



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2024 – 06:40 PM EDT

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

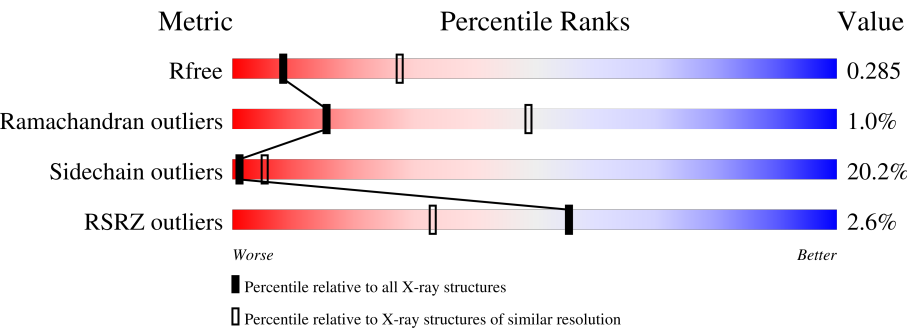
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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.





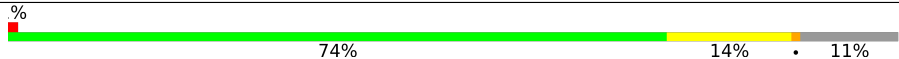
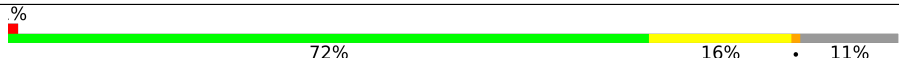
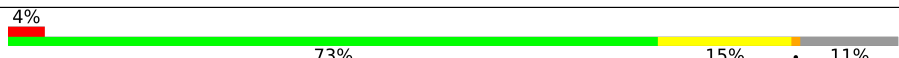
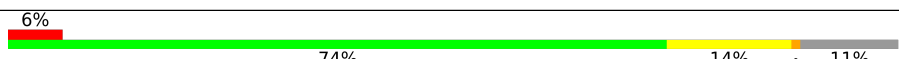
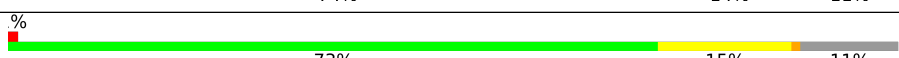
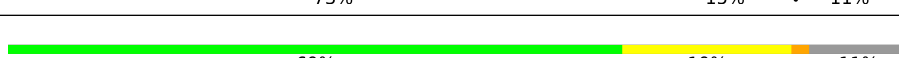
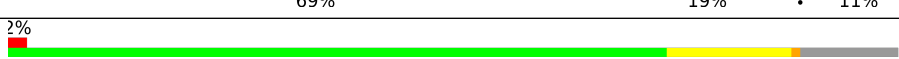

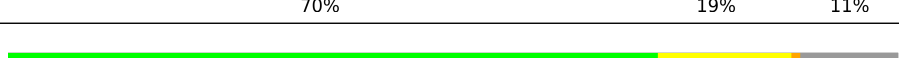







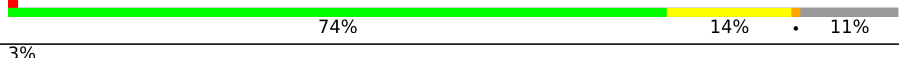
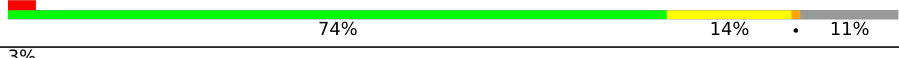

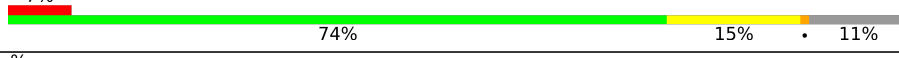



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	0	183	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>74%14%•11%</div></div>
1	1	183	<div><div>5%</div><div></div><div></div><div></div><div></div></div> <div>72%17%•11%</div>

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Mol	Chain	Length	Quality of chain
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	
1	U	183	
1	V	183	

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Mol	Chain	Length	Quality of chain
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	
1	t	183	
1	u	183	

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Mol	Chain	Length	Quality of chain
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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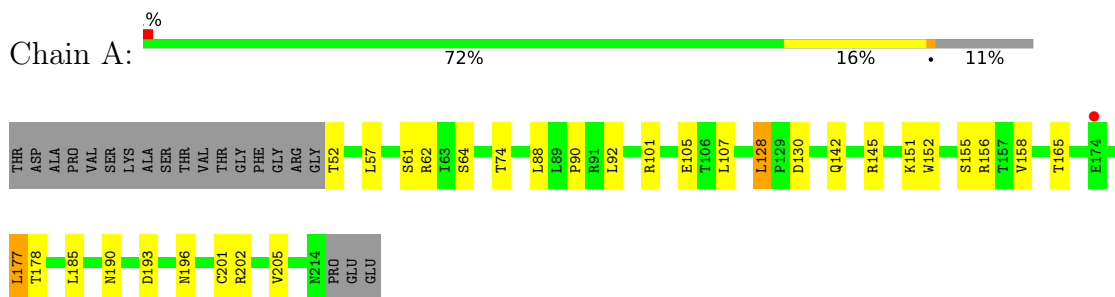
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Chain	Residue	Modelled	Actual	Comment	Reference
8	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
9	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
a	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
b	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
c	214	ASN	THR	SEE REMARK 999	UNP Q8JNX5
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

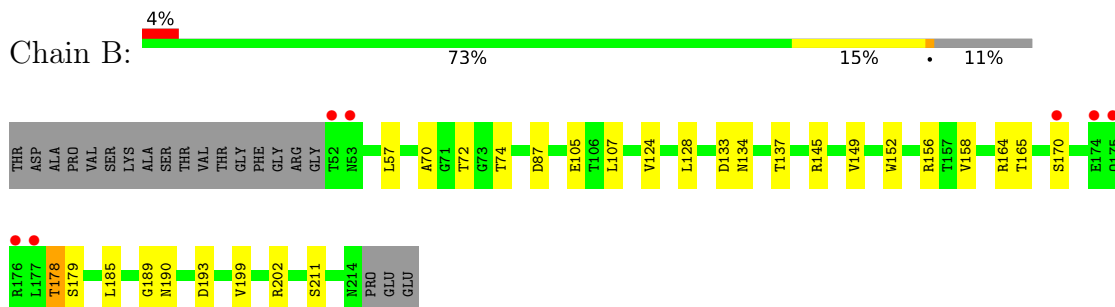
### 3 Residue-property plots [i](#)

