



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 07:34 PM GMT

PDB ID : 4RFT
Title : T=1 subviral particle of Grouper nervous necrosis virus capsid protein deletion mutant (delta 1-34 & 218-338)
Authors : Chen, N.C.; Chen, C.J.; Yoshimura, M.; Guan, H.H.; Chen, T.Y.
Deposited on : 2014-09-27
Resolution : 3.10 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
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

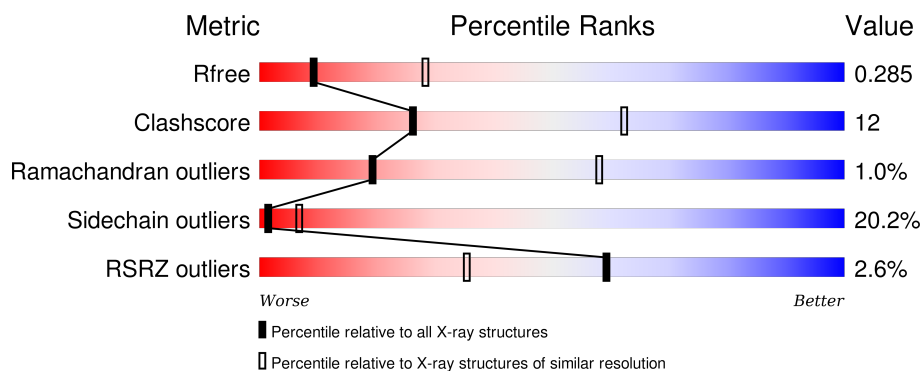
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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. 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	183	<div> <div>60%</div> <div>23%</div> <div>5%</div> <div>11%</div> </div>
1	1	183	<div> <div>5%</div> <div>54%</div> <div>28%</div> <div>7%</div> <div>11%</div> </div>
1	2	183	<div> <div>3%</div> <div>52%</div> <div>31%</div> <div>7%</div> <div>11%</div> </div>
1	3	183	<div> <div>3%</div> <div>61%</div> <div>23%</div> <div>5%</div> <div>11%</div> </div>
1	4	183	<div> <div>4%</div> <div>54%</div> <div>26%</div> <div>9%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	5	183	
1	6	183	
1	7	183	
1	8	183	
1	9	183	
1	A	183	
1	B	183	
1	C	183	
1	D	183	
1	E	183	
1	F	183	
1	G	183	
1	H	183	
1	I	183	
1	J	183	
1	K	183	
1	L	183	
1	M	183	
1	N	183	
1	O	183	
1	P	183	
1	Q	183	
1	R	183	
1	S	183	
1	T	183	

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Mol	Chain	Length	Quality of chain
1	U	183	
1	V	183	
1	W	183	
1	X	183	
1	Y	183	
1	Z	183	
1	a	183	
1	b	183	
1	c	183	
1	d	183	
1	e	183	
1	f	183	
1	g	183	
1	h	183	
1	i	183	
1	j	183	
1	k	183	
1	l	183	
1	m	183	
1	n	183	
1	o	183	
1	p	183	
1	q	183	
1	r	183	
1	s	183	

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Mol	Chain	Length	Quality of chain
1	t	183	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>72%</div><div>17%</div><div>•</div><div>11%</div></div></div>
1	u	183	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>74%</div><div>15%</div><div>•</div><div>11%</div></div></div>
1	v	183	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>72%</div><div>16%</div><div>•</div><div>11%</div></div></div>
1	w	183	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>72%</div><div>16%</div><div>•</div><div>11%</div></div></div>
1	x	183	<div><div><div></div><div></div><div></div></div><div><div>4%</div><div>74%</div><div>14%</div><div>•</div><div>11%</div></div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 75180 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	B	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	C	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	D	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	E	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	F	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	G	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	H	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	I	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	J	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	K	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	L	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	M	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	N	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	O	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	P	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	R	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	S	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	T	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	U	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	V	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	W	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	X	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	Y	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	Z	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	0	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	1	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	2	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	3	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	4	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	5	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	6	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	7	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	8	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	9	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	a	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	b	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	c	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	d	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	e	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	f	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	g	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	h	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	i	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	j	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	k	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	l	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	m	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	n	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	o	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	p	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	q	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	r	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	s	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	t	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	u	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	v	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	w	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			
1	x	163	Total	C	N	O	S	0	0	0
			1253	788	224	236	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
B	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
C	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
D	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
E	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
F	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
G	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
H	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
I	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
J	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
K	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
L	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
M	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
N	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
O	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
P	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
Q	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
R	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
S	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
T	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
U	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
V	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
W	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
X	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
Y	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
Z	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
0	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
1	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
2	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
3	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
4	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
5	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
6	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
7	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5

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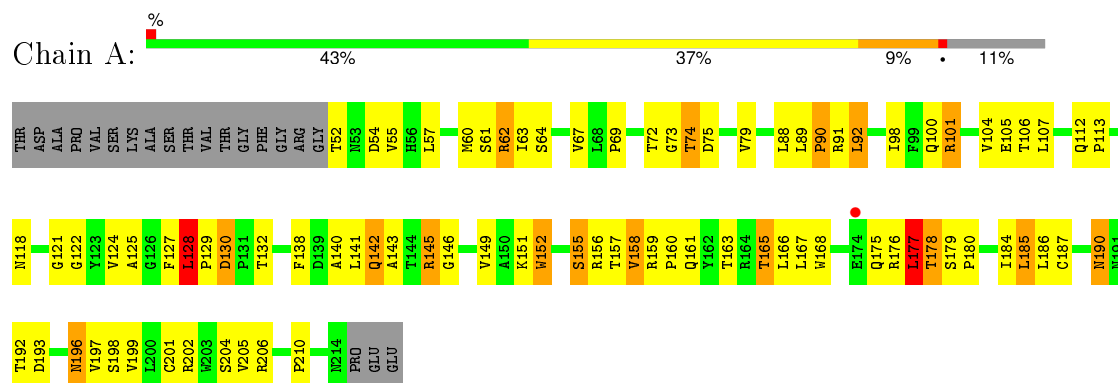
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Chain	Residue	Modelled	Actual	Comment	Reference
8	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
9	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
a	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
b	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
c	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
d	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
e	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
f	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
g	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
h	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
i	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
j	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
k	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
l	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
m	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
n	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
o	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
p	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
q	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
r	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
s	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
t	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
u	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
v	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
w	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
x	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5

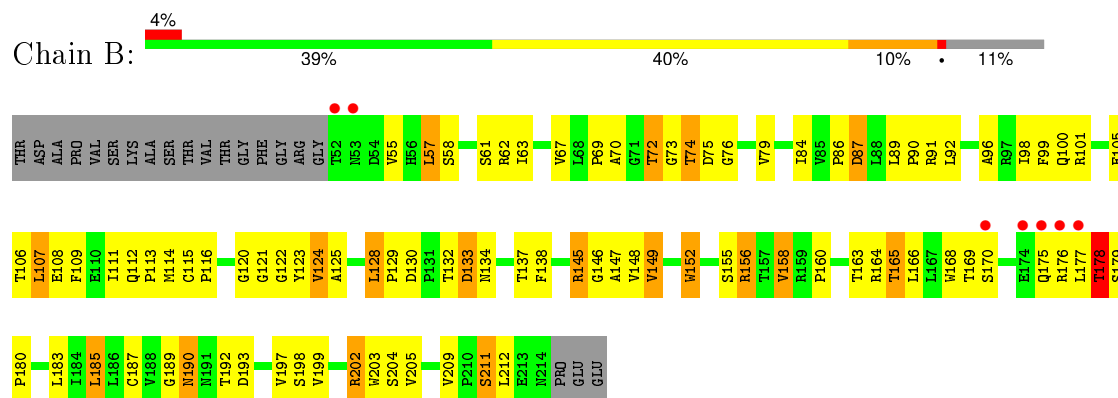
3 Residue-property plots [i](#)

