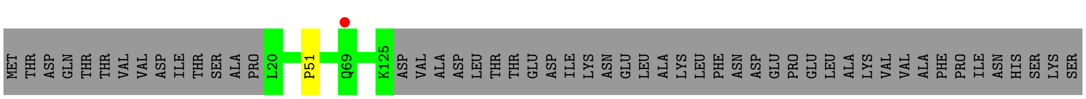
• Molecule 1: Small Terminase subunit

Chain AD:



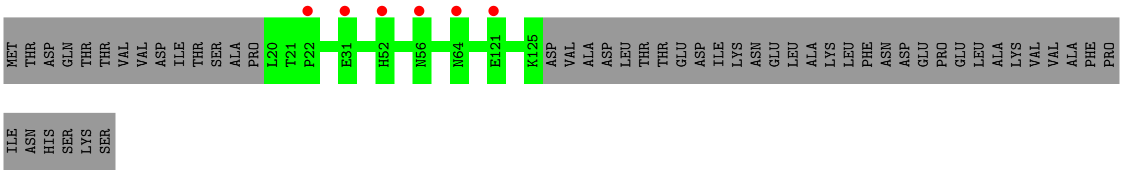
• Molecule 1: Small Terminase subunit

Chain AE:

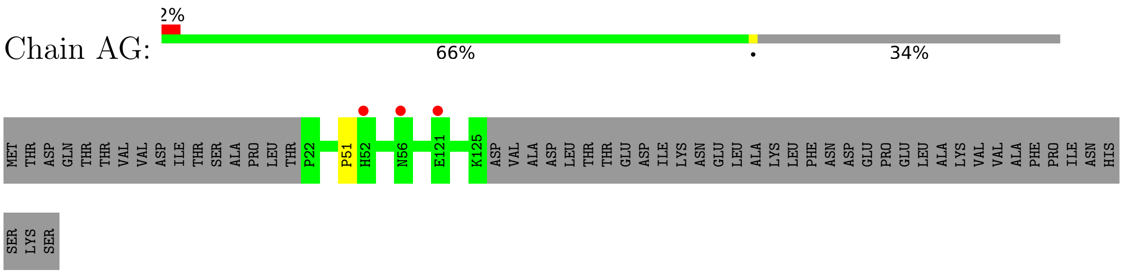


• Molecule 1: Small Terminase subunit

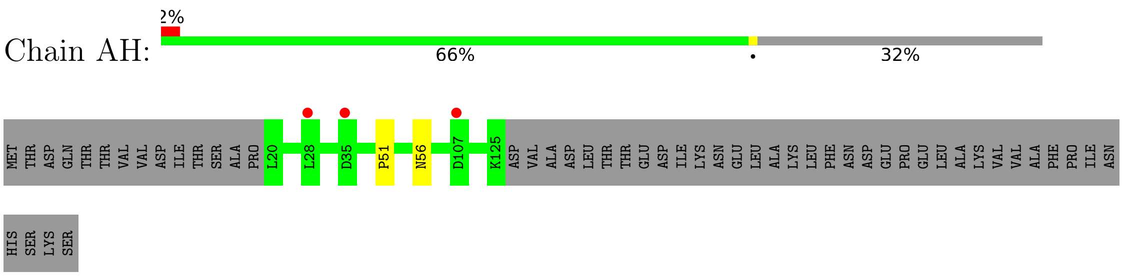
Chain AF:



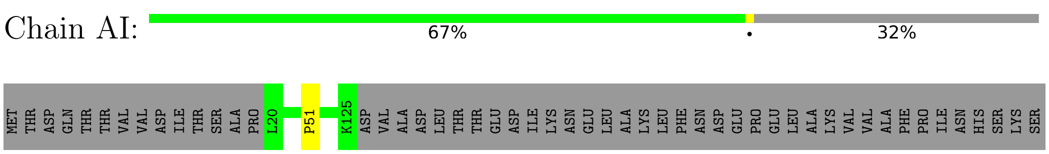
• Molecule 1: Small Terminase subunit



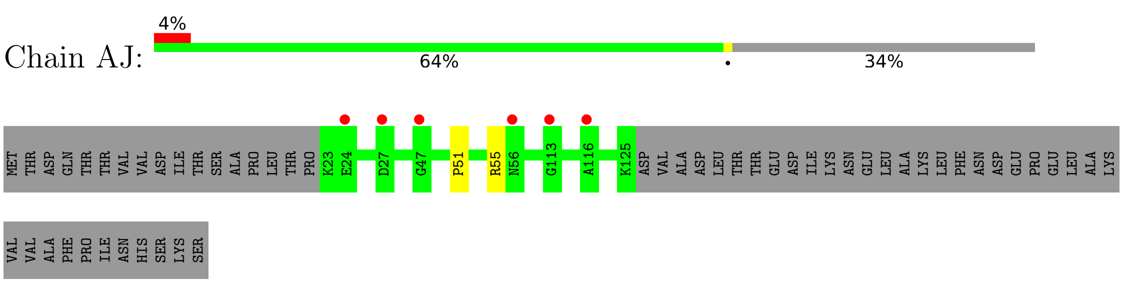
• Molecule 1: Small Terminase subunit



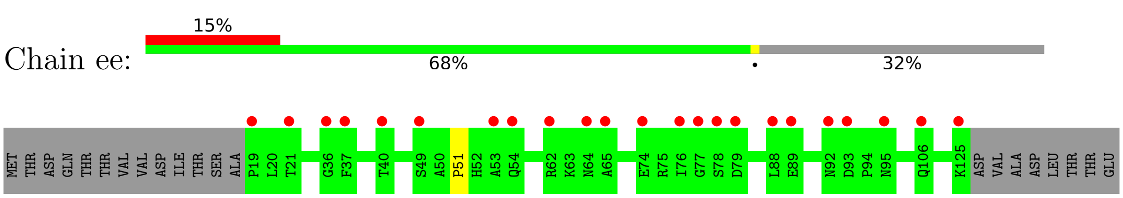
• Molecule 1: Small Terminase subunit



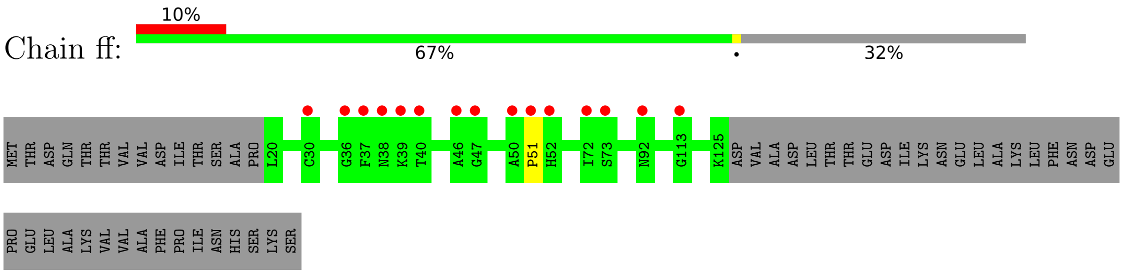
• Molecule 1: Small Terminase subunit



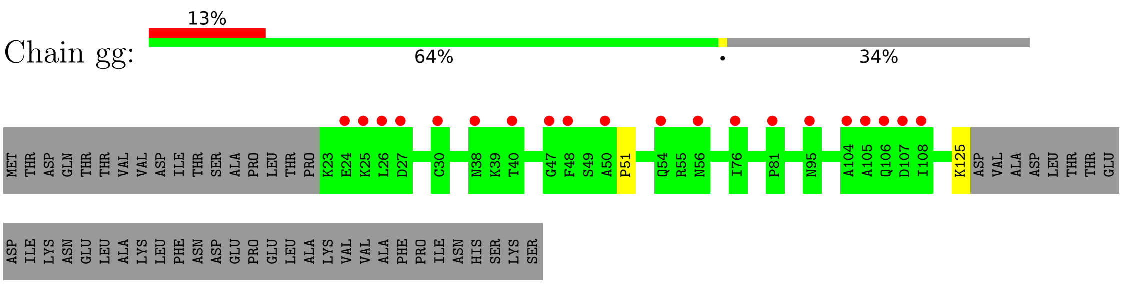
• Molecule 1: Small Terminase subunit



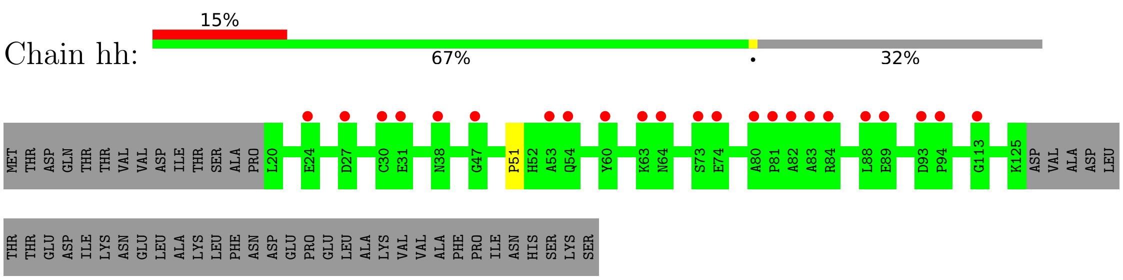
- Molecule 1: Small Terminase subunit



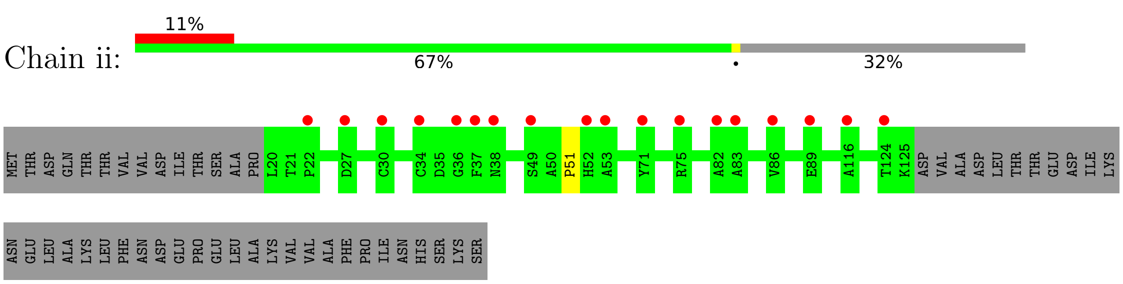
- Molecule 1: Small Terminase subunit



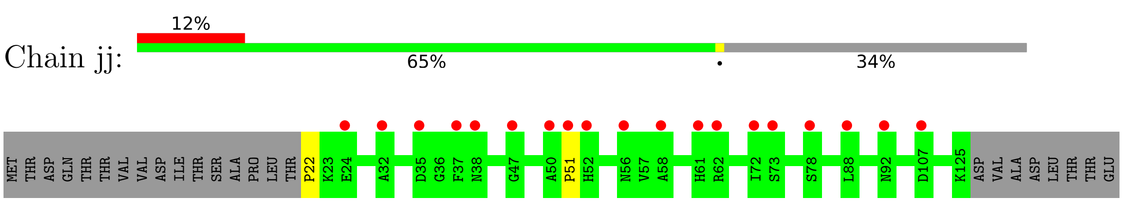
- Molecule 1: Small Terminase subunit



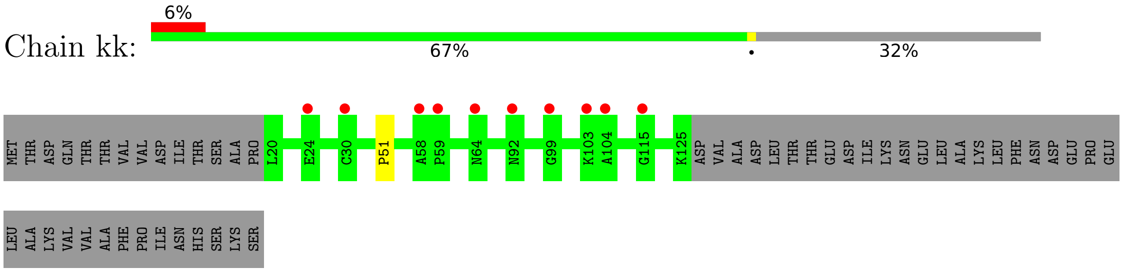