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

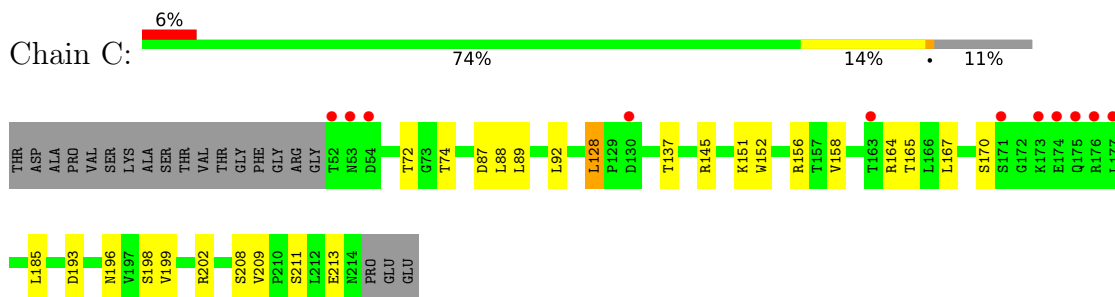
- Molecule 1: Coat protein



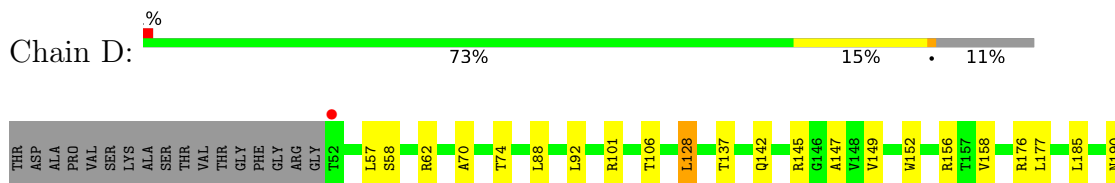
- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein

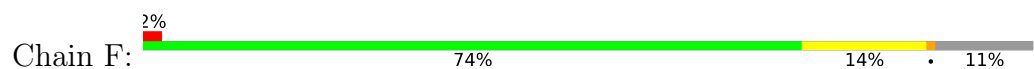




- Molecule 1: Coat protein



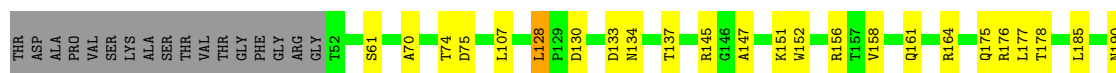
- Molecule 1: Coat protein



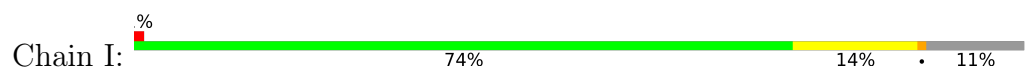
- Molecule 1: Coat protein



- Molecule 1: Coat protein

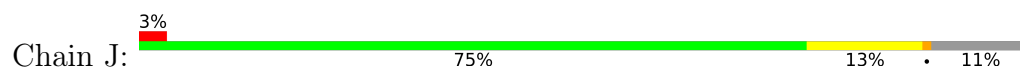


- Molecule 1: Coat protein

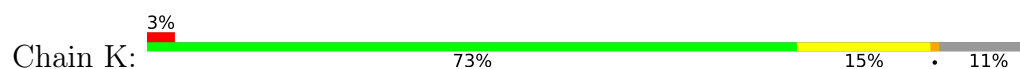




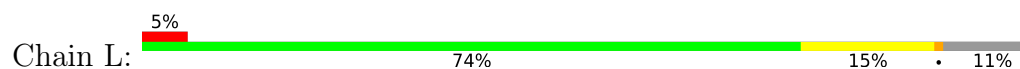
• Molecule 1: Coat protein



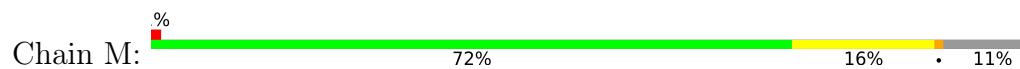
• Molecule 1: Coat protein



• Molecule 1: Coat protein



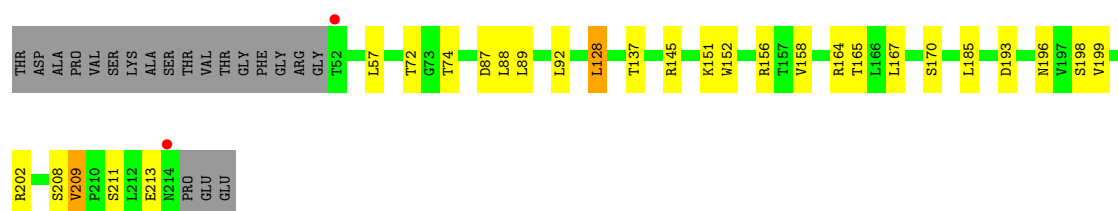
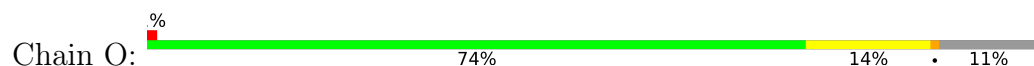
• Molecule 1: Coat protein



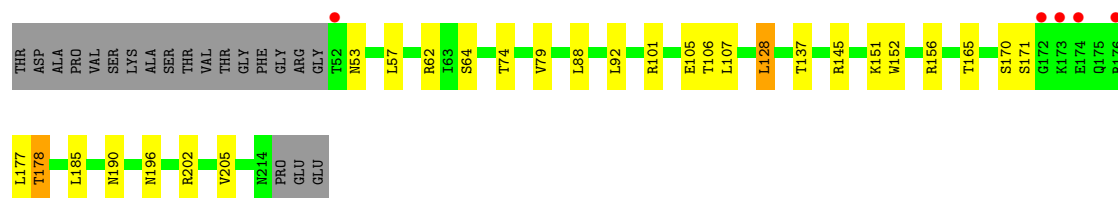
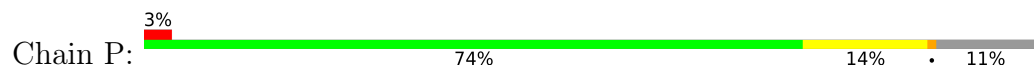
- Molecule 1: Coat protein



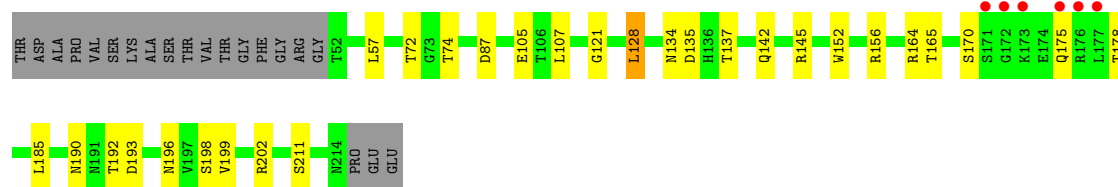
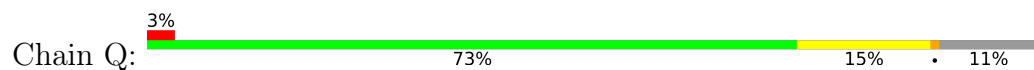
- Molecule 1: Coat protein