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

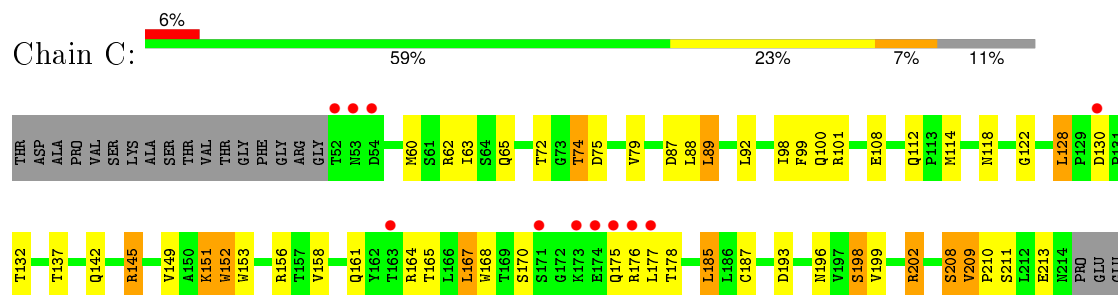
• Molecule 1: Coat protein



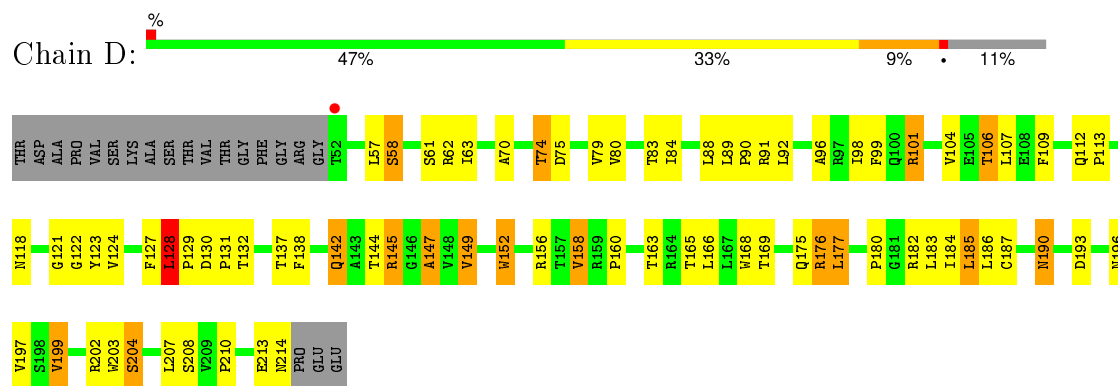
• Molecule 1: Coat protein



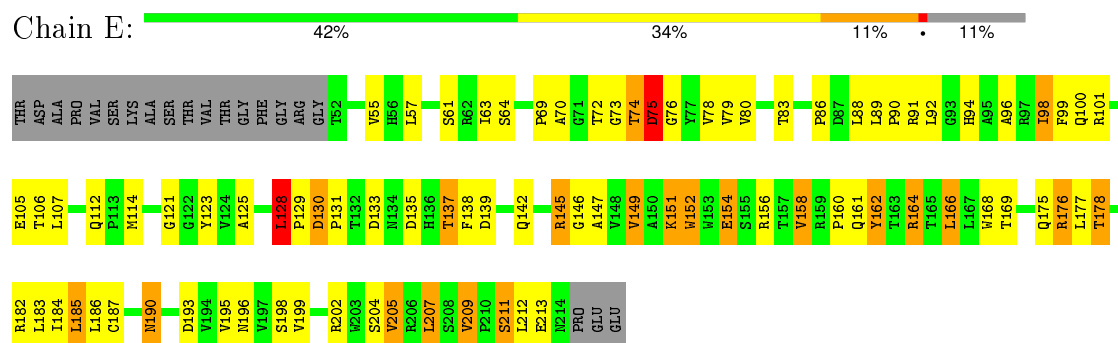
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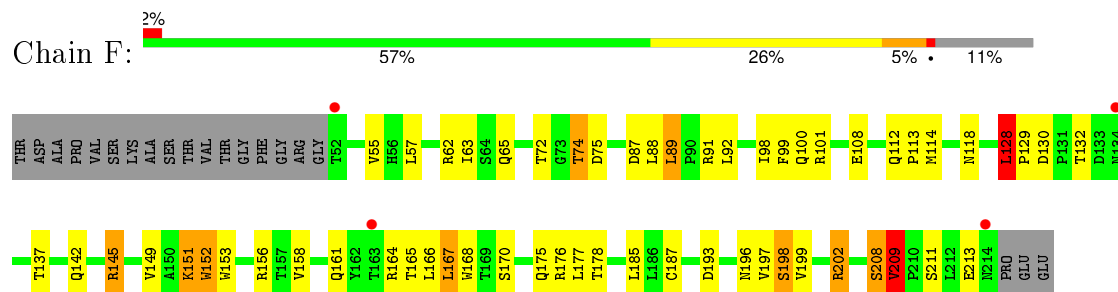
• Molecule 1: Coat protein



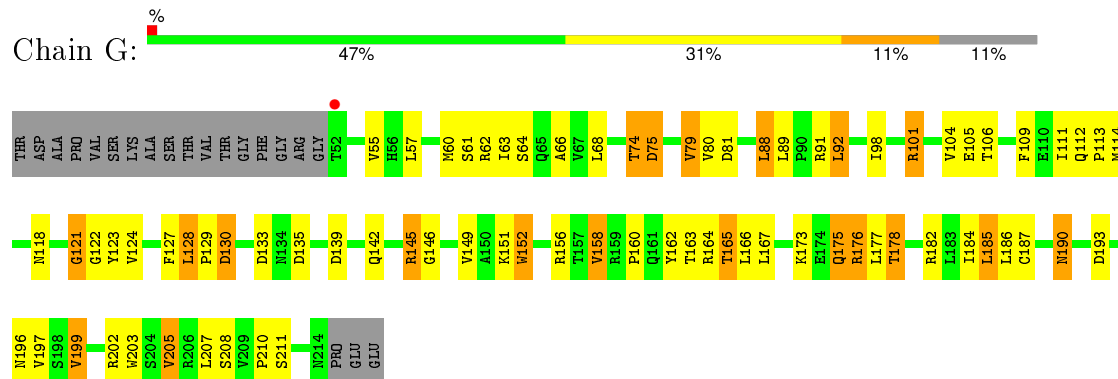
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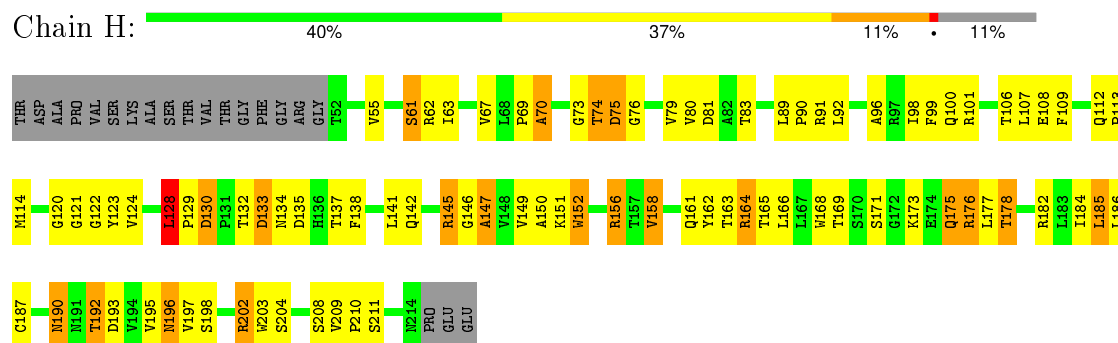
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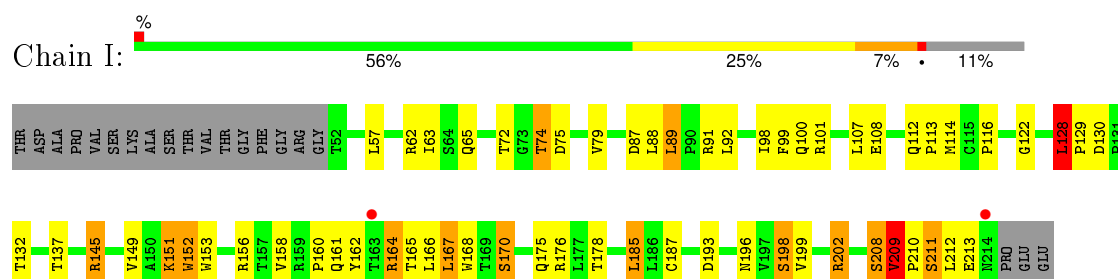
- Molecule 1: Coat protein



