



wwPDB X-ray Structure Validation Summary Report ⓘ

May 7, 2026 – 10:14 AM EDT

PDB ID : 7TJM / pdb_00007tjm
Title : Bacteriophage Q beta capsid protein in T3 symmetry
Authors : Jin, X.
Deposited on : 2022-01-16
Resolution : 3.54 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

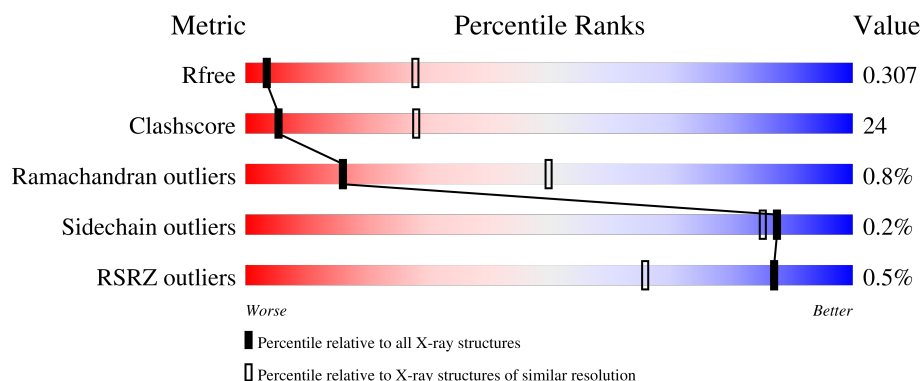
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.54 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1008 (3.58-3.50)
Clashscore	190562	1062 (3.58-3.50)
Ramachandran outliers	187476	1033 (3.58-3.50)
Sidechain outliers	187428	1034 (3.58-3.50)
RSRZ outliers	180081	1007 (3.58-3.50)

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

Mol	Chain	Length	Quality of chain
1	0	132	2% 52% 48%
1	1	132	% 62% 38%
1	2	132	% 52% 48%
1	3	132	% 55% 45%
1	4	132	% 56% 43%

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Mol	Chain	Length	Quality of chain
1	5	132	 52% 48%
1	6	132	 55% 44% .
1	7	132	 2% 58% 42%
1	8	132	 53% 47%
1	9	132	 % 55% 45% .
1	A	132	 55% 45%
1	B	132	 67% 33%
1	C	132	 65% 35%
1	D	132	 % 64% 36%
1	E	132	 61% 39%
1	F	132	 61% 39%
1	G	132	 60% 40%
1	H	132	 54% 45% .
1	I	132	 % 58% 42%
1	J	132	 61% 39%
1	K	132	 52% 48%
1	L	132	 62% 38%
1	M	132	 2% 58% 41% .
1	N	132	 50% 50%
1	O	132	 63% 37%
1	P	132	 % 52% 48%
1	Q	132	 % 55% 43% .
1	R	132	 62% 36% .
1	S	132	 % 53% 46% .
1	T	132	 % 58% 42%

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Mol	Chain	Length	Quality of chain
1	U	132	2% 59% 41%
1	V	132	55% 44%
1	W	132	48% 52%
1	X	132	54% 45%
1	Y	132	53% 45%
1	Z	132	% 52% 48%
1	a	132	47% 52%
1	b	132	% 61% 39%
1	c	132	57% 43%
1	d	132	2% 54% 45%
1	e	132	2% 61% 38%
1	f	132	% 56% 43%
1	g	132	61% 39%
1	h	132	% 49% 50%
1	i	132	52% 48%
1	j	132	56% 44%
1	k	132	57% 42%
1	l	132	% 61% 39%
1	m	132	% 49% 50%
1	n	132	51% 49%
1	o	132	2% 55% 44%
1	p	132	2% 55% 45%
1	q	132	58% 42%
1	r	132	% 48% 50%
1	s	132	2% 61% 39%

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Mol	Chain	Length	Quality of chain
1	t	132	% 61% 39%
1	u	132	% 55% 45%
1	v	132	57% 42%
1	w	132	56% 44%
1	x	132	59% 41%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 59580 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 Minor capsid protein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	S	0	0	0
			993	616	177	198	2			
1	a	132	Total	C	N	O	S	0	0	0
			993	616	177	198	2			
1	B	132	Total	C	N	O	S	0	0	0
			993	616	177	198	2			
1	b	132	Total	C	N	O	S	0	0	0
			993	616	177	198	2			
1	C	132	Total	C	N	O	S	0	0	0
			993	616	177	198	2			
1	c	132	Total	C	N	O	S	0	0	0
			993	616	177	198	2			
1	D	132	Total	C	N	O	S	0	0	0
			993	616	177	198	2			
1	d	132	Total	C	N	O	S	0	0	0
			993	616	177	198	2			
1	E	132	Total	C	N	O	S	0	0	0
			993	616	177	198	2			
1	e	132	Total	C	N	O	S	0	0	0
			993	616	177	198	2			
1	1	132	Total	C	N	O	S	0	0	0
			993	616	177	198	2			
1	U	132	Total	C	N	O	S	0	0	0
			993	616	177	198	2			
1	F	132	Total	C	N	O	S	0	0	0
			993	616	177	198	2			
1	f	132	Total	C	N	O	S	0	0	0
			993	616	177	198	2			
1	G	132	Total	C	N	O	S	0	0	0
			993	616	177	198	2			
1	g	132	Total	C	N	O	S	0	0	0
			993	616	177	198	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	h	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	I	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	i	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	J	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	j	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	5	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	Y	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	K	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	k	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	L	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	l	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	M	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	m	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	N	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	n	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	O	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	o	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	9	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	v	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	P	132	Total 993	C 616	N 177	O 198	S 2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	p	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	Q	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	q	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	R	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	r	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	S	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	s	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	T	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	t	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	w	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	x	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	2	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	V	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	3	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	W	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	4	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	X	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	6	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	Z	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	7	132	Total 993	C 616	N 177	O 198	S 2	0	0	0
1	u	132	Total 993	C 616	N 177	O 198	S 2	0	0	0