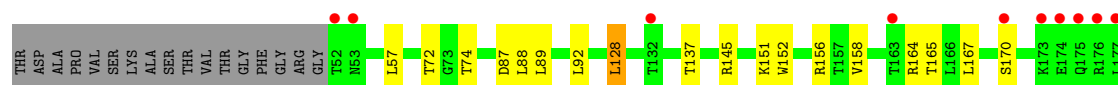
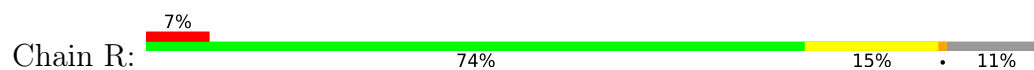
- Molecule 1: Coat protein

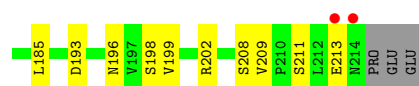


- Molecule 1: Coat protein

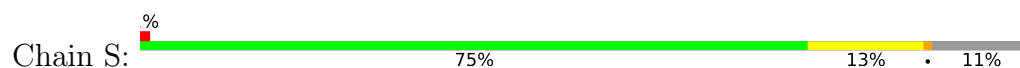


- Molecule 1: Coat protein

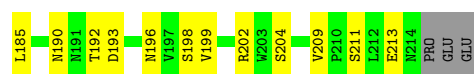




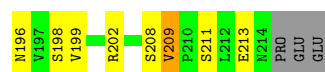
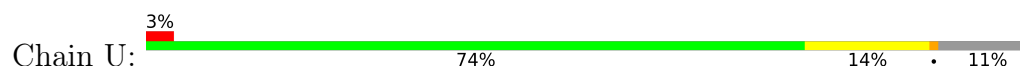
## ● Molecule 1: Coat protein



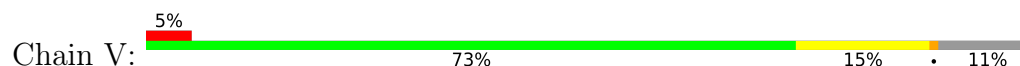
## ● Molecule 1: Coat protein



## ● Molecule 1: Coat protein



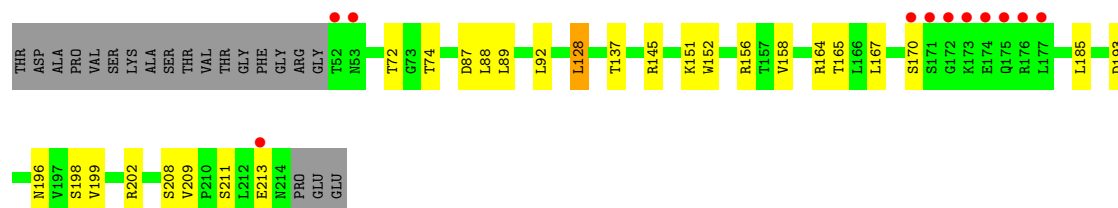
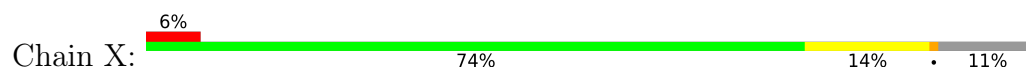
## ● Molecule 1: Coat protein



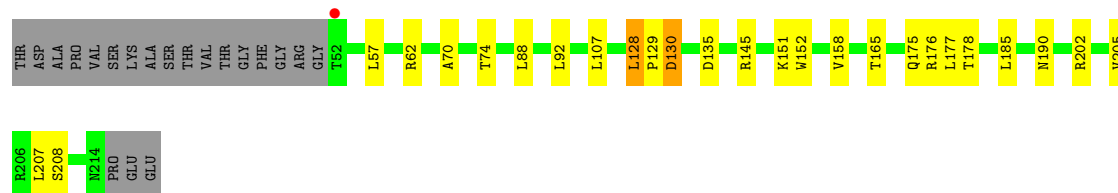
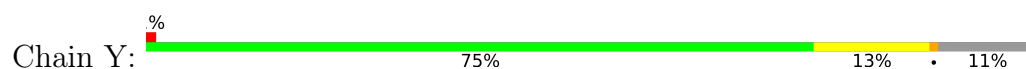
## ● Molecule 1: Coat protein



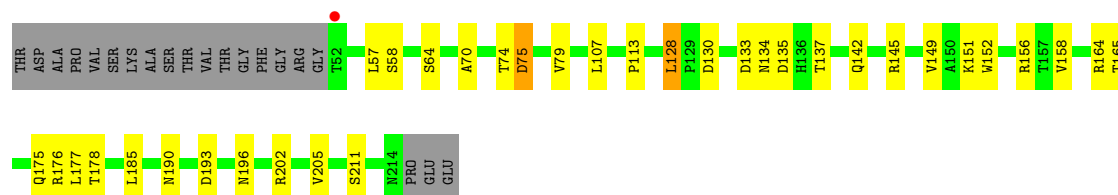
- Molecule 1: Coat protein



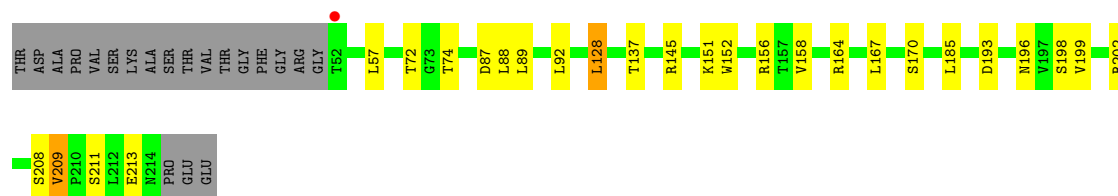
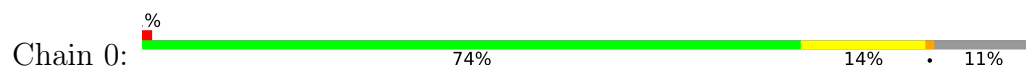
- Molecule 1: Coat protein