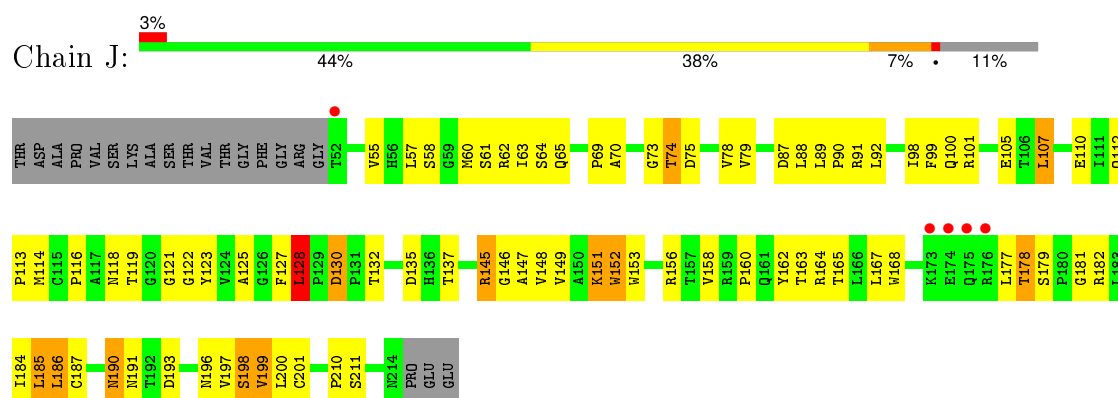
- Molecule 1: Coat protein



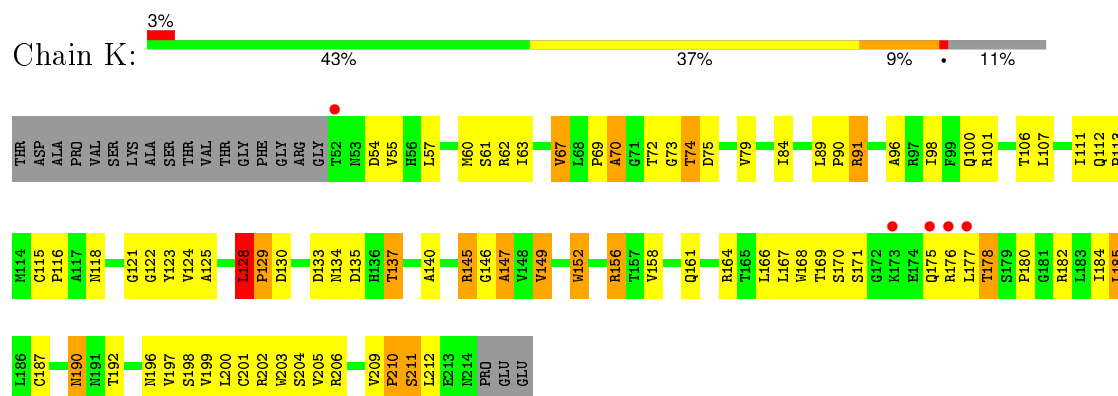
- Molecule 1: Coat protein



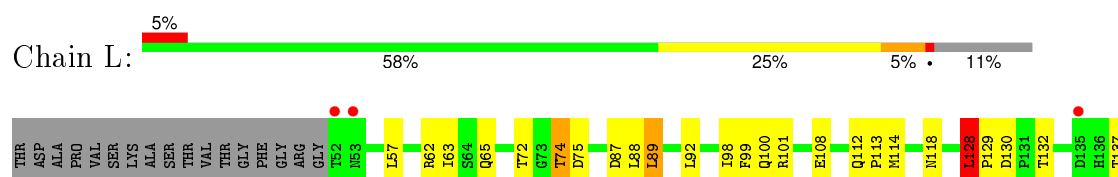
- Molecule 1: Coat protein



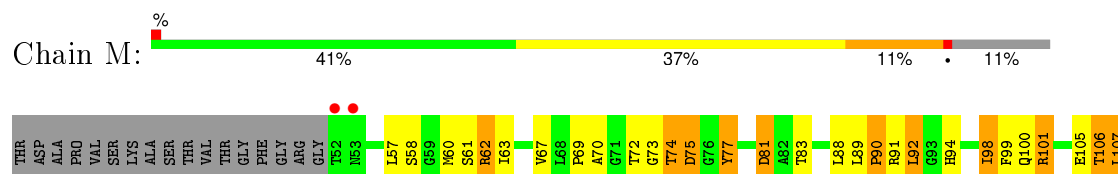
- Molecule 1: Coat protein



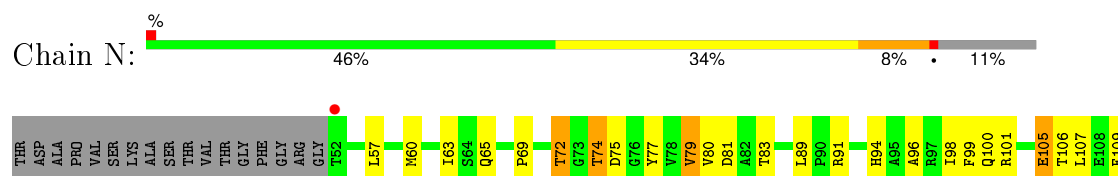
- Molecule 1: Coat protein



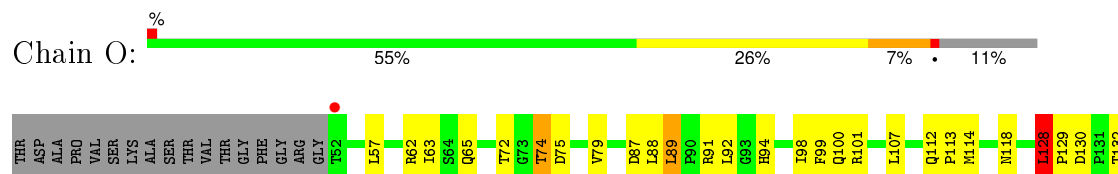
- Molecule 1: Coat protein



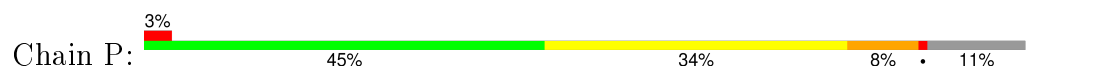
- Molecule 1: Coat protein

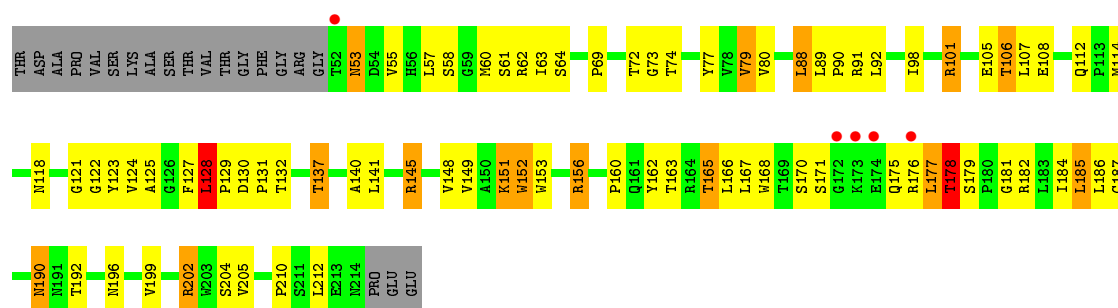


- Molecule 1: Coat protein

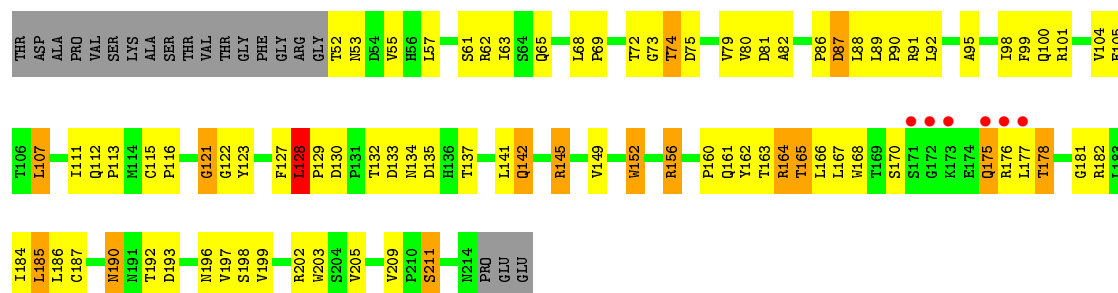


- Molecule 1: Coat protein

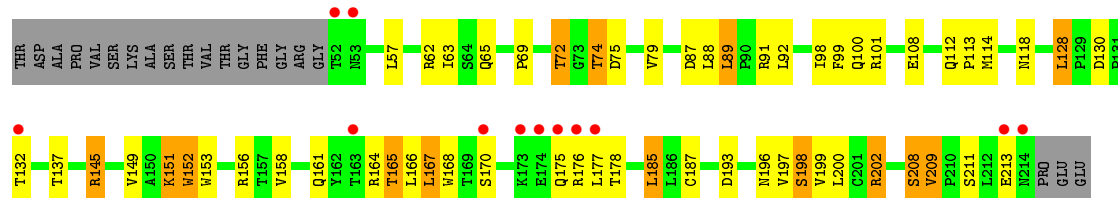




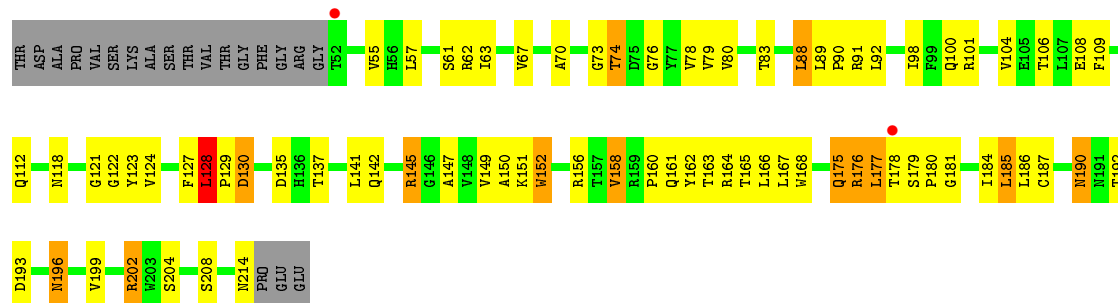
• Molecule 1: Coat protein



• Molecule 1: Coat protein

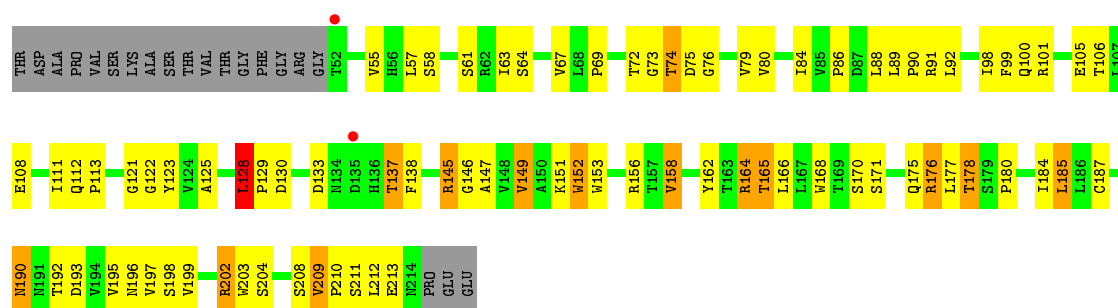


• Molecule 1: Coat protein

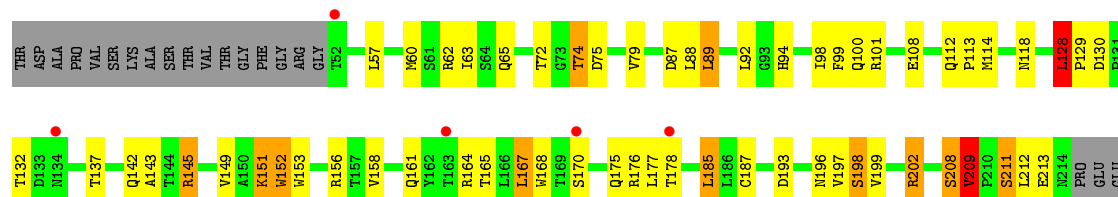


• Molecule 1: Coat protein

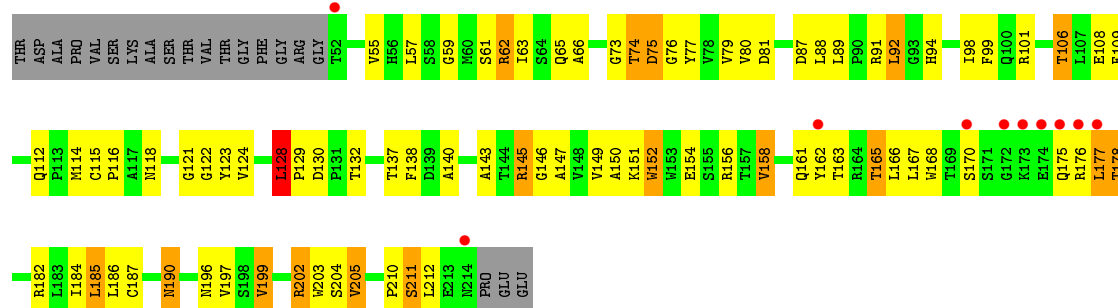
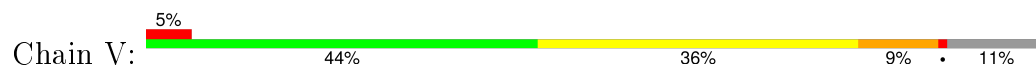