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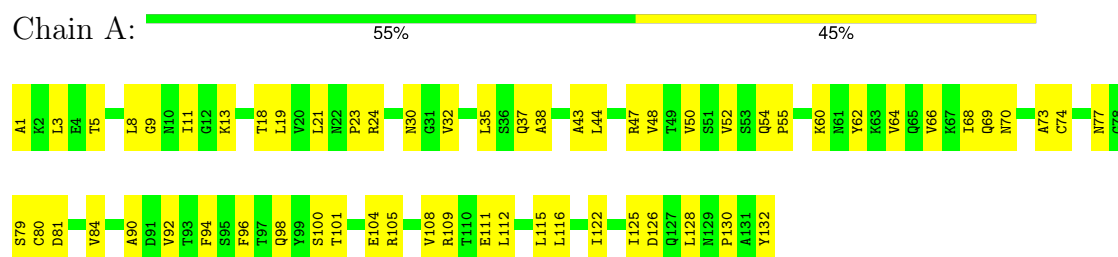
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	8	132	Total	C	N	O	S	0	0	0
			993	616	177	198	2			
1	0	132	Total	C	N	O	S	0	0	0
			993	616	177	198	2			

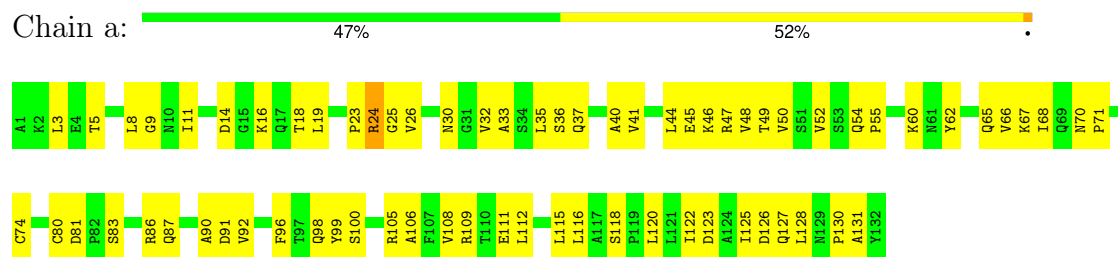
3 Residue-property plots

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

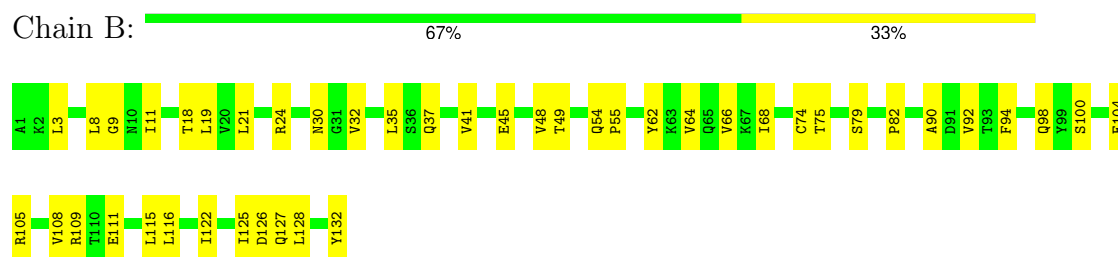
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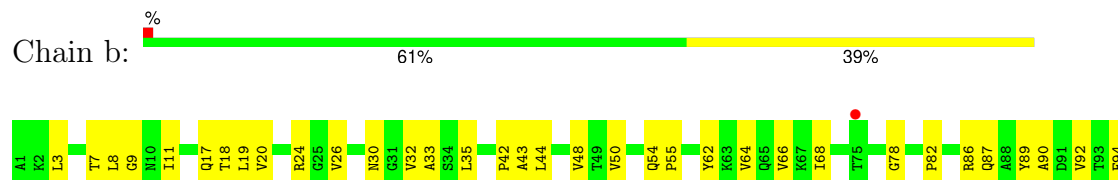
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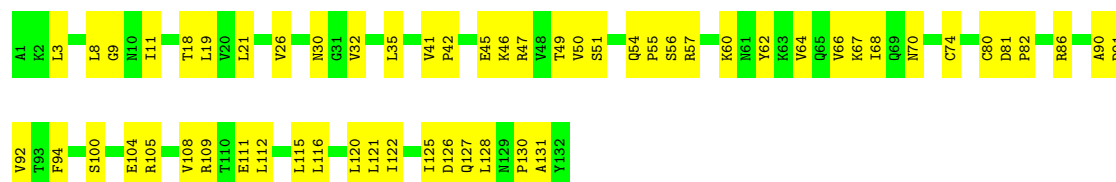