- Molecule 1: Coat protein

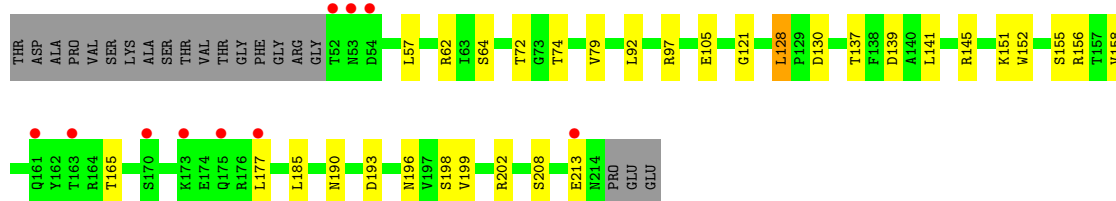


- Molecule 1: Coat protein



- Molecule 1: Coat protein

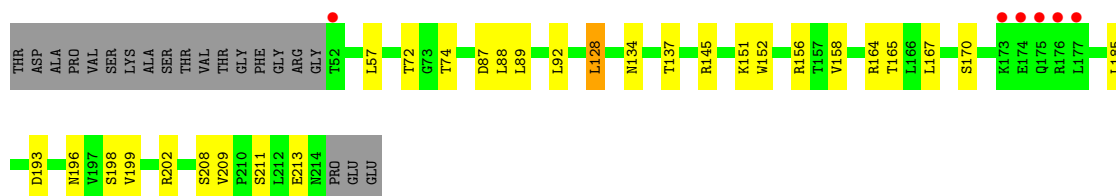




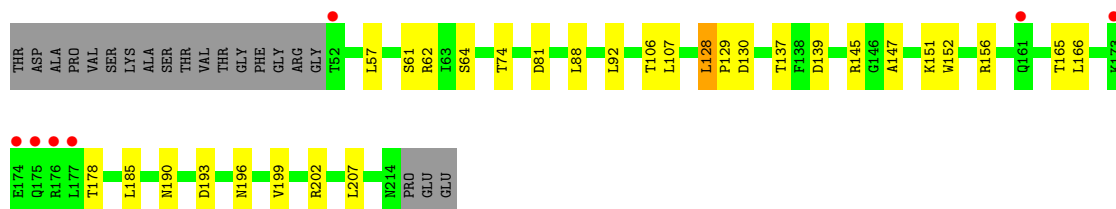
• Molecule 1: Coat protein



• Molecule 1: Coat protein

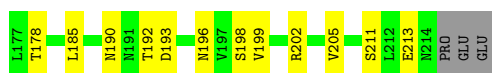


• Molecule 1: Coat protein

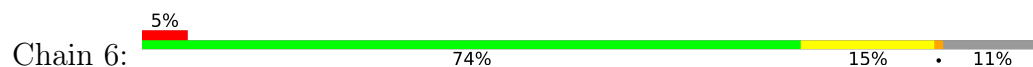


• Molecule 1: Coat protein

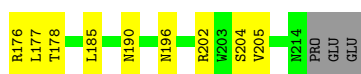




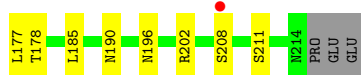
• Molecule 1: Coat protein



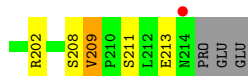
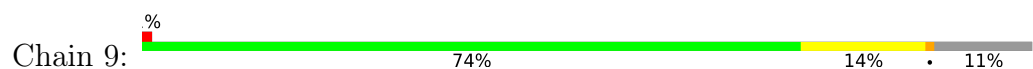
• Molecule 1: Coat protein



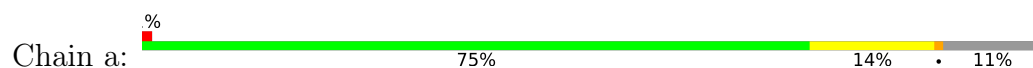
• Molecule 1: Coat protein

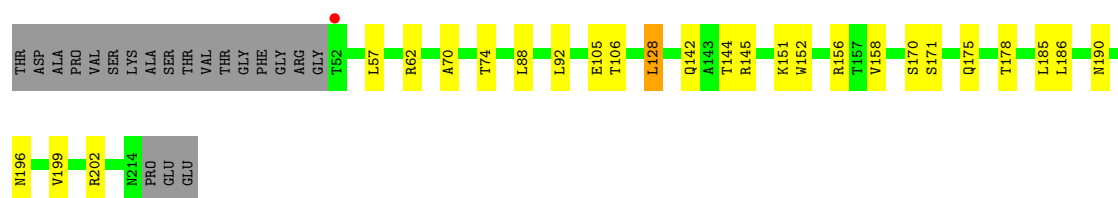


• Molecule 1: Coat protein

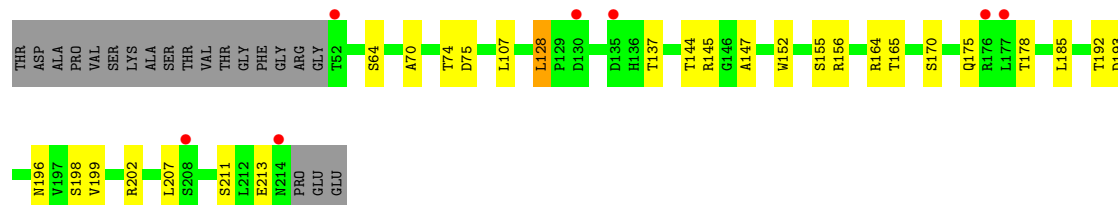
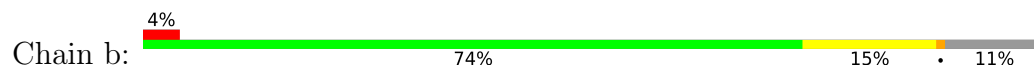