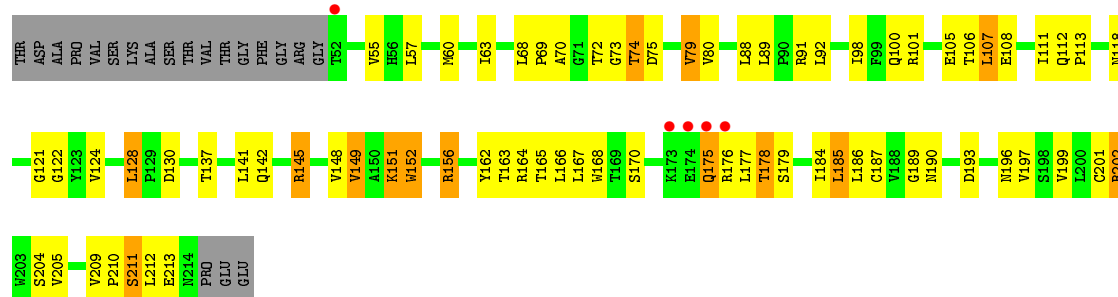
- Molecule 1: Coat protein



- Molecule 1: Coat protein



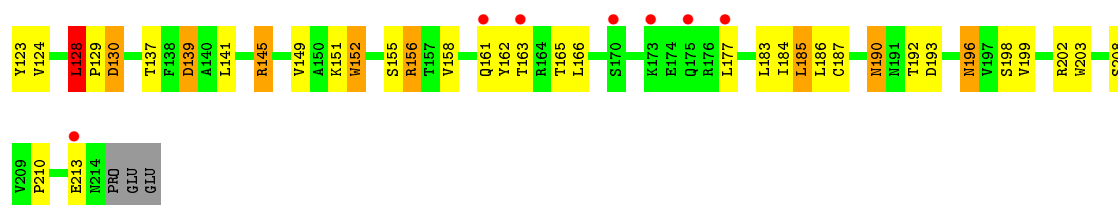
- Molecule 1: Coat protein



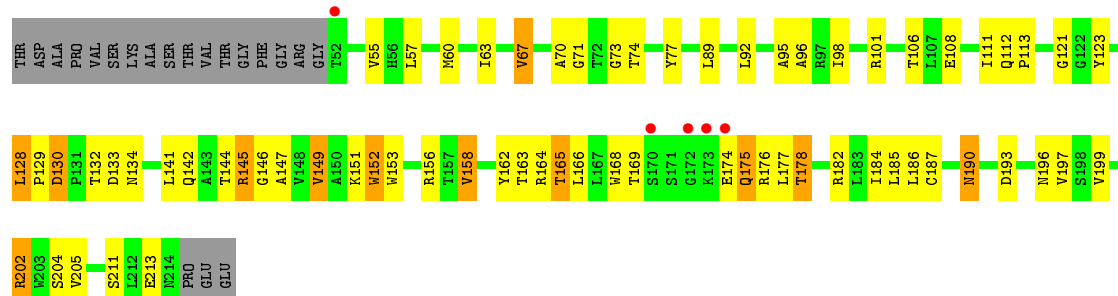
- Molecule 1: Coat protein



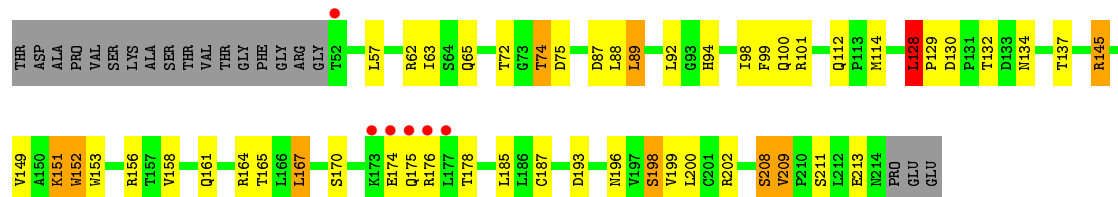




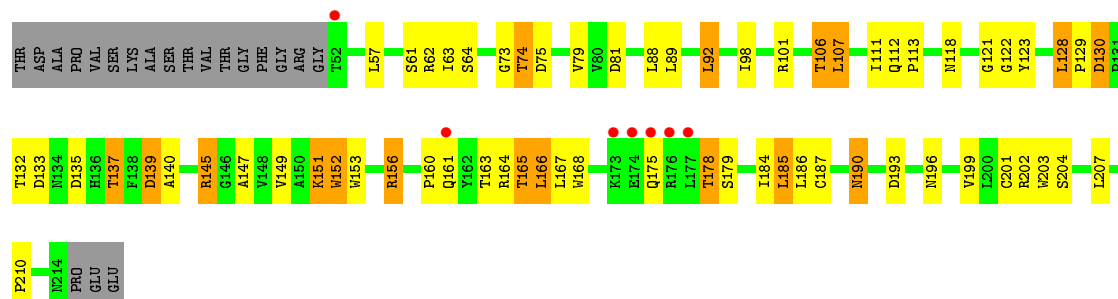
• Molecule 1: Coat protein



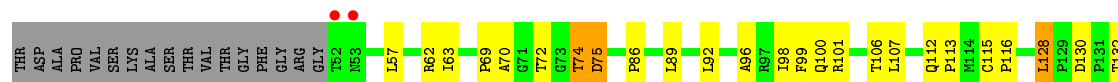
• Molecule 1: Coat protein

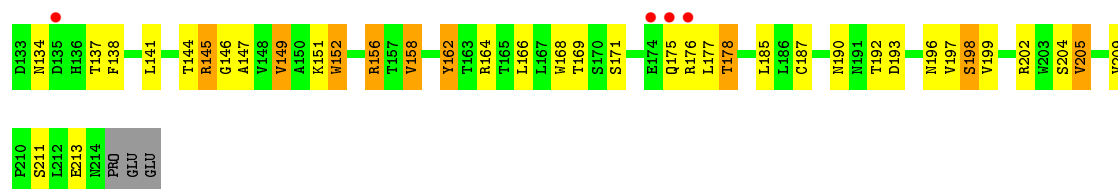


• Molecule 1: Coat protein

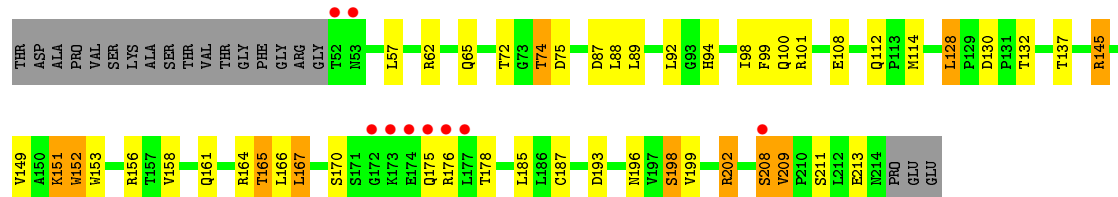


• Molecule 1: Coat protein

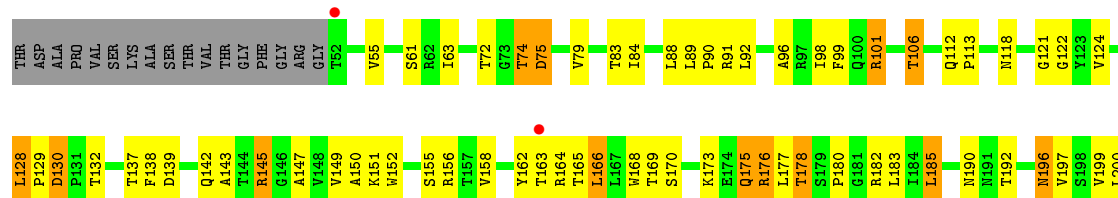




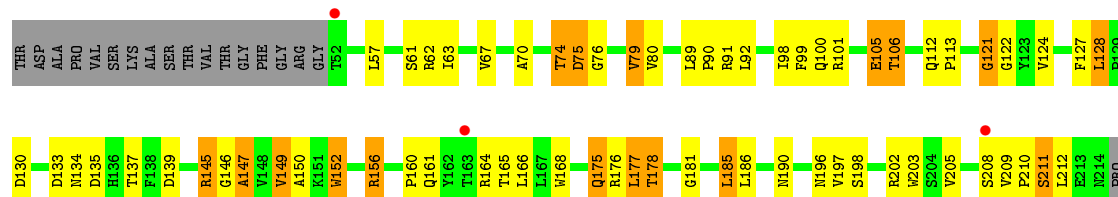
• Molecule 1: Coat protein



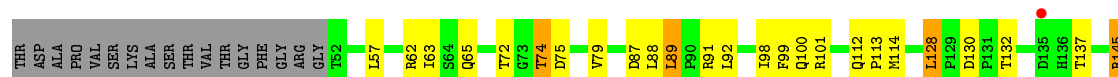
• Molecule 1: Coat protein



• Molecule 1: Coat protein

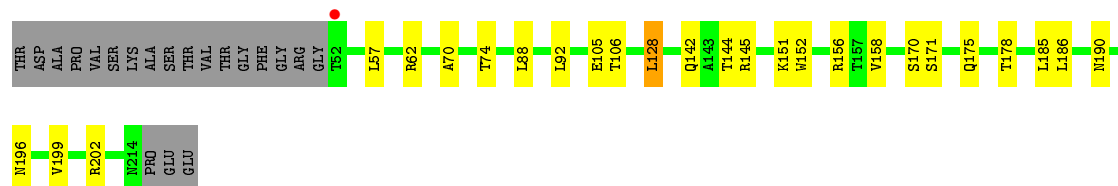
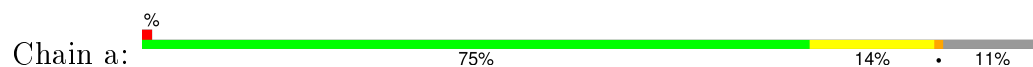