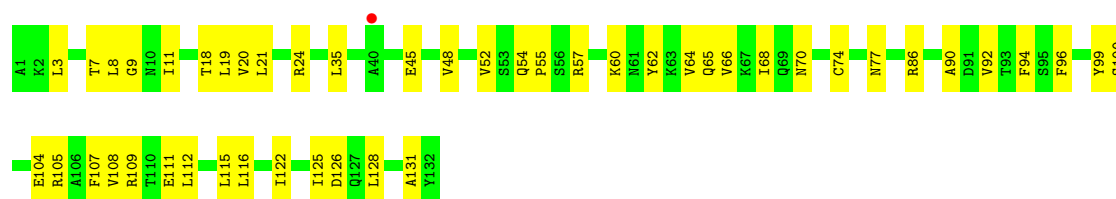
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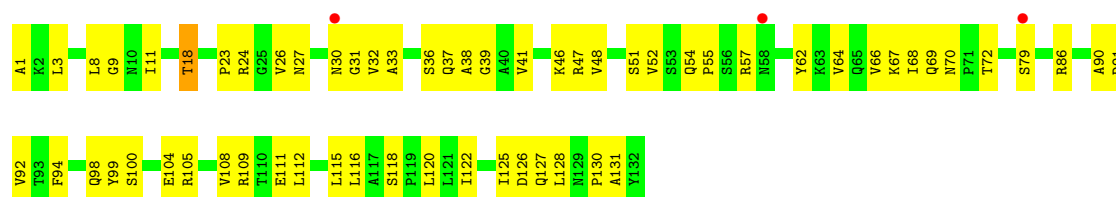
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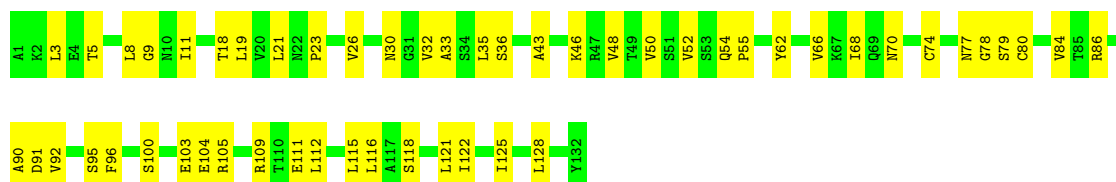


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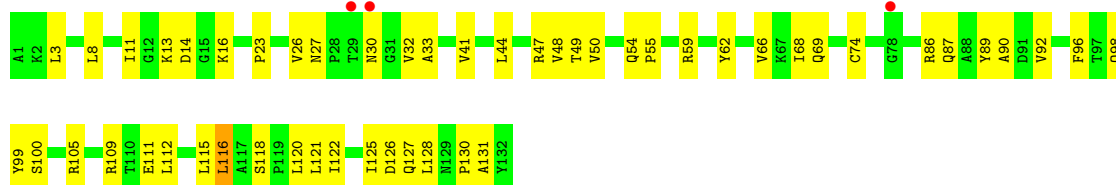


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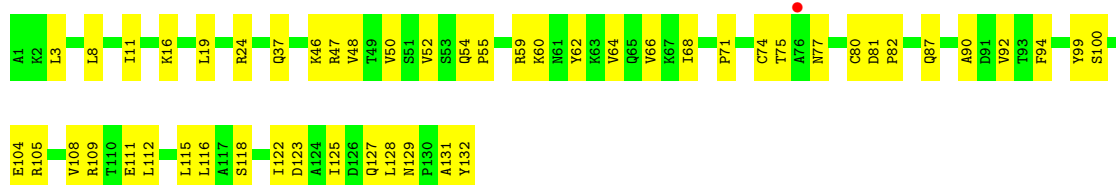