• Molecule 1: Coat protein

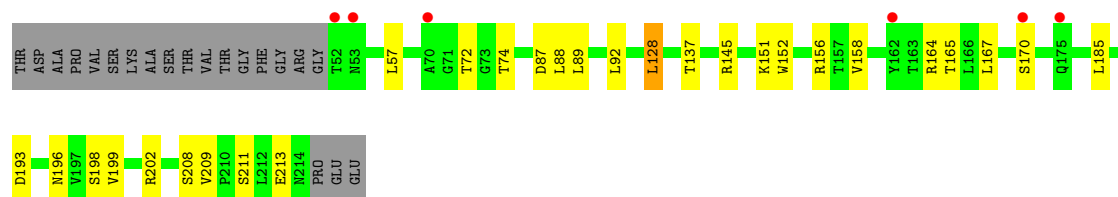




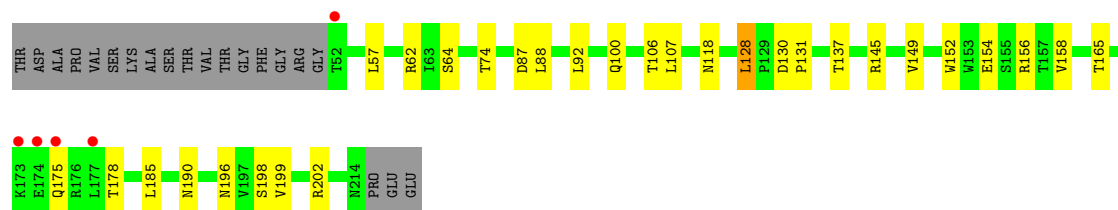
- Molecule 1: Coat protein



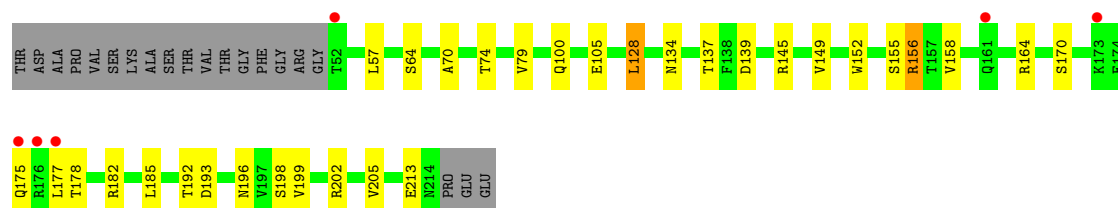
- Molecule 1: Coat protein



- Molecule 1: Coat protein



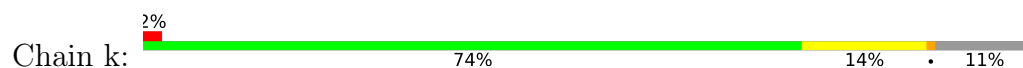
- Molecule 1: Coat protein



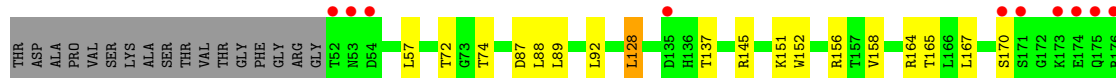




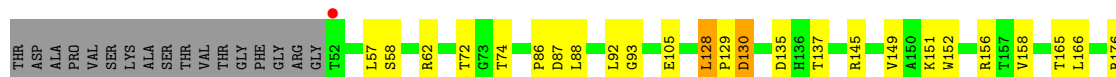
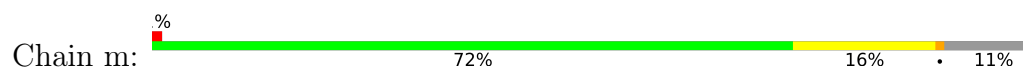
• Molecule 1: Coat protein



• Molecule 1: Coat protein



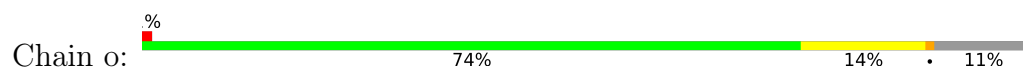
• Molecule 1: Coat protein

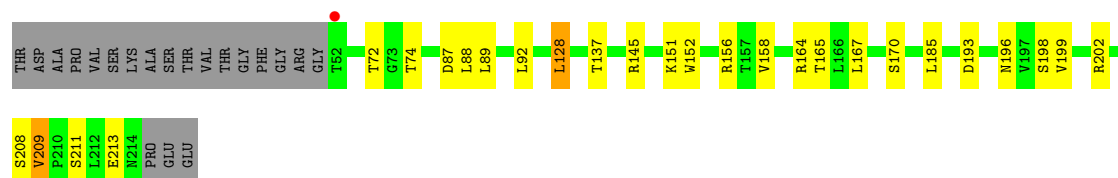


• Molecule 1: Coat protein

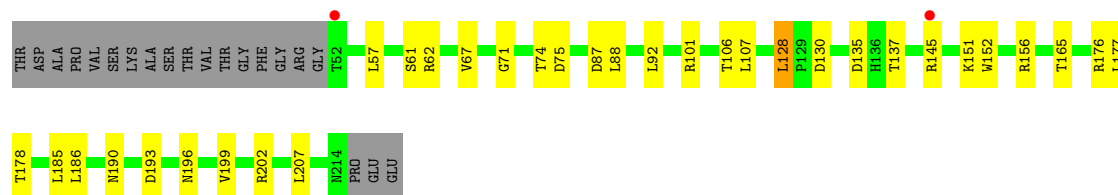


• Molecule 1: Coat protein

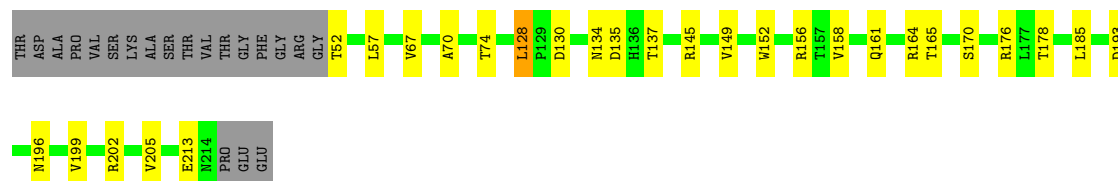




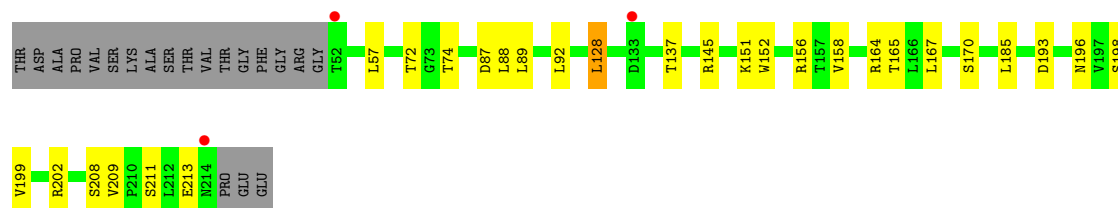
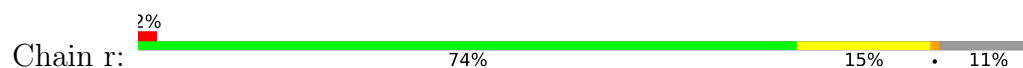
- Molecule 1: Coat protein