- Molecule 1: Small Terminase subunit



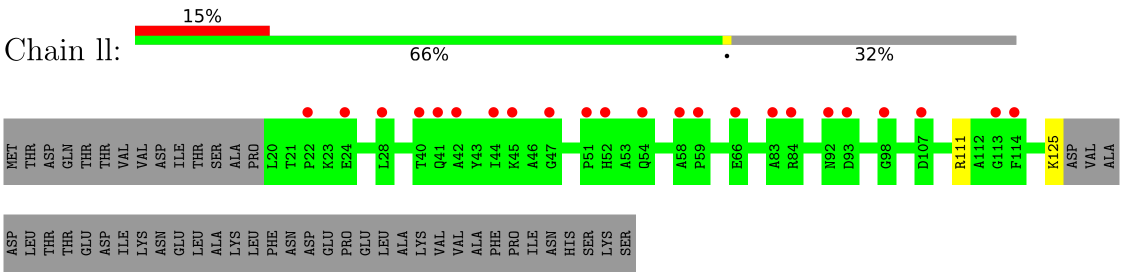
- Molecule 1: Small Terminase subunit



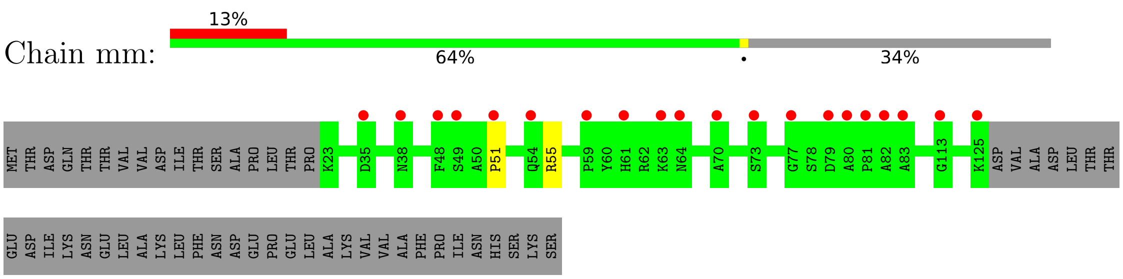
• Molecule 1: Small Terminase subunit



• Molecule 1: Small Terminase subunit



• Molecule 1: Small Terminase subunit



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| >$ = 0.39, $< L^2 >$ = 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.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (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(^{o})	Ideal(^{o})
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

All (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
1	r	22	PRO
1	l	47	GLY

5.3.2 Protein sidechains (i)

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	69/130 (53%)	68 (99%)	1 (1%)	67	80
1	3	67/130 (52%)	66 (98%)	1 (2%)	65	79
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	67/130 (52%)	66 (98%)	1 (2%)	65	79
1	O	66/130 (51%)	66 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	l	67/130 (52%)	67 (100%)	0	100	100
1	ll	67/130 (52%)	65 (97%)	2 (3%)	41	64
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

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	PRO
1	B	51	PRO
1	D	51	PRO
1	F	51	PRO
1	G	51	PRO
1	K	51	PRO
1	L	51	PRO
1	L	125	LYS
1	M	51	PRO
1	N	51	PRO
1	P	51	PRO
1	Q	75	ARG
1	Q	111	ARG
1	R	51	PRO