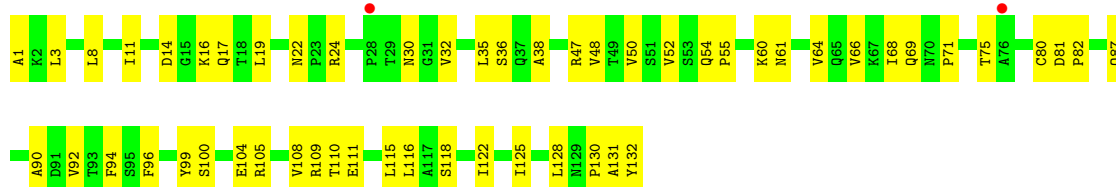
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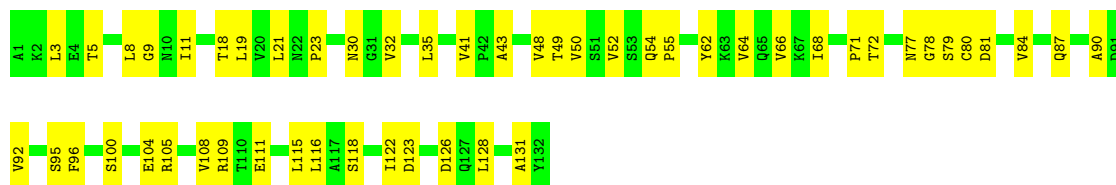
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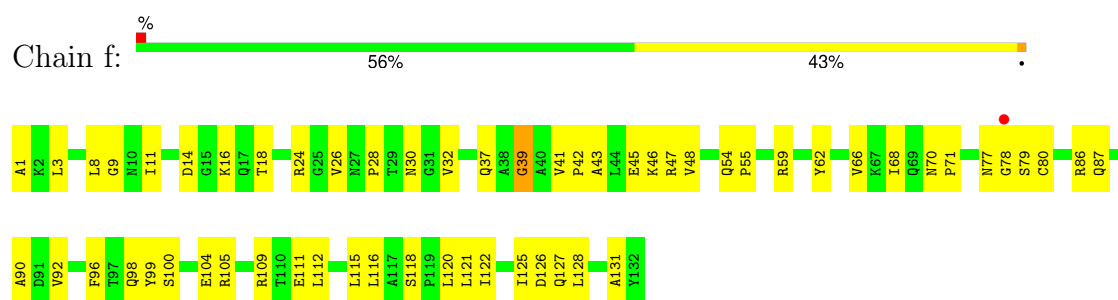
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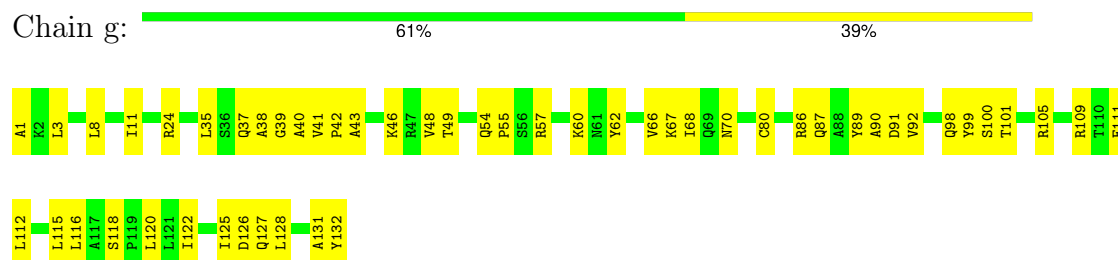
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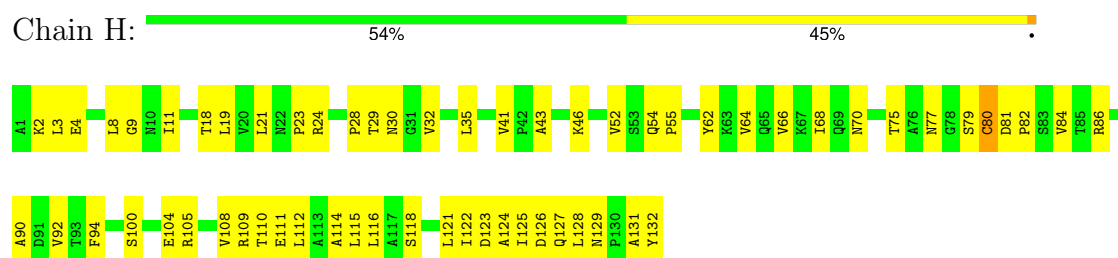
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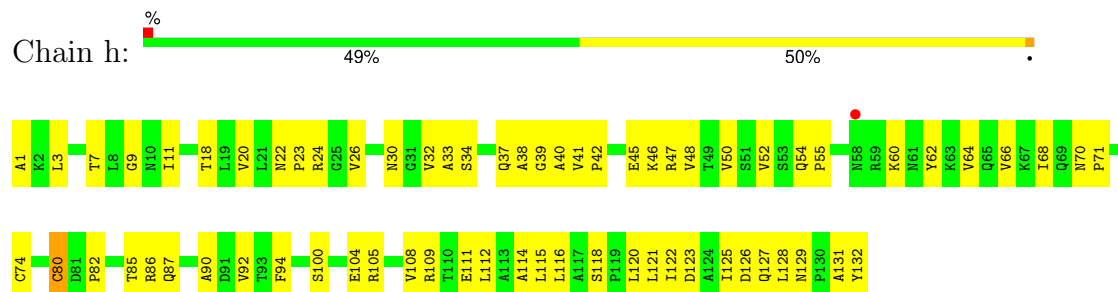
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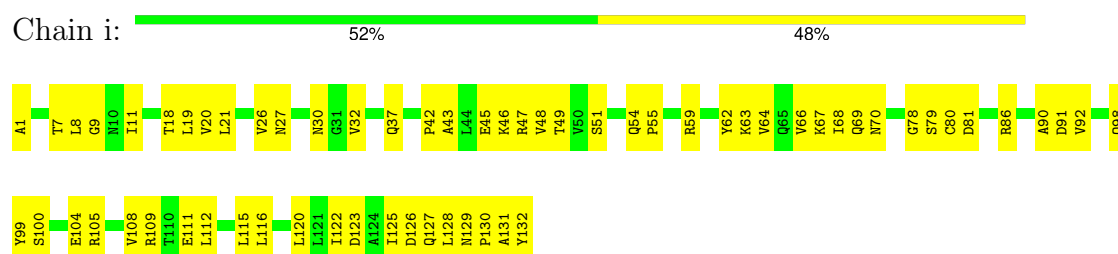
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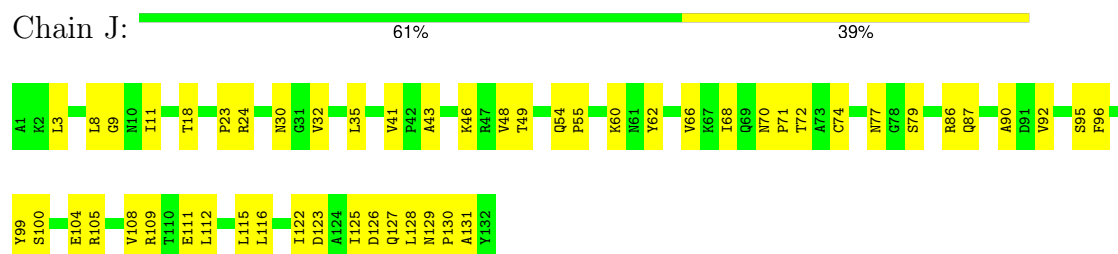
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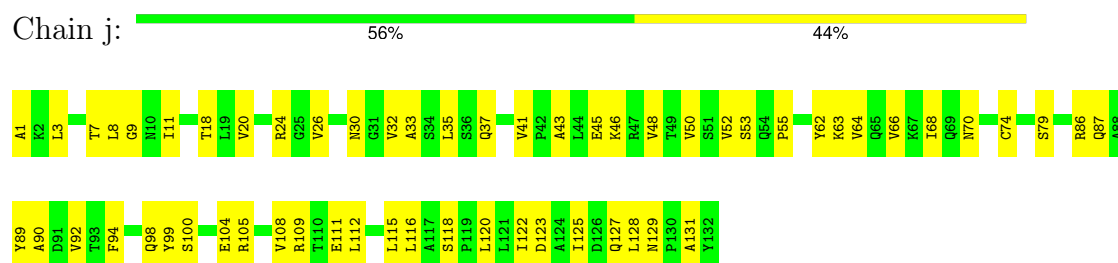
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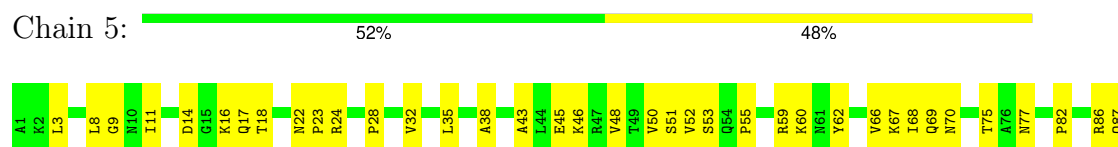
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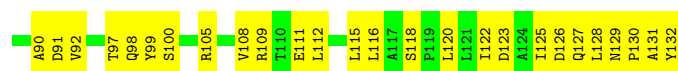