• Molecule 1: Coat protein

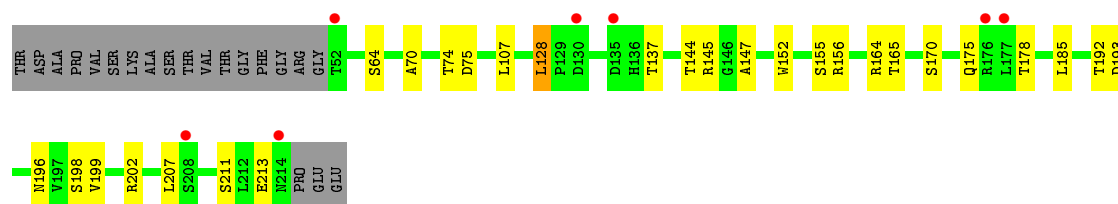




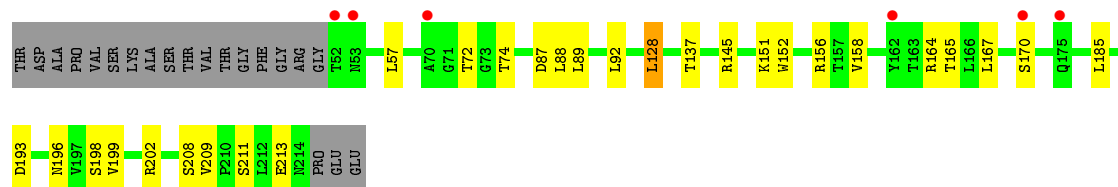
• Molecule 1: Coat protein



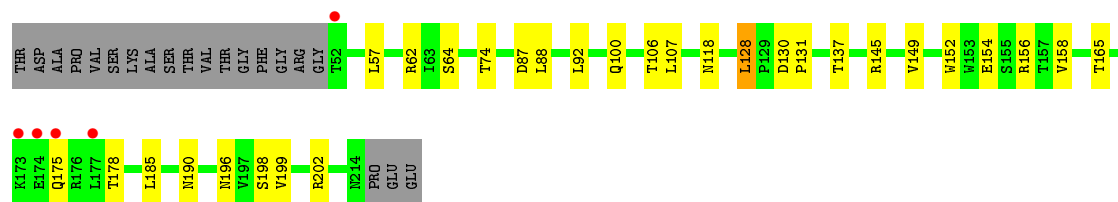
• Molecule 1: Coat protein



• Molecule 1: Coat protein

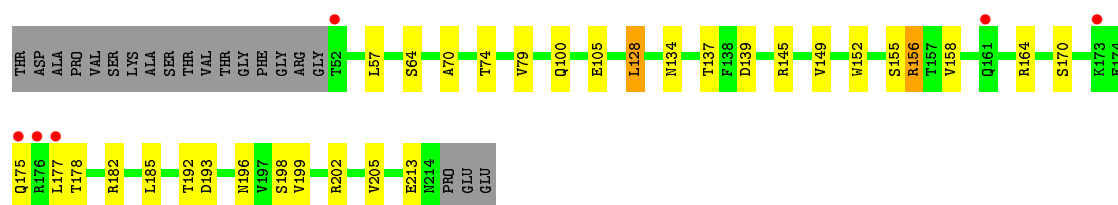


• Molecule 1: Coat protein

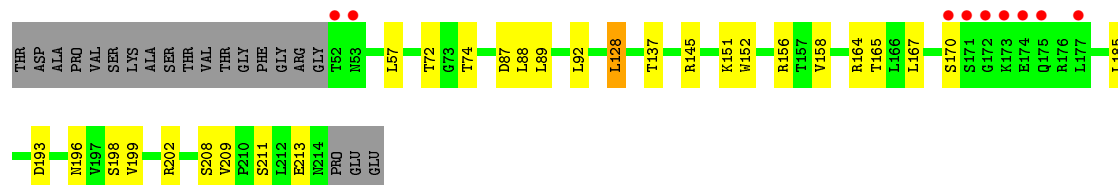


• Molecule 1: Coat protein





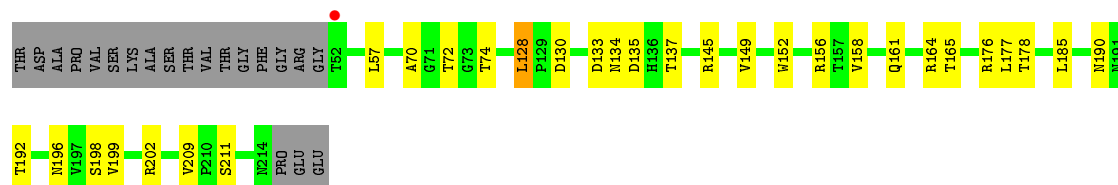
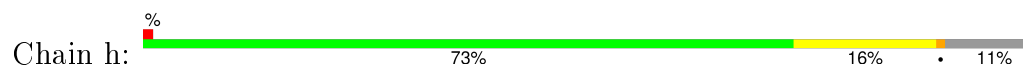
• Molecule 1: Coat protein



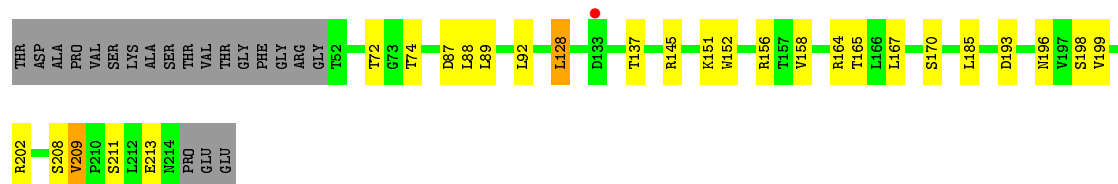
• Molecule 1: Coat protein



• Molecule 1: Coat protein

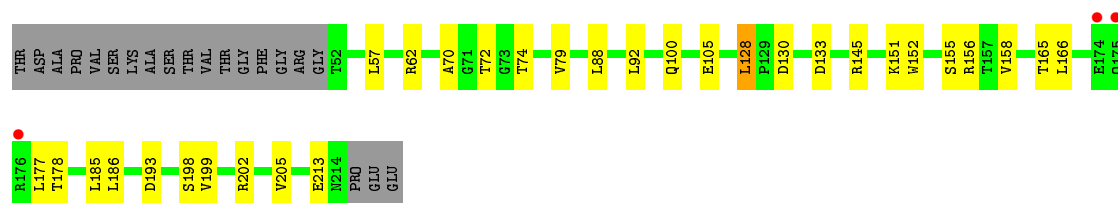


• Molecule 1: Coat protein

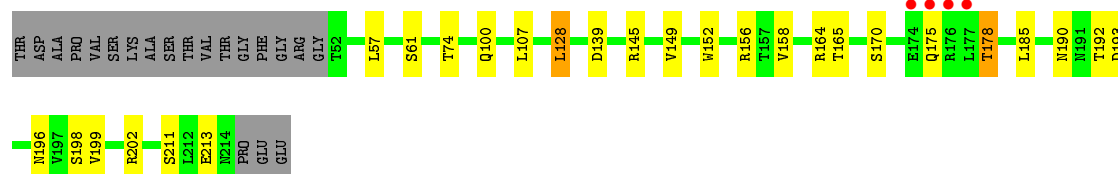
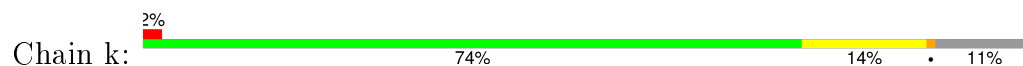


• Molecule 1: Coat protein

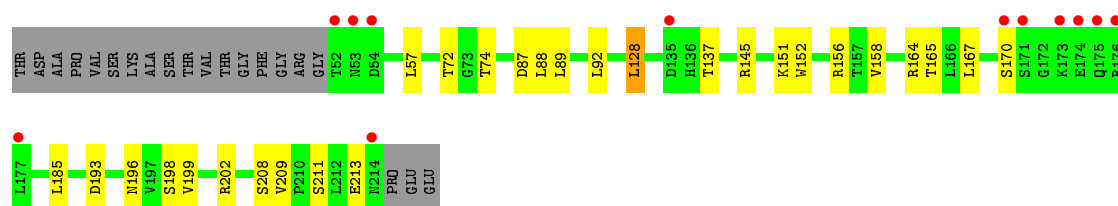




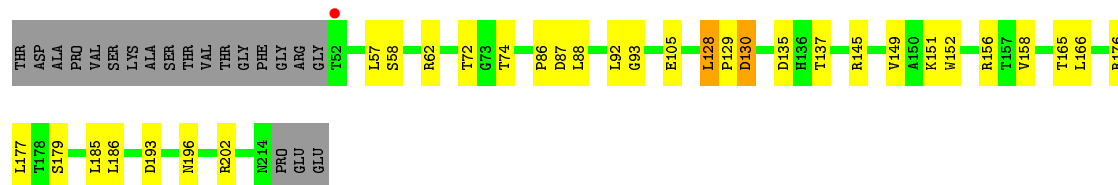
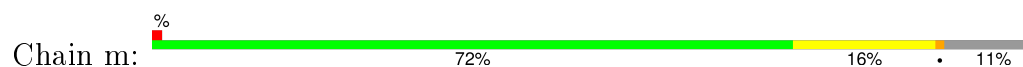
- Molecule 1: Coat protein



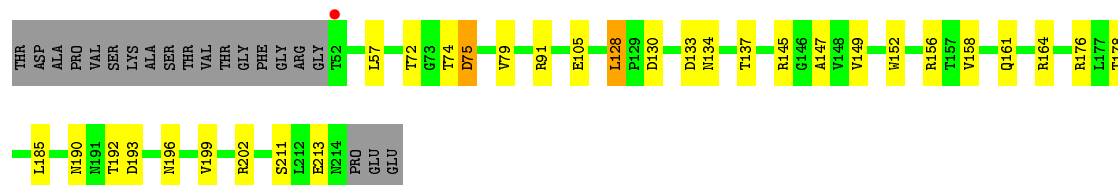
- Molecule 1: Coat protein



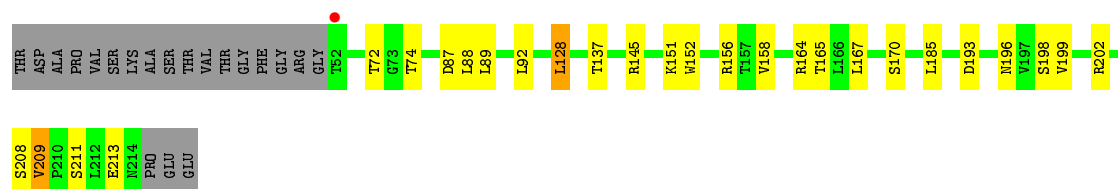
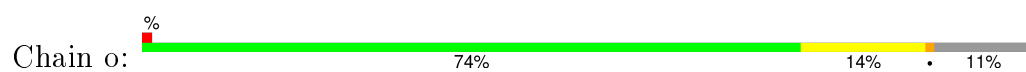
- Molecule 1: Coat protein