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Mol	Chain	Res	Type
1	S	125	LYS
1	T	51	PRO
1	U	125	LYS
1	V	51	PRO
1	W	51	PRO
1	X	51	PRO
1	Y	51	PRO
1	Z	51	PRO
1	Z	111	ARG
1	a	55	ARG
1	b	125	LYS
1	c	51	PRO
1	d	125	LYS
1	e	51	PRO
1	f	51	PRO
1	g	51	PRO
1	g	55	ARG
1	i	51	PRO
1	i	111	ARG
1	j	51	PRO
1	j	55	ARG
1	k	51	PRO
1	m	51	PRO
1	o	51	PRO
1	q	51	PRO
1	r	111	ARG
1	s	51	PRO
1	s	55	ARG
1	t	51	PRO
1	v	51	PRO
1	x	51	PRO
1	y	51	PRO
1	0	111	ARG
1	1	55	ARG
1	2	51	PRO
1	3	51	PRO
1	4	51	PRO
1	4	125	LYS
1	5	51	PRO
1	6	51	PRO
1	7	51	PRO
1	7	111	ARG

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Mol	Chain	Res	Type
1	8	51	PRO
1	9	51	PRO
1	9	125	LYS
1	AA	51	PRO
1	AA	55	ARG
1	AC	51	PRO
1	AD	51	PRO
1	AD	125	LYS
1	AE	51	PRO
1	AG	51	PRO
1	AH	51	PRO
1	AI	51	PRO
1	AJ	51	PRO
1	AJ	55	ARG
1	ee	51	PRO
1	ff	51	PRO
1	gg	51	PRO
1	gg	125	LYS
1	hh	51	PRO
1	ii	51	PRO
1	jj	51	PRO
1	kk	51	PRO
1	ll	111	ARG
1	ll	125	LYS
1	mm	51	PRO
1	mm	55	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	61	HIS
1	M	52	HIS
1	N	61	HIS
1	Q	61	HIS
1	V	61	HIS
1	Z	61	HIS
1	a	52	HIS
1	c	56	ASN
1	f	52	HIS
1	i	61	HIS
1	j	52	HIS
1	j	118	GLN

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Mol	Chain	Res	Type
1	n	41	GLN
1	AD	61	HIS
1	AF	95	ASN
1	AF	106	GLN
1	AJ	61	HIS
1	ff	41	GLN
1	gg	61	HIS
1	jj	38	ASN
1	kk	52	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	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, 142, 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, 154, 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