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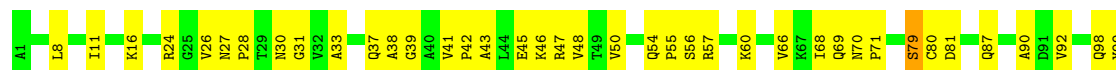
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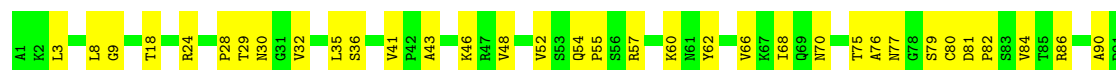
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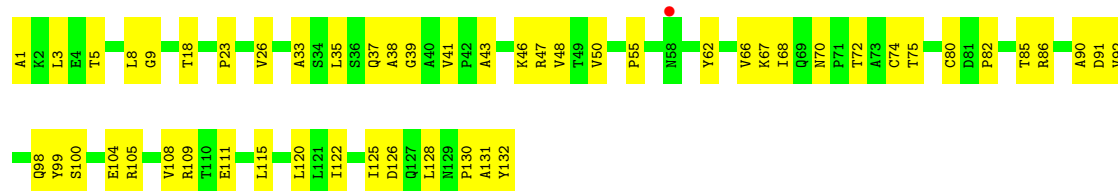


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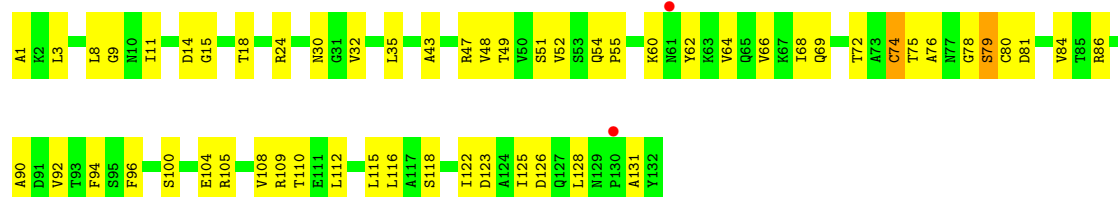


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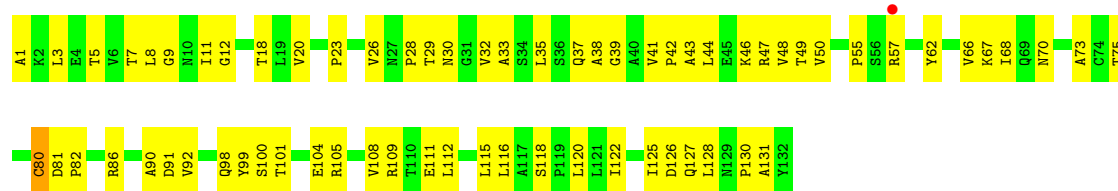