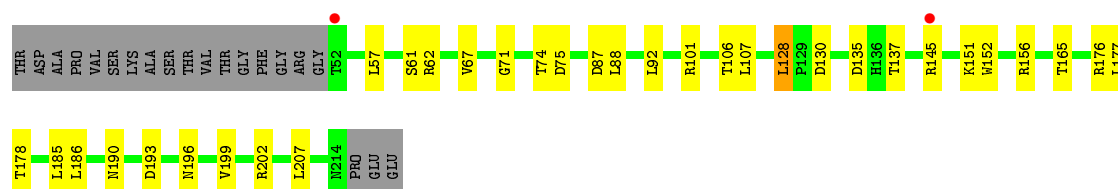
- Molecule 1: Coat protein



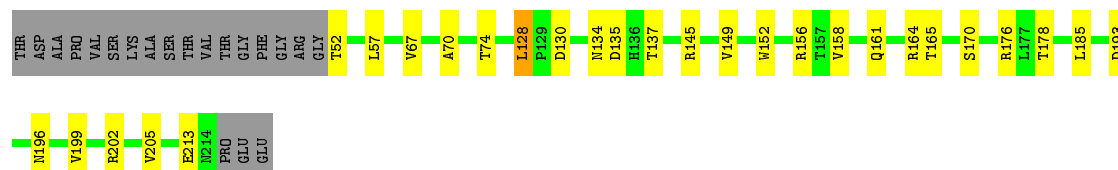
- Molecule 1: Coat protein



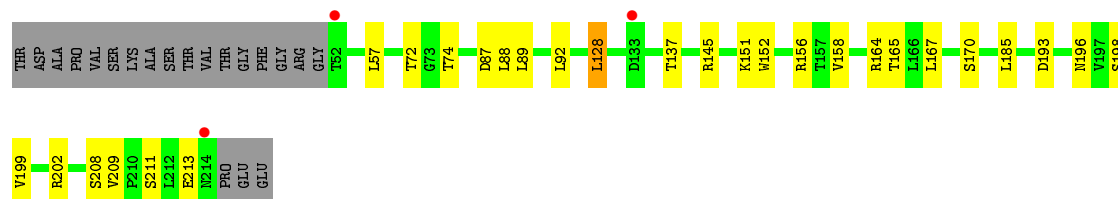
• Molecule 1: Coat protein



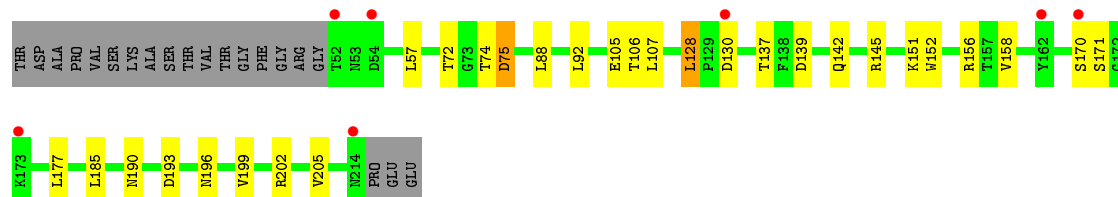
• Molecule 1: Coat protein



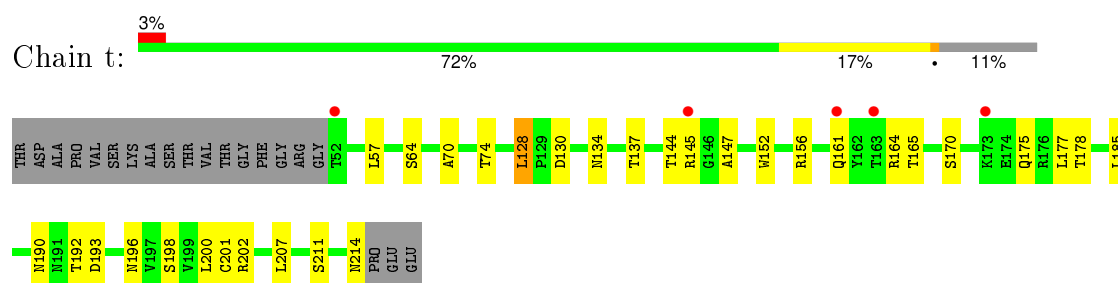
• Molecule 1: Coat protein



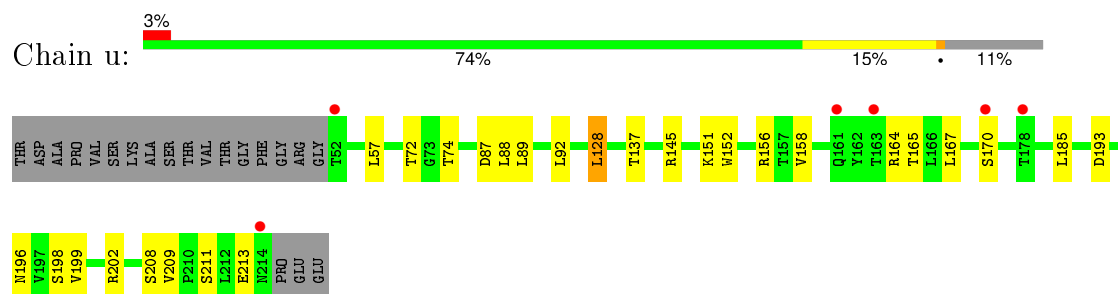
• Molecule 1: Coat protein



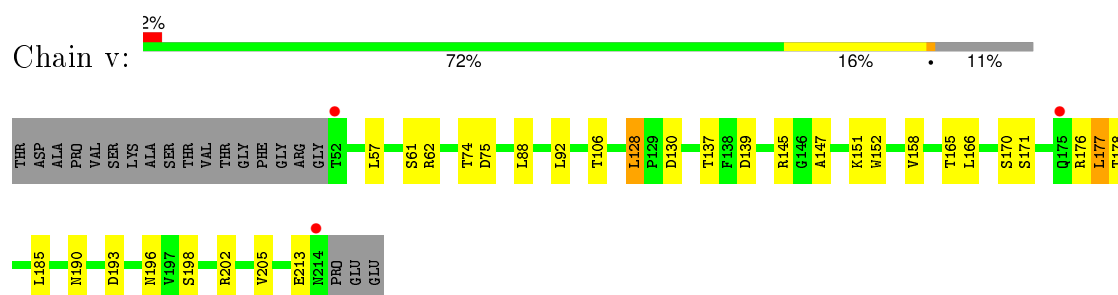
• Molecule 1: Coat protein



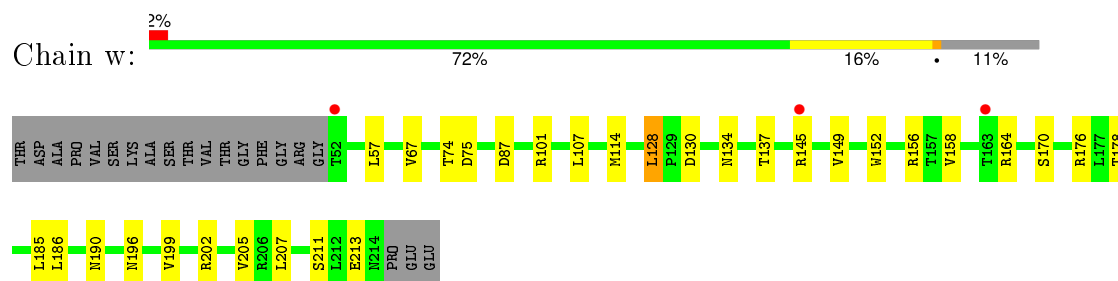
• Molecule 1: Coat protein



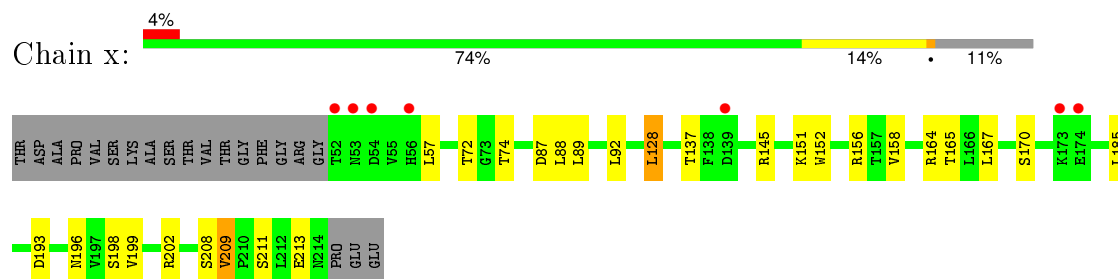
• Molecule 1: Coat protein



• Molecule 1: Coat protein



• Molecule 1: Coat protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	288.95Å 288.95Å 175.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.37 – 3.10 26.37 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.1 (26.37-3.10) 98.3 (26.37-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.238 , 0.288 0.238 , 0.285	Depositor DCC
R_{free} test set	12823 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 9.5	EDS
Estimated twinning fraction	0.448 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 255488 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	75180	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.53	0/1281	0.75	1/1753 (0.1%)
1	1	0.55	0/1281	0.80	2/1753 (0.1%)
1	2	0.52	0/1281	0.78	0/1753
1	3	0.53	0/1281	0.74	1/1753 (0.1%)
1	4	0.54	0/1281	0.79	1/1753 (0.1%)
1	5	0.54	0/1281	0.77	1/1753 (0.1%)
1	6	0.49	0/1281	0.74	1/1753 (0.1%)
1	7	0.61	0/1281	0.86	0/1753
1	8	0.59	0/1281	0.85	1/1753 (0.1%)
1	9	0.54	0/1281	0.76	1/1753 (0.1%)
1	A	0.55	0/1281	0.82	2/1753 (0.1%)
1	B	0.54	0/1281	0.78	0/1753
1	C	0.51	0/1281	0.75	1/1753 (0.1%)
1	D	0.55	0/1281	0.83	1/1753 (0.1%)
1	E	0.55	0/1281	0.84	1/1753 (0.1%)
1	F	0.51	0/1281	0.74	1/1753 (0.1%)
1	G	0.60	0/1281	0.85	0/1753
1	H	0.58	0/1281	0.82	1/1753 (0.1%)
1	I	0.55	0/1281	0.77	1/1753 (0.1%)
1	J	0.53	0/1281	0.81	1/1753 (0.1%)
1	K	0.53	0/1281	0.78	1/1753 (0.1%)
1	L	0.50	0/1281	0.72	1/1753 (0.1%)
1	M	0.62	0/1281	0.85	1/1753 (0.1%)
1	N	0.60	0/1281	0.84	1/1753 (0.1%)
1	O	0.53	0/1281	0.75	1/1753 (0.1%)
1	P	0.56	0/1281	0.82	1/1753 (0.1%)
1	Q	0.57	0/1281	0.81	1/1753 (0.1%)
1	R	0.50	0/1281	0.73	1/1753 (0.1%)
1	S	0.56	0/1281	0.84	1/1753 (0.1%)
1	T	0.57	0/1281	0.82	1/1753 (0.1%)
1	U	0.50	0/1281	0.74	1/1753 (0.1%)
1	V	0.56	0/1281	0.80	1/1753 (0.1%)
1	W	0.57	0/1281	0.79	1/1753 (0.1%)
1	X	0.52	0/1281	0.74	1/1753 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Y	0.58	0/1281	0.84	2/1753 (0.1%)
1	Z	0.53	0/1281	0.77	1/1753 (0.1%)
1	a	0.50	0/1281	0.76	1/1753 (0.1%)
1	b	0.53	0/1281	0.77	1/1753 (0.1%)
1	c	0.47	0/1281	0.72	1/1753 (0.1%)
1	d	0.59	0/1281	0.81	1/1753 (0.1%)
1	e	0.54	0/1281	0.78	3/1753 (0.2%)
1	f	0.46	0/1281	0.72	1/1753 (0.1%)
1	g	0.55	0/1281	0.79	2/1753 (0.1%)
1	h	0.57	0/1281	0.83	1/1753 (0.1%)
1	i	0.55	0/1281	0.76	1/1753 (0.1%)
1	j	0.56	0/1281	0.86	2/1753 (0.1%)
1	k	0.56	0/1281	0.79	1/1753 (0.1%)
1	l	0.50	0/1281	0.73	1/1753 (0.1%)
1	m	0.63	0/1281	0.85	2/1753 (0.1%)
1	n	0.58	0/1281	0.83	1/1753 (0.1%)
1	o	0.56	0/1281	0.76	1/1753 (0.1%)
1	p	0.57	0/1281	0.82	1/1753 (0.1%)
1	q	0.55	0/1281	0.78	1/1753 (0.1%)
1	r	0.49	0/1281	0.73	1/1753 (0.1%)
1	s	0.48	0/1281	0.79	1/1753 (0.1%)
1	t	0.54	0/1281	0.78	1/1753 (0.1%)
1	u	0.46	0/1281	0.72	1/1753 (0.1%)
1	v	0.53	0/1281	0.78	2/1753 (0.1%)
1	w	0.52	0/1281	0.81	1/1753 (0.1%)
1	x	0.51	0/1281	0.74	1/1753 (0.1%)
All	All	0.54	0/76860	0.79	65/105180 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	4	0	1
1	E	0	1
1	Y	0	2
1	b	0	1
1	m	0	1
1	t	0	1
1	w	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	128	LEU	CA-CB-CG	8.91	135.78	115.30
1	t	128	LEU	CA-CB-CG	8.16	134.06	115.30
1	N	128	LEU	CA-CB-CG	7.52	132.60	115.30
1	S	128	LEU	CA-CB-CG	7.37	132.25	115.30
1	4	128	LEU	CA-CB-CG	7.32	132.14	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	4	207	LEU	Peptide
1	E	207	LEU	Peptide
1	Y	129	PRO	Peptide
1	Y	207	LEU	Peptide
1	b	207	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1253	0	1242	41	0
1	1	1253	0	1242	39	0
1	2	1253	0	1242	42	0
1	3	1253	0	1242	31	1
1	4	1253	0	1242	42	0
1	5	1253	0	1242	41	0
1	6	1253	0	1242	32	0
1	7	1253	0	1242	62	0
1	8	1253	0	1242	49	0
1	9	1253	0	1242	54	0
1	A	1253	0	1242	74	0
1	B	1253	0	1242	84	0
1	C	1253	0	1242	44	0
1	D	1253	0	1242	77	0
1	E	1253	0	1242	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1253	0	1242	51	0
1	G	1253	0	1242	85	0
1	H	1253	0	1242	98	0
1	I	1253	0	1242	76	0
1	J	1253	0	1242	77	0
1	K	1253	0	1242	79	0
1	L	1253	0	1242	46	0
1	M	1253	0	1242	96	0
1	N	1253	0	1242	72	1