All (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
1	ff	51	PRO	5.9
1	ll	42	ALA	5.6
1	1	47	GLY	5.6
1	jj	24	GLU	5.4
1	gg	47	GLY	5.3
1	hh	82	ALA	5.3
1	hh	81	PRO	5.2
1	gg	105	ALA	5.2
1	hh	83	ALA	5.1
1	O	52	HIS	5.0
1	kk	115	GLY	4.9
1	ee	78	SER	4.9
1	ii	52	HIS	4.9
1	mm	113	GLY	4.7
1	gg	106	GLN	4.7
1	ll	47	GLY	4.6
1	hh	53	ALA	4.6
1	ll	84	ARG	4.5
1	j	92	ASN	4.5
1	Q	38	ASN	4.4
1	ll	114	PHE	4.3
1	ii	75	ARG	4.3
1	g	47	GLY	4.2
1	ee	77	GLY	4.2
1	gg	104	ALA	4.2
1	hh	94	PRO	4.1
1	ee	49	SER	4.1
1	6	74	GLU	4.1
1	kk	104	ALA	4.1
1	9	22	PRO	4.1
1	3	64	ASN	3.9
1	ii	82	ALA	3.9
1	ll	51	PRO	3.9
1	mm	73	SER	3.9
1	ee	40	THR	3.9
1	hh	27	ASP	3.9
1	X	64	ASN	3.8
1	gg	107	ASP	3.8
1	1	51	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	jj	38	ASN	3.8
1	hh	88	LEU	3.8
1	s	51	PRO	3.7
1	i	63	LYS	3.7
1	mm	38	ASN	3.7
1	3	45	LYS	3.7
1	ee	64	ASN	3.7
1	ll	59	PRO	3.7
1	b	65	ALA	3.6
1	G	38	ASN	3.6
1	l	38	ASN	3.6
1	hh	80	ALA	3.6
1	ll	83	ALA	3.6
1	jj	47	GLY	3.6
1	p	58	ALA	3.5
1	mm	77	GLY	3.5
1	L	54	GLN	3.5
1	s	47	GLY	3.5
1	AJ	47	GLY	3.5
1	AD	56	ASN	3.5
1	ff	36	GLY	3.4
1	g	92	ASN	3.4
1	X	52	HIS	3.4
1	r	27	ASP	3.4
1	m	69	GLN	3.4
1	mm	63	LYS	3.4
1	mm	61	HIS	3.4
1	gg	30	CYS	3.4
1	kk	24	GLU	3.4
1	ee	54	GLN	3.4
1	O	47	GLY	3.4
1	a	70	ALA	3.3
1	ee	37	PHE	3.3
1	jj	73	SER	3.3
1	ii	83	ALA	3.3
1	p	63	LYS	3.3
1	q	92	ASN	3.3
1	ff	50	ALA	3.3
1	ee	74	GLU	3.3
1	hh	24	GLU	3.3
1	hh	73	SER	3.3
1	ff	37	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	kk	58	ALA	3.2
1	d	41	GLN	3.2
1	i	51	PRO	3.2
1	mm	83	ALA	3.2
1	i	56	ASN	3.2
1	6	64	ASN	3.2
1	z	56	ASN	3.2
1	O	58	ALA	3.2
1	s	124	THR	3.2
1	2	53	ALA	3.2
1	y	52	HIS	3.2
1	W	36	GLY	3.1
1	ee	36	GLY	3.1
1	jj	37	PHE	3.1
1	o	49	SER	3.1
1	u	92	ASN	3.1
1	jj	52	HIS	3.1
1	v	115	GLY	3.1
1	E	52	HIS	3.1
1	hh	74	GLU	3.1
1	ii	36	GLY	3.1
1	ll	45	LYS	3.0
1	y	95	ASN	3.0
1	ii	30	CYS	3.0
1	ll	113	GLY	3.0
1	mm	79	ASP	3.0
1	ii	37	PHE	3.0
1	c	40	THR	3.0
1	ii	86	VAL	3.0
1	mm	81	PRO	3.0
1	n	95	ASN	3.0
1	gg	56	ASN	3.0
1	hh	47	GLY	3.0
1	b	107	ASP	3.0
1	b	51	PRO	3.0
1	mm	82	ALA	2.9
1	ee	65	ALA	2.9
1	F	28	LEU	2.9
1	AH	28	LEU	2.9
1	mm	35	ASP	2.9
1	r	41	GLN	2.9
1	ll	52	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	jj	72	ILE	2.9
1	mm	59	PRO	2.9
1	hh	93	ASP	2.9
1	ff	113	GLY	2.9
1	ll	93	ASP	2.9