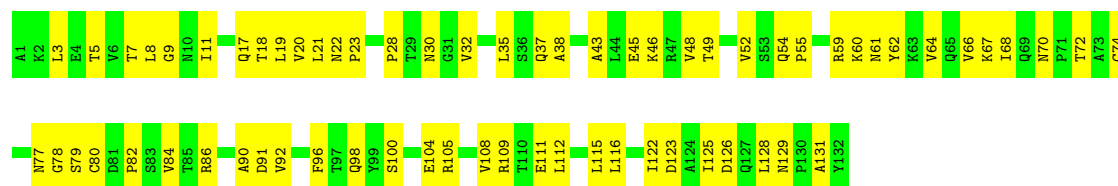
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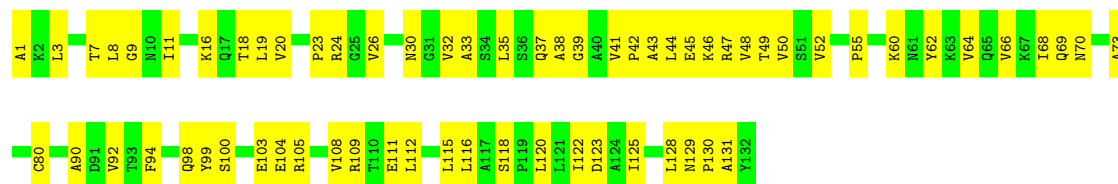
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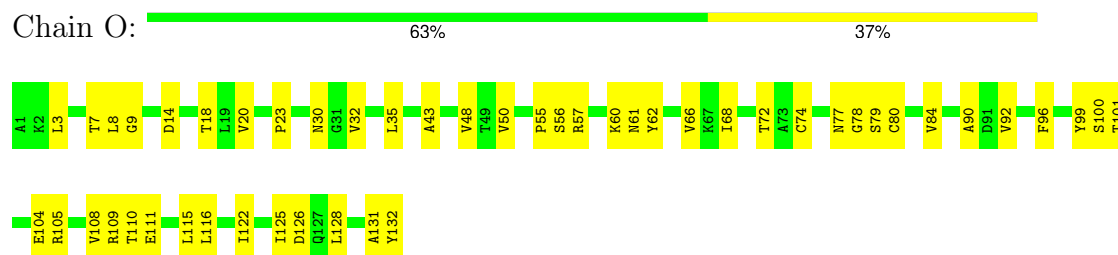
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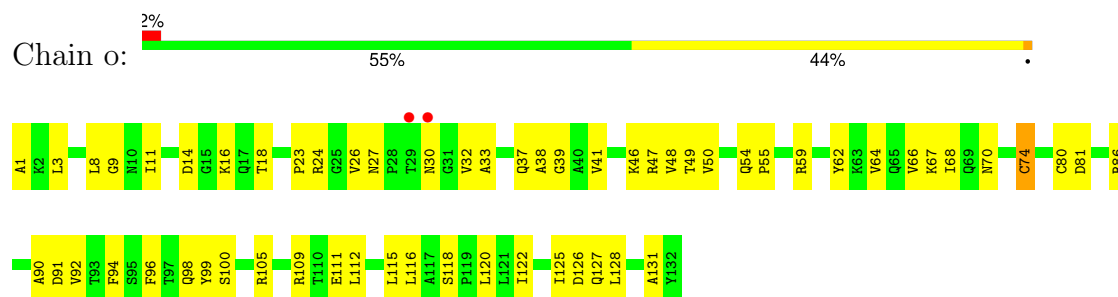
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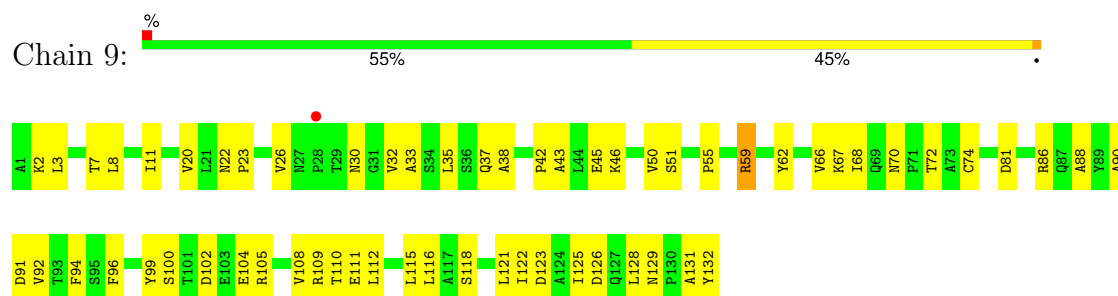
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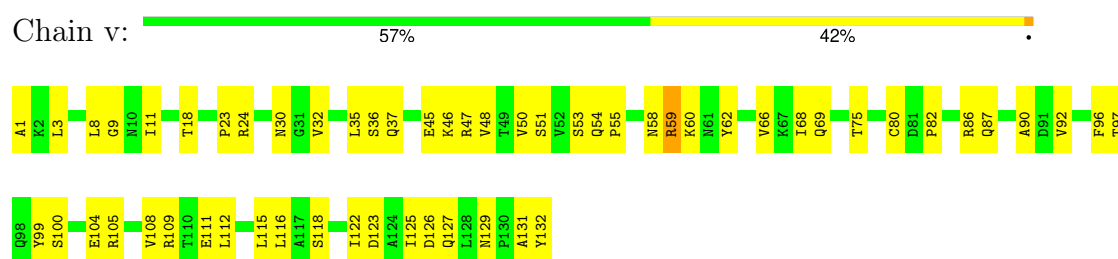
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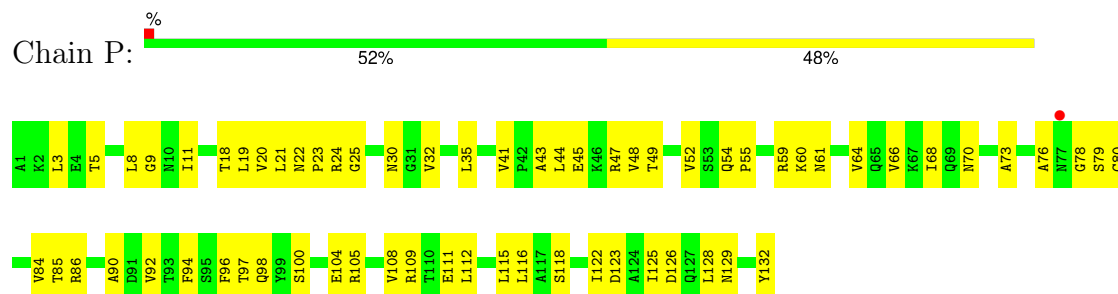
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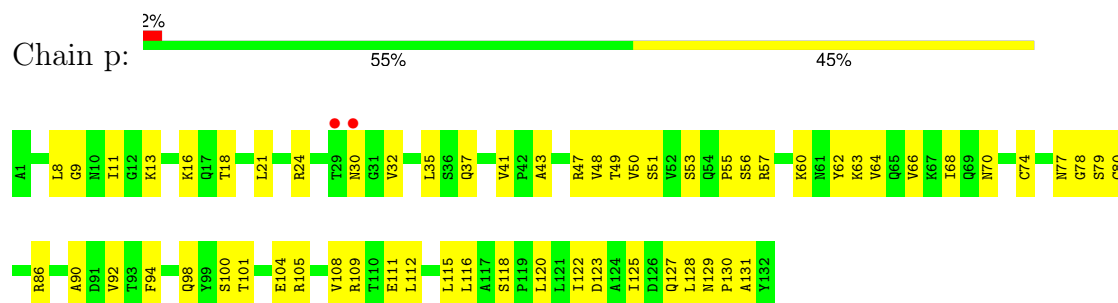
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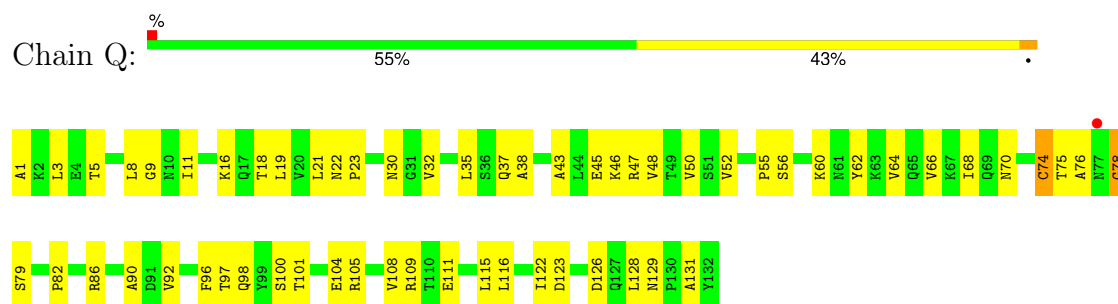
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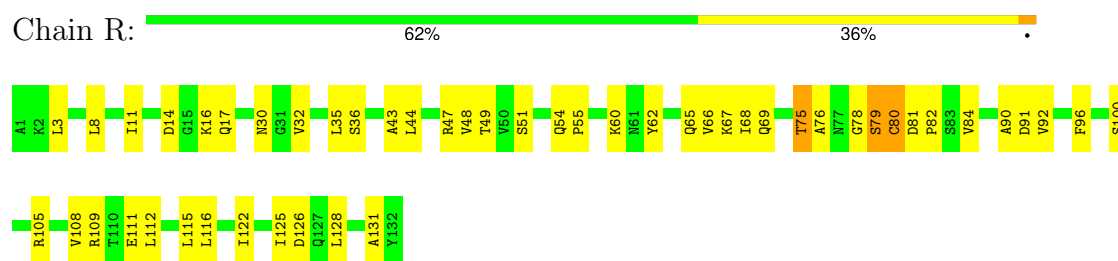
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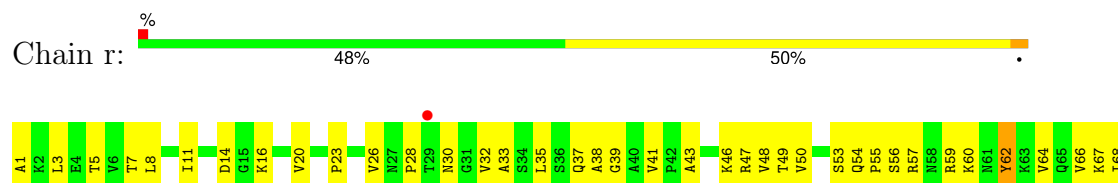
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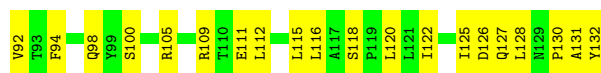
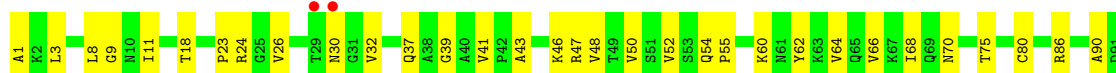