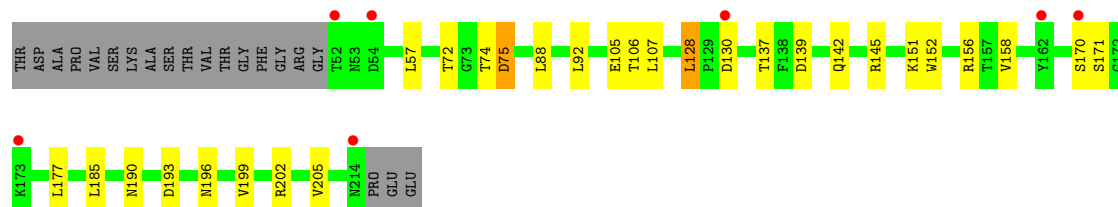
- Molecule 1: Coat protein



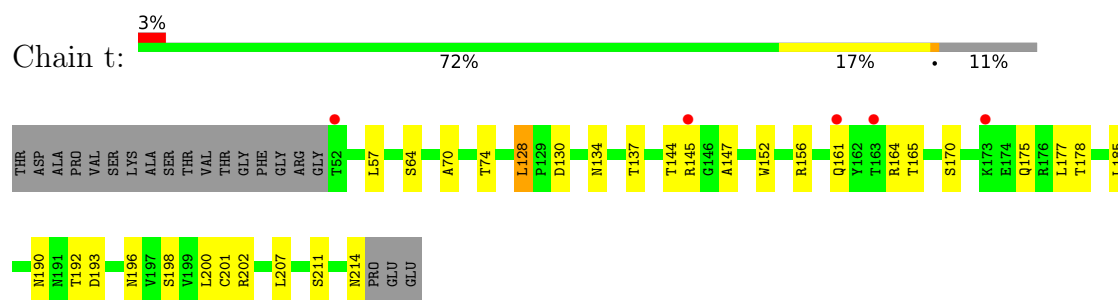
- Molecule 1: Coat protein



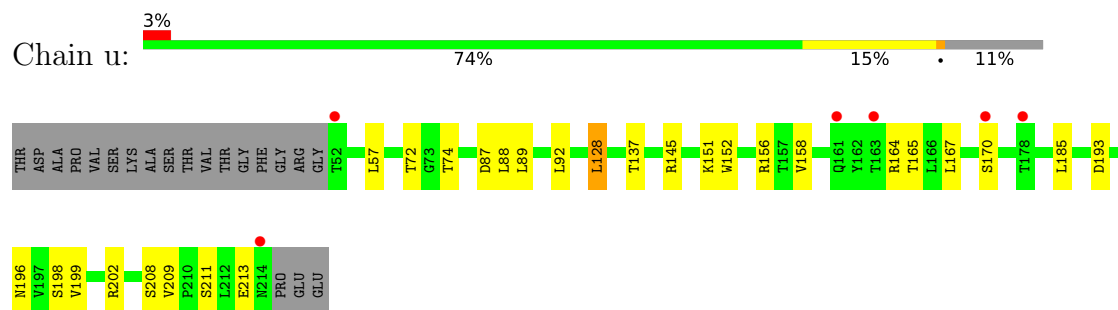
- Molecule 1: Coat protein



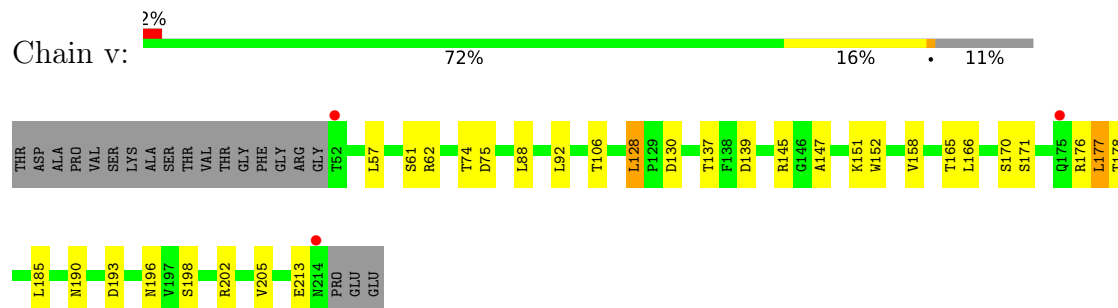
- Molecule 1: Coat protein



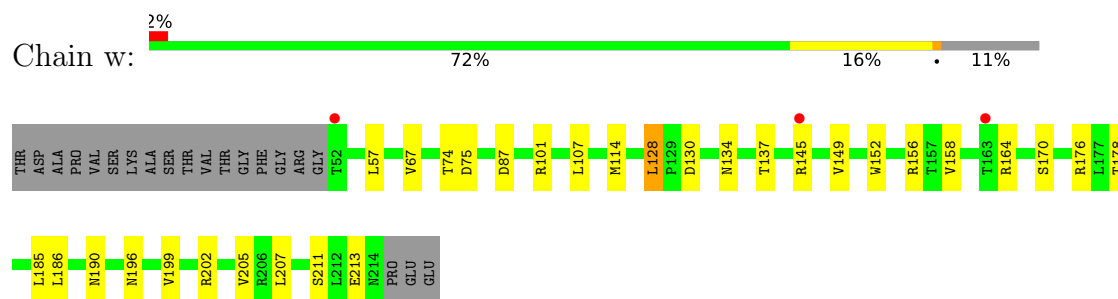
• Molecule 1: Coat protein



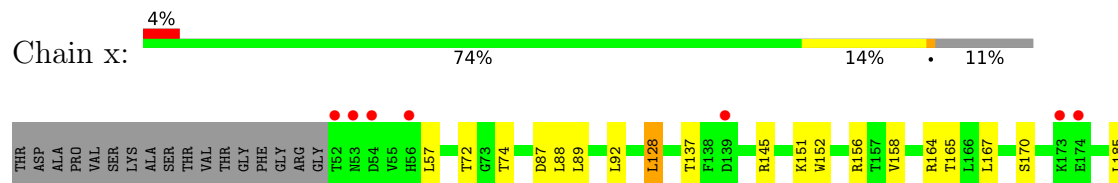
• Molecule 1: Coat protein



• Molecule 1: Coat protein



• Molecule 1: Coat protein



D193	N196	V197	S198	V199	R202	S208	V209	P210	S211	L212	E213	N214	PRO	GLU	GLU
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.5	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 9.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.448 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	75180	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	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 [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	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	25	59
1	1	161/183 (88%)	142 (88%)	17 (11%)	2 (1%)	13	44
1	2	161/183 (88%)	136 (84%)	22 (14%)	3 (2%)	8	33
1	3	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	25	59
1	4	161/183 (88%)	141 (88%)	18 (11%)	2 (1%)	13	44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5	161/183 (88%)	148 (92%)	9 (6%)	4 (2%)	5	27
1	6	161/183 (88%)	152 (94%)	8 (5%)	1 (1%)	25	59
1	7	161/183 (88%)	141 (88%)	18 (11%)	2 (1%)	13	44
1	8	161/183 (88%)	145 (90%)	12 (8%)	4 (2%)	5	27
1	9	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	25	59
1	A	161/183 (88%)	148 (92%)	11 (7%)	2 (1%)	13	44
1	B	161/183 (88%)	142 (88%)	16 (10%)	3 (2%)	8	33
1	C	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	25	59
1	D	161/183 (88%)	149 (92%)	10 (6%)	2 (1%)	13	44
1	E	161/183 (88%)	147 (91%)	12 (8%)	2 (1%)	13	44
1	F	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	25	59
1	G	161/183 (88%)	144 (89%)	16 (10%)	1 (1%)	25	59
1	H	161/183 (88%)	143 (89%)	15 (9%)	3 (2%)	8	33
1	I	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	25	59
1	J	161/183 (88%)	145 (90%)	15 (9%)	1 (1%)	25	59
1	K	161/183 (88%)	142 (88%)	16 (10%)	3 (2%)	8	33
1	L	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	25	59
1	M	161/183 (88%)	141 (88%)	16 (10%)	4 (2%)	5	27
1	N	161/183 (88%)	143 (89%)	18 (11%)	0	100	100
1	O	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	25	59
1	P	161/183 (88%)	139 (86%)	20 (12%)	2 (1%)	13	44
1	Q	161/183 (88%)	145 (90%)	15 (9%)	1 (1%)	25	59
1	R	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	25	59
1	S	161/183 (88%)	146 (91%)	13 (8%)	2 (1%)	13	44
1	T	161/183 (88%)	146 (91%)	15 (9%)	0	100	100
1	U	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	25	59
1	V	161/183 (88%)	145 (90%)	14 (9%)	2 (1%)	13	44
1	W	161/183 (88%)	142 (88%)	17 (11%)	2 (1%)	13	44
1	X	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	25	59
1	Y	161/183 (88%)	147 (91%)	13 (8%)	1 (1%)	25	59
1	Z	161/183 (88%)	143 (89%)	15 (9%)	3 (2%)	8	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	161/183 (88%)	140 (87%)	20 (12%)	1 (1%)	25	59
1	b	161/183 (88%)	141 (88%)	17 (11%)	3 (2%)	8	33
1	c	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	25	59
1	d	161/183 (88%)	148 (92%)	12 (8%)	1 (1%)	25	59
1	e	161/183 (88%)	143 (89%)	17 (11%)	1 (1%)	25	59
1	f	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	25	59
1	g	161/183 (88%)	146 (91%)	14 (9%)	1 (1%)	25	59
1	h	161/183 (88%)	145 (90%)	15 (9%)	1 (1%)	25	59
1	i	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	25	59
1	j	161/183 (88%)	146 (91%)	13 (8%)	2 (1%)	13	44