1	gg	54	GLN	2.9
1	3	23	LYS	2.9
1	l	27	ASP	2.9
1	mm	80	ALA	2.9
1	ff	46	ALA	2.9
1	x	56	ASN	2.8
1	X	55	ARG	2.8
1	AJ	24	GLU	2.8
1	M	94	PRO	2.8
1	ee	95	ASN	2.8
1	8	70	ALA	2.8
1	K	44	ILE	2.8
1	gg	26	LEU	2.8
1	A	116	ALA	2.8
1	ff	30	CYS	2.8
1	L	93	ASP	2.7
1	i	88	LEU	2.7
1	hh	31	GLU	2.7
1	V	20	LEU	2.7
1	L	53	ALA	2.7
1	ii	27	ASP	2.7
1	jj	78	SER	2.7
1	7	35	ASP	2.7
1	S	65	ALA	2.7
1	0	41	GLN	2.7
1	ll	28	LEU	2.7
1	AG	56	ASN	2.7
1	ll	24	GLU	2.7
1	x	50	ALA	2.7
1	O	37	PHE	2.7
1	e	51	PRO	2.7
1	c	38	ASN	2.7
1	4	92	ASN	2.7
1	jj	62	ARG	2.7
1	hh	30	CYS	2.7
1	AJ	27	ASP	2.7
1	ee	125	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	AF	121	GLU	2.6
1	AA	41	GLN	2.6
1	j	47	GLY	2.6
1	mm	49	SER	2.6
1	F	56	ASN	2.6
1	ll	22	PRO	2.6
1	mm	48	PHE	2.6
1	ee	89	GLU	2.6
1	u	38	ASN	2.6
1	hh	38	ASN	2.6
1	ii	124	THR	2.6
1	O	49	SER	2.6
1	gg	27	ASP	2.6
1	ii	34	CYS	2.6
1	ff	92	ASN	2.6
1	ee	79	ASP	2.6
1	U	41	GLN	2.6
1	ll	41	GLN	2.6
1	B	54	GLN	2.6
1	gg	48	PHE	2.6
1	1	92	ASN	2.6
1	hh	89	GLU	2.5
1	w	124	THR	2.5
1	AH	35	ASP	2.5
1	ii	22	PRO	2.5
1	a	92	ASN	2.5
1	AA	24	GLU	2.5
1	A	49	SER	2.5
1	mm	54	GLN	2.5
1	ll	40	THR	2.5
1	F	20	LEU	2.5
1	jj	88	LEU	2.5
1	t	52	HIS	2.5
1	AG	52	HIS	2.5
1	c	49	SER	2.5
1	jj	58	ALA	2.5
1	g	40	THR	2.5
1	t	22	PRO	2.5
1	a	93	ASP	2.5
1	E	41	GLN	2.5
1	p	24	GLU	2.5
1	2	52	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	Z	124	THR	2.5
1	ee	92	ASN	2.5
1	hh	60	TYR	2.5
1	G	49	SER	2.4
1	ll	66	GLU	2.4
1	O	30	CYS	2.4
1	4	54	GLN	2.4
1	AJ	116	ALA	2.4
1	ff	40	THR	2.4
1	hh	113	GLY	2.4
1	ii	49	SER	2.4
1	N	110	ASP	2.4
1	Z	64	ASN	2.4
1	AF	22	PRO	2.4
1	x	49	SER	2.4
1	m	28	LEU	2.4
1	AF	64	ASN	2.4
1	AD	47	GLY	2.4
1	kk	59	PRO	2.4
1	s	95	ASN	2.4
1	ll	44	ILE	2.4
1	Q	78	SER	2.4
1	G	52	HIS	2.4
1	F	27	ASP	2.4
1	AH	107	ASP	2.4
1	g	95	ASN	2.4
1	ff	47	GLY	2.4
1	ll	98	GLY	2.4
1	ii	38	ASN	2.4
1	R	36	GLY	2.4
1	f	82	ALA	2.4
1	z	92	ASN	2.4
1	ll	92	ASN	2.4
1	jj	50	ALA	2.4
1	6	22	PRO	2.3
1	jj	51	PRO	2.3
1	AC	64	ASN	2.3
1	kk	64	ASN	2.3
1	B	92	ASN	2.3
1	AD	92	ASN	2.3
1	gg	38	ASN	2.3
1	mm	64	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	X	62	ARG	2.3
1	AG	121	GLU	2.3
1	Q	77	GLY	2.3
1	L	92	ASN	2.3
1	kk	92	ASN	2.3
1	8	56	ASN	2.3
1	ff	73	SER	2.3
1	h	95	ASN	2.3
1	ll	107	ASP	2.3
1	mm	70	ALA	2.3
1	O	24	GLU	2.3
1	W	74	GLU	2.3