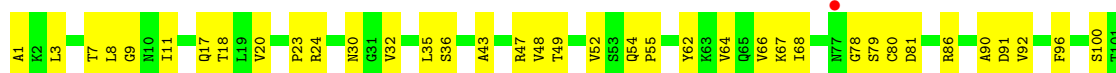
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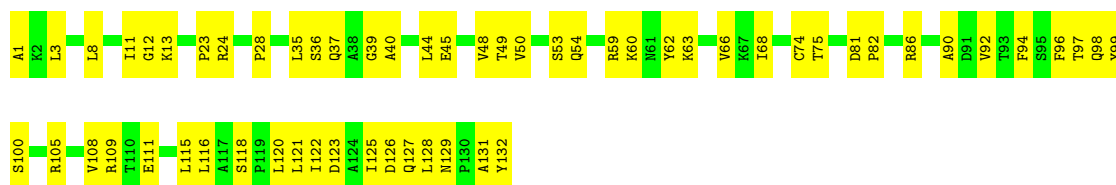


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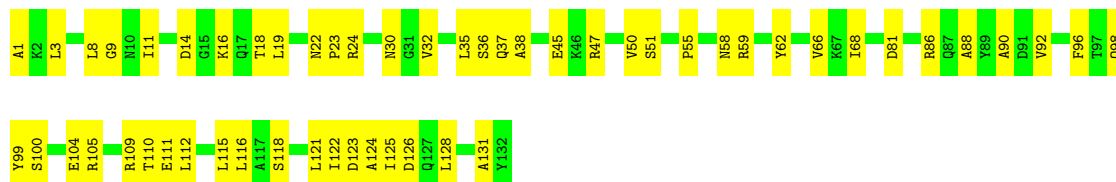