1	O	1253	0	1242	66	0
1	P	1253	0	1242	73	0
1	Q	1253	0	1242	84	0
1	R	1253	0	1242	48	0
1	S	1253	0	1242	73	0
1	T	1253	0	1242	84	0
1	U	1253	0	1242	59	0
1	V	1253	0	1242	86	0
1	W	1253	0	1242	75	0
1	X	1253	0	1242	49	0
1	Y	1253	0	1242	58	0
1	Z	1253	0	1242	56	0
1	a	1253	0	1242	0	0
1	b	1253	0	1242	0	0
1	c	1253	0	1242	0	0
1	d	1253	0	1242	0	0
1	e	1253	0	1242	0	0
1	f	1253	0	1242	0	0
1	g	1253	0	1242	0	0
1	h	1253	0	1242	0	0
1	i	1253	0	1242	0	0
1	j	1253	0	1242	0	0
1	k	1253	0	1242	0	0
1	l	1253	0	1242	0	0
1	m	1253	0	1242	0	0
1	n	1253	0	1242	0	0
1	o	1253	0	1242	0	0
1	p	1253	0	1242	0	0
1	q	1253	0	1242	0	0
1	r	1253	0	1242	0	0
1	s	1253	0	1242	0	0
1	t	1253	0	1242	0	0
1	u	1253	0	1242	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	v	1253	0	1242	0	0
1	w	1253	0	1242	0	0
1	x	1253	0	1242	0	0
All	All	75180	0	74520	1835	1

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

The worst 5 of 1835 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:101:ARG:HE	1:N:166:LEU:HD21	1.02	1.07
1:T:101:ARG:HE	1:T:166:LEU:HD21	1.23	1.03
1:Q:101:ARG:HE	1:Q:166:LEU:HD21	1.21	1.02
1:H:91:ARG:O	1:M:98:ILE:HD11	1.61	1.00
1:V:163:THR:HA	1:X:101:ARG:HH22	1.64	1.00

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:77:TYR:OH	1:3:134:ASN:OD1[3_654]	1.87	0.33

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	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	1	161/183 (88%)	142 (88%)	17 (11%)	2 (1%)	16	52
1	2	161/183 (88%)	136 (84%)	22 (14%)	3 (2%)	10	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	4	161/183 (88%)	141 (88%)	18 (11%)	2 (1%)	16	52
1	5	161/183 (88%)	148 (92%)	9 (6%)	4 (2%)	7	32
1	6	161/183 (88%)	152 (94%)	8 (5%)	1 (1%)	30	68
1	7	161/183 (88%)	141 (88%)	18 (11%)	2 (1%)	16	52
1	8	161/183 (88%)	145 (90%)	12 (8%)	4 (2%)	7	32
1	9	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	30	68
1	A	161/183 (88%)	148 (92%)	11 (7%)	2 (1%)	16	52
1	B	161/183 (88%)	142 (88%)	16 (10%)	3 (2%)	10	40
1	C	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	D	161/183 (88%)	149 (92%)	10 (6%)	2 (1%)	16	52
1	E	161/183 (88%)	147 (91%)	12 (8%)	2 (1%)	16	52
1	F	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	G	161/183 (88%)	144 (89%)	16 (10%)	1 (1%)	30	68
1	H	161/183 (88%)	143 (89%)	15 (9%)	3 (2%)	10	40
1	I	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	J	161/183 (88%)	145 (90%)	15 (9%)	1 (1%)	30	68
1	K	161/183 (88%)	142 (88%)	16 (10%)	3 (2%)	10	40
1	L	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	M	161/183 (88%)	141 (88%)	16 (10%)	4 (2%)	7	32
1	N	161/183 (88%)	143 (89%)	18 (11%)	0	100	100
1	O	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	30	68
1	P	161/183 (88%)	139 (86%)	20 (12%)	2 (1%)	16	52
1	Q	161/183 (88%)	145 (90%)	15 (9%)	1 (1%)	30	68
1	R	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	30	68
1	S	161/183 (88%)	146 (91%)	13 (8%)	2 (1%)	16	52
1	T	161/183 (88%)	146 (91%)	15 (9%)	0	100	100
1	U	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	30	68
1	V	161/183 (88%)	145 (90%)	14 (9%)	2 (1%)	16	52
1	W	161/183 (88%)	142 (88%)	17 (11%)	2 (1%)	16	52
1	X	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	30	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	161/183 (88%)	147 (91%)	13 (8%)	1 (1%)	30	68
1	Z	161/183 (88%)	143 (89%)	15 (9%)	3 (2%)	10	40
1	a	161/183 (88%)	140 (87%)	20 (12%)	1 (1%)	30	68
1	b	161/183 (88%)	141 (88%)	17 (11%)	3 (2%)	10	40
1	c	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	d	161/183 (88%)	148 (92%)	12 (8%)	1 (1%)	30	68
1	e	161/183 (88%)	143 (89%)	17 (11%)	1 (1%)	30	68
1	f	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	g	161/183 (88%)	146 (91%)	14 (9%)	1 (1%)	30	68
1	h	161/183 (88%)	145 (90%)	15 (9%)	1 (1%)	30	68
1	i	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	30	68
1	j	161/183 (88%)	146 (91%)	13 (8%)	2 (1%)	16	52
1	k	161/183 (88%)	143 (89%)	17 (11%)	1 (1%)	30	68
1	l	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	30	68
1	m	161/183 (88%)	144 (89%)	16 (10%)	1 (1%)	30	68
1	n	161/183 (88%)	146 (91%)	13 (8%)	2 (1%)	16	52
1	o	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	30	68
1	p	161/183 (88%)	144 (89%)	15 (9%)	2 (1%)	16	52
1	q	161/183 (88%)	145 (90%)	15 (9%)	1 (1%)	30	68
1	r	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	s	161/183 (88%)	134 (83%)	26 (16%)	1 (1%)	30	68
1	t	161/183 (88%)	147 (91%)	12 (8%)	2 (1%)	16	52
1	u	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	30	68
1	v	161/183 (88%)	143 (89%)	16 (10%)	2 (1%)	16	52
1	w	161/183 (88%)	146 (91%)	14 (9%)	1 (1%)	30	68
1	x	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	30	68
All	All	9660/10980 (88%)	8763 (91%)	803 (8%)	94 (1%)	19	58