1	gg	25	LYS	2.3
1	L	64	ASN	2.3
1	AJ	113	GLY	2.3
1	E	62	ARG	2.3
1	6	88	LEU	2.3
1	mm	51	PRO	2.3
1	G	110	ASP	2.3
1	9	27	ASP	2.3
1	jj	107	ASP	2.3
1	Q	52	HIS	2.3
1	ff	72	ILE	2.3
1	O	56	ASN	2.3
1	ii	89	GLU	2.3
1	p	54	GLN	2.3
1	l	64	ASN	2.3
1	AA	27	ASP	2.3
1	jj	56	ASN	2.3
1	kk	99	GLY	2.3
1	ii	71	TYR	2.3
1	AD	24	GLU	2.3
1	X	58	ALA	2.3
1	AA	74	GLU	2.2
1	a	56	ASN	2.2
1	q	56	ASN	2.2
1	S	107	ASP	2.2
1	s	110	ASP	2.2
1	ee	19	PRO	2.2
1	P	56	ASN	2.2
1	j	93	ASP	2.2
1	9	54	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	AE	69	GLN	2.2
1	F	74	GLU	2.2
1	Q	59	PRO	2.2
1	q	94	PRO	2.2
1	r	54	GLN	2.2
1	v	116	ALA	2.2
1	mm	125	LYS	2.2
1	ee	106	GLN	2.2
1	W	22	PRO	2.2
1	M	61	HIS	2.2
1	W	31	GLU	2.2
1	1	124	THR	2.2
1	ee	76	ILE	2.2
1	ee	88	LEU	2.2
1	P	69	GLN	2.2
1	o	74	GLU	2.2
1	AJ	56	ASN	2.2
1	7	69	GLN	2.2
1	O	124	THR	2.2
1	6	56	ASN	2.2
1	ee	21	THR	2.2
1	G	106	GLN	2.2
1	j	70	ALA	2.2
1	6	78	SER	2.2
1	hh	63	LYS	2.2
1	0	31	GLU	2.2
1	0	47	GLY	2.1
1	i	40	THR	2.1
1	0	56	ASN	2.1
1	r	47	GLY	2.1
1	gg	50	ALA	2.1
1	g	39	LYS	2.1
1	f	27	ASP	2.1
1	o	79	ASP	2.1
1	D	36	GLY	2.1
1	2	58	ALA	2.1
1	gg	108	ILE	2.1
1	h	69	GLN	2.1
1	AF	52	HIS	2.1
1	A	34	CYS	2.1
1	i	64	ASN	2.1
1	u	77	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	jj	61	HIS	2.1
1	T	58	ALA	2.1
1	z	94	PRO	2.1
1	b	71	TYR	2.1
1	jj	35	ASP	2.1
1	t	64	ASN	2.1
1	gg	95	ASN	2.1
1	H	115	GLY	2.1
1	P	74	GLU	2.1
1	ll	58	ALA	2.1
1	gg	24	GLU	2.1
1	9	21	THR	2.1
1	9	124	THR	2.1
1	D	31	GLU	2.1
1	M	64	ASN	2.1
1	AF	31	GLU	2.1
1	1	48	PHE	2.1
1	ee	53	ALA	2.1
1	AC	52	HIS	2.1
1	c	110	ASP	2.1
1	m	31	GLU	2.1
1	ee	93	ASP	2.1
1	L	58	ALA	2.1
1	U	109	LEU	2.1
1	9	24	GLU	2.1
1	L	56	ASN	2.1
1	Q	56	ASN	2.1
1	hh	64	ASN	2.1
1	8	69	GLN	2.1
1	kk	103	LYS	2.1
1	ff	52	HIS	2.0
1	9	99	GLY	2.0
1	AA	47	GLY	2.0
1	ee	62	ARG	2.0
1	l	89	GLU	2.0
1	jj	32	ALA	2.0
1	J	35	ASP	2.0
1	m	63	LYS	2.0
1	V	56	ASN	2.0
1	g	62	ARG	2.0
1	ii	116	ALA	2.0
1	P	37	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	AF	56	ASN	2.0
1	gg	76	ILE	2.0
1	r	26	LEU	2.0
1	7	94	PRO	2.0
1	E	31	GLU	2.0
1	U	31	GLU	2.0
1	kk	30	CYS	2.0
1	J	53	ALA	2.0
1	T	50	ALA	2.0
1	4	58	ALA	2.0
1	ii	53	ALA	2.0
1	X	56	ASN	2.0
1	ff	39	LYS	2.0
1	b	94	PRO	2.0
1	gg	81	PRO	2.0
1	hh	84	ARG	2.0

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.