1	k	161/183 (88%)	143 (89%)	17 (11%)	1 (1%)	25	59
1	l	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	25	59
1	m	161/183 (88%)	144 (89%)	16 (10%)	1 (1%)	25	59
1	n	161/183 (88%)	146 (91%)	13 (8%)	2 (1%)	13	44
1	o	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	25	59
1	p	161/183 (88%)	144 (89%)	15 (9%)	2 (1%)	13	44
1	q	161/183 (88%)	145 (90%)	15 (9%)	1 (1%)	25	59
1	r	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	25	59
1	s	161/183 (88%)	134 (83%)	26 (16%)	1 (1%)	25	59
1	t	161/183 (88%)	147 (91%)	12 (8%)	2 (1%)	13	44
1	u	161/183 (88%)	151 (94%)	9 (6%)	1 (1%)	25	59
1	v	161/183 (88%)	143 (89%)	16 (10%)	2 (1%)	13	44
1	w	161/183 (88%)	146 (91%)	14 (9%)	1 (1%)	25	59
1	x	161/183 (88%)	150 (93%)	10 (6%)	1 (1%)	25	59
All	All	9660/10980 (88%)	8763 (91%)	803 (8%)	94 (1%)	15	49

5 of 94 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	THR
1	C	209	VAL
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	6
1	1	138/153 (90%)	109 (79%)	29 (21%)	1	5
1	2	138/153 (90%)	112 (81%)	26 (19%)	1	6
1	3	138/153 (90%)	111 (80%)	27 (20%)	1	6
1	4	138/153 (90%)	111 (80%)	27 (20%)	1	6
1	5	138/153 (90%)	111 (80%)	27 (20%)	1	6
1	6	138/153 (90%)	111 (80%)	27 (20%)	1	6
1	7	138/153 (90%)	108 (78%)	30 (22%)	1	4
1	8	138/153 (90%)	112 (81%)	26 (19%)	1	6
1	9	138/153 (90%)	111 (80%)	27 (20%)	1	6
1	A	138/153 (90%)	109 (79%)	29 (21%)	1	5
1	B	138/153 (90%)	111 (80%)	27 (20%)	1	6
1	C	138/153 (90%)	112 (81%)	26 (19%)	1	6
1	D	138/153 (90%)	111 (80%)	27 (20%)	1	6
1	E	138/153 (90%)	102 (74%)	36 (26%)	0	1
1	F	138/153 (90%)	110 (80%)	28 (20%)	1	5
1	G	138/153 (90%)	105 (76%)	33 (24%)	0	2
1	H	138/153 (90%)	112 (81%)	26 (19%)	1	6
1	I	138/153 (90%)	110 (80%)	28 (20%)	1	5
1	J	138/153 (90%)	114 (83%)	24 (17%)	2	9
1	K	138/153 (90%)	112 (81%)	26 (19%)	1	6
1	L	138/153 (90%)	111 (80%)	27 (20%)	1	6
1	M	138/153 (90%)	109 (79%)	29 (21%)	1	5
1	N	138/153 (90%)	106 (77%)	32 (23%)	1	3
1	O	138/153 (90%)	110 (80%)	28 (20%)	1	5
1	P	138/153 (90%)	111 (80%)	27 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	138/153 (90%)	110 (80%)	28 (20%)	1	5
1	R	138/153 (90%)	111 (80%)	27 (20%)	1	6
1	S	138/153 (90%)	115 (83%)	23 (17%)	2	9
1	T	138/153 (90%)	104 (75%)	34 (25%)	0	2
1	U	138/153 (90%)	110 (80%)	28 (20%)	1	5
1	V	138/153 (90%)	111 (80%)	27 (20%)	1	6
1	W	138/153 (90%)	115 (83%)	23 (17%)	2	9
1	X	138/153 (90%)	112 (81%)	26 (19%)	1	6
1	Y	138/153 (90%)	115 (83%)	23 (17%)	2	9
1	Z	138/153 (90%)	105 (76%)	33 (24%)	0	2
1	a	138/153 (90%)	113 (82%)	25 (18%)	1	7
1	b	138/153 (90%)	114 (83%)	24 (17%)	2	9
1	c	138/153 (90%)	111 (80%)	27 (20%)	1	6
1	d	138/153 (90%)	109 (79%)	29 (21%)	1	5
1	e	138/153 (90%)	108 (78%)	30 (22%)	1	4
1	f	138/153 (90%)	111 (80%)	27 (20%)	1	6
1	g	138/153 (90%)	106 (77%)	32 (23%)	1	3
1	h	138/153 (90%)	109 (79%)	29 (21%)	1	5
1	i	138/153 (90%)	111 (80%)	27 (20%)	1	6
1	j	138/153 (90%)	110 (80%)	28 (20%)	1	5
1	k	138/153 (90%)	111 (80%)	27 (20%)	1	6
1	l	138/153 (90%)	111 (80%)	27 (20%)	1	6
1	m	138/153 (90%)	108 (78%)	30 (22%)	1	4
1	n	138/153 (90%)	108 (78%)	30 (22%)	1	4
1	o	138/153 (90%)	111 (80%)	27 (20%)	1	6
1	p	138/153 (90%)	107 (78%)	31 (22%)	1	3
1	q	138/153 (90%)	111 (80%)	27 (20%)	1	6
1	r	138/153 (90%)	111 (80%)	27 (20%)	1	6
1	s	138/153 (90%)	109 (79%)	29 (21%)	1	5
1	t	138/153 (90%)	109 (79%)	29 (21%)	1	5
1	u	138/153 (90%)	111 (80%)	27 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	v	138/153 (90%)	108 (78%)	30 (22%)	1	4
1	w	138/153 (90%)	109 (79%)	29 (21%)	1	5
1	x	138/153 (90%)	110 (80%)	28 (20%)	1	5
All	All	8280/9180 (90%)	6606 (80%)	1674 (20%)	1	5