5 of 94 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	THR
1	C	209	VAL

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Mol	Chain	Res	Type
1	H	70	ALA
1	K	70	ALA
1	W	70	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	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	1	138/153 (90%)	109 (79%)	29 (21%)	1	6
1	2	138/153 (90%)	112 (81%)	26 (19%)	2	8
1	3	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	4	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	5	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	6	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	7	138/153 (90%)	108 (78%)	30 (22%)	1	5
1	8	138/153 (90%)	112 (81%)	26 (19%)	2	8
1	9	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	A	138/153 (90%)	109 (79%)	29 (21%)	1	6
1	B	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	C	138/153 (90%)	112 (81%)	26 (19%)	2	8
1	D	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	E	138/153 (90%)	102 (74%)	36 (26%)	0	2
1	F	138/153 (90%)	110 (80%)	28 (20%)	1	6
1	G	138/153 (90%)	105 (76%)	33 (24%)	1	3
1	H	138/153 (90%)	112 (81%)	26 (19%)	2	8
1	I	138/153 (90%)	110 (80%)	28 (20%)	1	6
1	J	138/153 (90%)	114 (83%)	24 (17%)	2	11
1	K	138/153 (90%)	112 (81%)	26 (19%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	M	138/153 (90%)	109 (79%)	29 (21%)	1	6
1	N	138/153 (90%)	106 (77%)	32 (23%)	1	4
1	O	138/153 (90%)	110 (80%)	28 (20%)	1	6
1	P	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	Q	138/153 (90%)	110 (80%)	28 (20%)	1	6
1	R	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	S	138/153 (90%)	115 (83%)	23 (17%)	3	11
1	T	138/153 (90%)	104 (75%)	34 (25%)	1	3
1	U	138/153 (90%)	110 (80%)	28 (20%)	1	6
1	V	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	W	138/153 (90%)	115 (83%)	23 (17%)	3	11
1	X	138/153 (90%)	112 (81%)	26 (19%)	2	8
1	Y	138/153 (90%)	115 (83%)	23 (17%)	3	11
1	Z	138/153 (90%)	105 (76%)	33 (24%)	1	3
1	a	138/153 (90%)	113 (82%)	25 (18%)	2	9
1	b	138/153 (90%)	114 (83%)	24 (17%)	2	11
1	c	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	d	138/153 (90%)	109 (79%)	29 (21%)	1	6
1	e	138/153 (90%)	108 (78%)	30 (22%)	1	5
1	f	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	g	138/153 (90%)	106 (77%)	32 (23%)	1	4
1	h	138/153 (90%)	109 (79%)	29 (21%)	1	6
1	i	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	j	138/153 (90%)	110 (80%)	28 (20%)	1	6
1	k	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	l	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	m	138/153 (90%)	108 (78%)	30 (22%)	1	5
1	n	138/153 (90%)	108 (78%)	30 (22%)	1	5
1	o	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	p	138/153 (90%)	107 (78%)	31 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	q	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	r	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	s	138/153 (90%)	109 (79%)	29 (21%)	1	6
1	t	138/153 (90%)	109 (79%)	29 (21%)	1	6
1	u	138/153 (90%)	111 (80%)	27 (20%)	1	7
1	v	138/153 (90%)	108 (78%)	30 (22%)	1	5
1	w	138/153 (90%)	109 (79%)	29 (21%)	1	6
1	x	138/153 (90%)	110 (80%)	28 (20%)	1	6
All	All	8280/9180 (90%)	6606 (80%)	1674 (20%)	1	7

5 of 1674 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	79	VAL
1	7	177	LEU
1	t	177	LEU
1	1	208	SER
1	4	152	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 195 such sidechains are listed below:

Mol	Chain	Res	Type
1	0	175	GLN
1	7	118	ASN
1	t	214	ASN
1	1	118	ASN
1	4	118	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	163/183 (89%)	0.07	1 (0%) 90 80	28, 44, 82, 144	0
1	1	163/183 (89%)	0.22	10 (6%) 25 10	30, 49, 106, 153	0
1	2	163/183 (89%)	0.19	5 (3%) 52 28	36, 55, 110, 160	0
1	3	163/183 (89%)	0.19	6 (3%) 45 22	26, 45, 109, 163	0
1	4	163/183 (89%)	0.19	7 (4%) 39 18	30, 52, 109, 171	0
1	5	163/183 (89%)	0.13	6 (3%) 45 22	30, 51, 104, 156	0
1	6	163/183 (89%)	0.40	9 (5%) 29 12	32, 56, 122, 194	0
1	7	163/183 (89%)	-0.08	2 (1%) 81 64	26, 41, 72, 127	0
1	8	163/183 (89%)	-0.06	3 (1%) 71 50	26, 42, 76, 120	0
1	9	163/183 (89%)	0.06	2 (1%) 81 64	25, 43, 86, 112	0
1	A	163/183 (89%)	-0.03	1 (0%) 90 80	31, 47, 89, 132	0
1	B	163/183 (89%)	0.15	7 (4%) 39 18	29, 47, 101, 189	0
1	C	163/183 (89%)	0.28	11 (6%) 21 7	26, 50, 111, 183	0
1	D	163/183 (89%)	-0.05	1 (0%) 90 80	32, 46, 81, 112	0
1	E	163/183 (89%)	-0.06	0 100 100	24, 43, 79, 126	0
1	F	163/183 (89%)	0.25	4 (2%) 61 37	32, 53, 101, 137	0
1	G	163/183 (89%)	-0.07	1 (0%) 90 80	25, 43, 74, 114	0
1	H	163/183 (89%)	-0.05	0 100 100	26, 41, 76, 105	0
1	I	163/183 (89%)	0.05	2 (1%) 81 64	27, 44, 81, 118	0
1	J	163/183 (89%)	0.16	5 (3%) 52 28	27, 52, 110, 177	0
1	K	163/183 (89%)	0.17	5 (3%) 52 28	26, 53, 106, 171	0
1	L	163/183 (89%)	0.28	9 (5%) 29 12	27, 54, 123, 169	0
1	M	163/183 (89%)	-0.06	2 (1%) 81 64	23, 38, 71, 137	0
1	N	163/183 (89%)	-0.08	2 (1%) 81 64	23, 37, 74, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	O	163/183 (89%)	0.09	2 (1%) 81 64	28, 46, 84, 129	0
1	P	163/183 (89%)	0.13	5 (3%) 52 28	25, 47, 100, 159	0
1	Q	163/183 (89%)	0.12	6 (3%) 45 22	26, 45, 113, 151	0
1	R	163/183 (89%)	0.35	12 (7%) 17 6	29, 54, 124, 176	0
1	S	163/183 (89%)	-0.05	2 (1%) 81 64	29, 45, 81, 123	0
1	T	163/183 (89%)	0.01	2 (1%) 81 64	26, 44, 81, 120	0
1	U	163/183 (89%)	0.27	5 (3%) 52 28	36, 52, 96, 140	0
1	V	163/183 (89%)	0.24	10 (6%) 25 10	28, 53, 116, 150	0
1	W	163/183 (89%)	0.09	5 (3%) 52 28	27, 47, 104, 156	0
1	X	163/183 (89%)	0.35	11 (6%) 21 7	28, 47, 116, 193	0
1	Y	163/183 (89%)	-0.06	1 (0%) 90 80	25, 42, 79, 121	0
1	Z	163/183 (89%)	-0.02	1 (0%) 90 80	31, 48, 81, 143	0
1	a	163/183 (89%)	0.25	1 (0%) 90 80	36, 62, 110, 149	0
1	b	163/183 (89%)	0.15	7 (4%) 39 18	31, 53, 104, 147	0
1	c	163/183 (89%)	0.41	6 (3%) 45 22	36, 66, 120, 135	0
1	d	163/183 (89%)	0.07	5 (3%) 52 28	25, 43, 103, 156	0
1	e	163/183 (89%)	0.18	6 (3%) 45 22	28, 49, 106, 153	0
1	f	163/183 (89%)	0.34	9 (5%) 29 12	37, 59, 114, 159	0
1	g	163/183 (89%)	-0.09	1 (0%) 90 80	29, 48, 81, 120	0
1	h	163/183 (89%)	-0.04	1 (0%) 90 80	26, 43, 79, 121	0
1	i	163/183 (89%)	0.07	1 (0%) 90 80	26, 45, 87, 114	0
1	j	163/183 (89%)	0.13	3 (1%) 71 50	26, 49, 102, 165	0
1	k	163/183 (89%)	0.07	4 (2%) 61 37	34, 47, 102, 151	0
1	l	163/183 (89%)	0.43	12 (7%) 17 6	31, 52, 115, 265	0
1	m	163/183 (89%)	-0.11	1 (0%) 90 80	25, 36, 71, 115	0
1	n	163/183 (89%)	0.00	1 (0%) 90 80	28, 44, 78, 137	0
1	o	163/183 (89%)	0.04	1 (0%) 90 80	26, 39, 79, 124	0
1	p	163/183 (89%)	-0.05	2 (1%) 81 64	28, 43, 90, 120	0
1	q	163/183 (89%)	0.06	0 100 100	26, 47, 95, 118	0
1	r	163/183 (89%)	0.18	3 (1%) 71 50	38, 57, 99, 128	0
1	s	163/183 (89%)	0.23	7 (4%) 39 18	39, 61, 103, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	t	163/183 (89%)	0.15	5 (3%)	52	28	33, 52, 103, 141	0
1	u	163/183 (89%)	0.44	6 (3%)	45	22	41, 65, 114, 144	0
1	v	163/183 (89%)	0.15	3 (1%)	71	50	35, 55, 93, 129	0
1	w	163/183 (89%)	-0.02	3 (1%)	71	50	29, 44, 93, 117	0
1	x	163/183 (89%)	0.18	7 (4%)	39	18	26, 49, 97, 122	0
All	All	9780/10980 (89%)	0.12	258 (2%)	59	35	23, 48, 102, 265	0

The worst 5 of 258 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	l	174	GLU	12.7
1	l	175	GLN	12.0
1	l	177	LEU	10.3
1	f	52	THR	9.9
1	l	176	ARG	9.7

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 carbohydrates 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.