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

Mol	Chain	Res	Type
1	7	151	LYS
1	f	158	VAL
1	v	151	LYS
1	8	137	THR
1	7	145	ARG

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

Mol	Chain	Res	Type
1	8	214	ASN
1	g	196	ASN
1	a	65	GLN
1	d	100	GLN
1	j	100	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	0	163/183 (89%)	0.07	1 (0%) 89 78	28, 44, 82, 144	0
1	1	163/183 (89%)	0.22	10 (6%) 21 9	30, 49, 106, 153	0
1	2	163/183 (89%)	0.19	5 (3%) 49 26	36, 55, 110, 160	0
1	3	163/183 (89%)	0.19	6 (3%) 41 21	26, 45, 109, 163	0
1	4	163/183 (89%)	0.20	7 (4%) 35 17	30, 52, 109, 171	0
1	5	163/183 (89%)	0.13	6 (3%) 41 21	30, 51, 104, 156	0
1	6	163/183 (89%)	0.40	9 (5%) 25 11	32, 56, 122, 194	0
1	7	163/183 (89%)	-0.08	2 (1%) 79 61	26, 41, 72, 127	0
1	8	163/183 (89%)	-0.06	3 (1%) 68 47	26, 42, 76, 120	0
1	9	163/183 (89%)	0.06	2 (1%) 79 61	25, 43, 86, 112	0
1	A	163/183 (89%)	-0.02	1 (0%) 89 78	31, 47, 89, 132	0
1	B	163/183 (89%)	0.15	7 (4%) 35 17	29, 47, 101, 189	0
1	C	163/183 (89%)	0.28	11 (6%) 17 7	26, 50, 111, 183	0
1	D	163/183 (89%)	-0.05	1 (0%) 89 78	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%) 57 34	32, 53, 101, 137	0
1	G	163/183 (89%)	-0.07	1 (0%) 89 78	25, 42, 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%) 79 61	27, 44, 81, 118	0
1	J	163/183 (89%)	0.16	5 (3%) 49 26	27, 52, 110, 177	0
1	K	163/183 (89%)	0.17	5 (3%) 49 26	26, 53, 106, 171	0
1	L	163/183 (89%)	0.28	9 (5%) 25 11	26, 54, 123, 169	0
1	M	163/183 (89%)	-0.06	2 (1%) 79 61	23, 38, 71, 137	0
1	N	163/183 (89%)	-0.08	2 (1%) 79 61	23, 37, 74, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	O	163/183 (89%)	0.09	2 (1%) 79 61	28, 46, 84, 129	0
1	P	163/183 (89%)	0.13	5 (3%) 49 26	25, 47, 100, 159	0
1	Q	163/183 (89%)	0.12	6 (3%) 41 21	26, 45, 113, 151	0
1	R	163/183 (89%)	0.36	12 (7%) 14 5	29, 54, 124, 176	0
1	S	163/183 (89%)	-0.05	2 (1%) 79 61	29, 45, 81, 123	0
1	T	163/183 (89%)	0.01	2 (1%) 79 61	26, 44, 81, 120	0
1	U	163/183 (89%)	0.27	5 (3%) 49 26	36, 52, 96, 140	0
1	V	163/183 (89%)	0.24	10 (6%) 21 9	28, 53, 116, 150	0
1	W	163/183 (89%)	0.09	5 (3%) 49 26	27, 47, 104, 156	0
1	X	163/183 (89%)	0.35	11 (6%) 17 7	28, 47, 116, 193	0
1	Y	163/183 (89%)	-0.06	1 (0%) 89 78	25, 42, 79, 121	0
1	Z	163/183 (89%)	-0.02	1 (0%) 89 78	31, 48, 81, 143	0
1	a	163/183 (89%)	0.25	1 (0%) 89 78	36, 62, 110, 149	0
1	b	163/183 (89%)	0.15	7 (4%) 35 17	31, 53, 104, 147	0
1	c	163/183 (89%)	0.41	6 (3%) 41 21	36, 66, 120, 135	0
1	d	163/183 (89%)	0.07	5 (3%) 49 26	25, 43, 103, 156	0
1	e	163/183 (89%)	0.18	6 (3%) 41 21	28, 49, 106, 153	0
1	f	163/183 (89%)	0.34	9 (5%) 25 11	37, 59, 114, 159	0
1	g	163/183 (89%)	-0.09	1 (0%) 89 78	29, 48, 81, 120	0
1	h	163/183 (89%)	-0.04	1 (0%) 89 78	26, 43, 79, 121	0
1	i	163/183 (89%)	0.07	1 (0%) 89 78	26, 45, 87, 114	0
1	j	163/183 (89%)	0.13	3 (1%) 68 47	26, 49, 102, 165	0
1	k	163/183 (89%)	0.07	4 (2%) 57 34	34, 47, 102, 151	0
1	l	163/183 (89%)	0.43	12 (7%) 14 5	31, 52, 115, 265	0
1	m	163/183 (89%)	-0.11	1 (0%) 89 78	25, 36, 71, 115	0
1	n	163/183 (89%)	0.00	1 (0%) 89 78	28, 44, 78, 137	0
1	o	163/183 (89%)	0.04	1 (0%) 89 78	26, 39, 79, 124	0
1	p	163/183 (89%)	-0.05	2 (1%) 79 61	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%) 68 47	38, 57, 99, 128	0
1	s	163/183 (89%)	0.23	7 (4%) 35 17	39, 61, 103, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	t	163/183 (89%)	0.15	5 (3%)	49	26	33, 52, 103, 141	0
1	u	163/183 (89%)	0.44	6 (3%)	41	21	41, 65, 114, 144	0
1	v	163/183 (89%)	0.15	3 (1%)	68	47	35, 55, 93, 129	0
1	w	163/183 (89%)	-0.02	3 (1%)	68	47	29, 44, 93, 117	0
1	x	163/183 (89%)	0.18	7 (4%)	35	17	26, 49, 97, 122	0
All	All	9780/10980 (89%)	0.12	258 (2%)	56	33	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	10.2
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 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.