- Molecule 1: Minor capsid protein A1

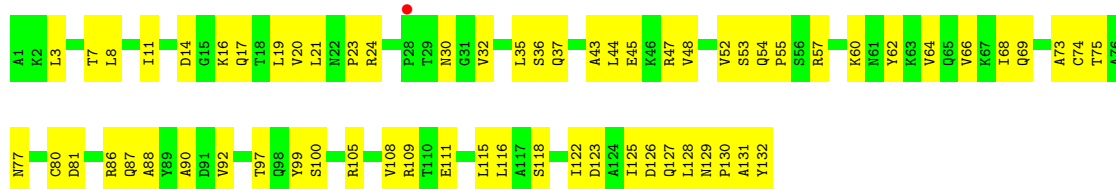




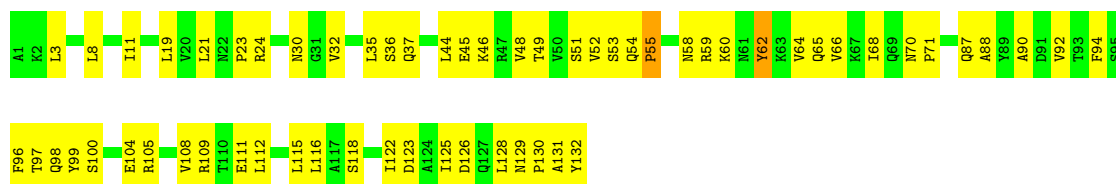
- Molecule 1: Minor capsid protein A1



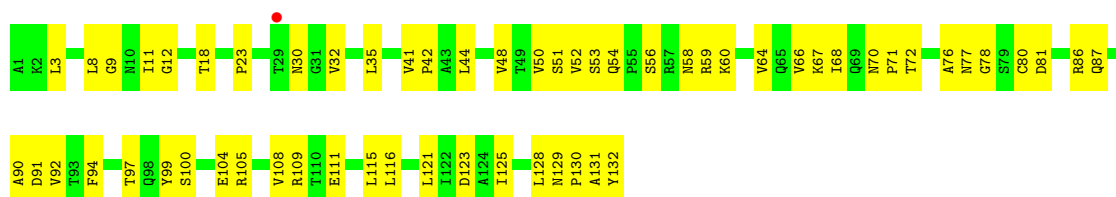
- Molecule 1: Minor capsid protein A1



- Molecule 1: Minor capsid protein A1

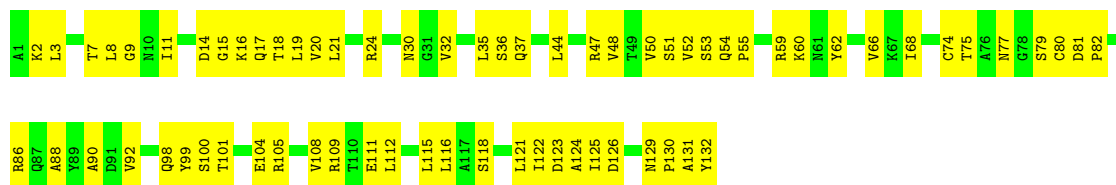


- Molecule 1: Minor capsid protein A1



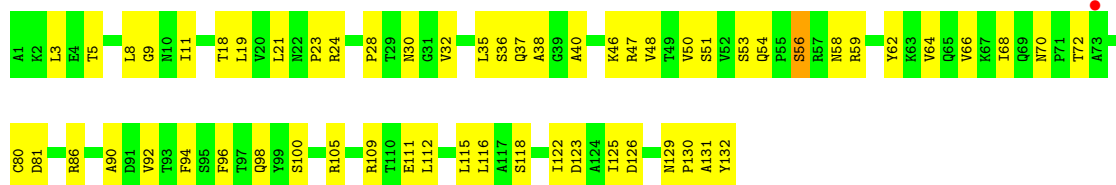
- Molecule 1: Minor capsid protein A1

Chain W:  48% 52%



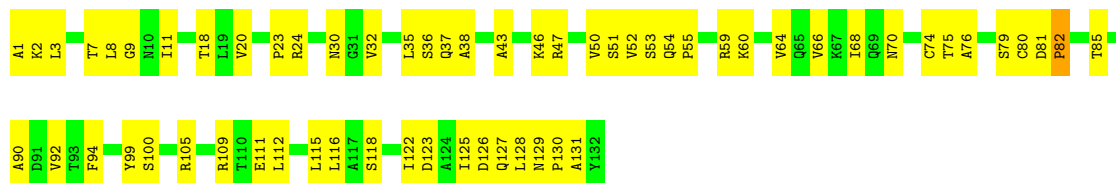
• Molecule 1: Minor capsid protein A1

Chain 4:  56% 43%



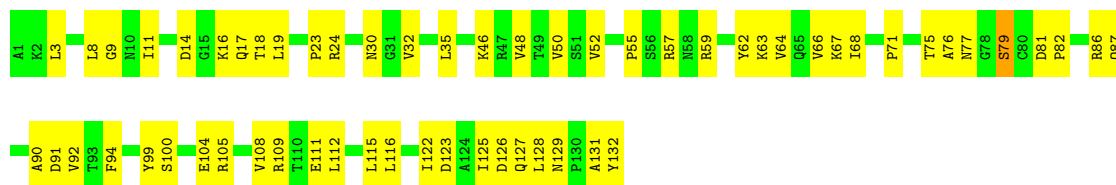
• Molecule 1: Minor capsid protein A1

Chain X:  54% 45%



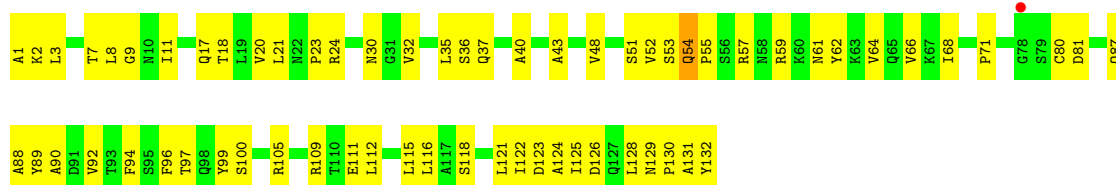
• Molecule 1: Minor capsid protein A1

Chain 6:  55% 44%

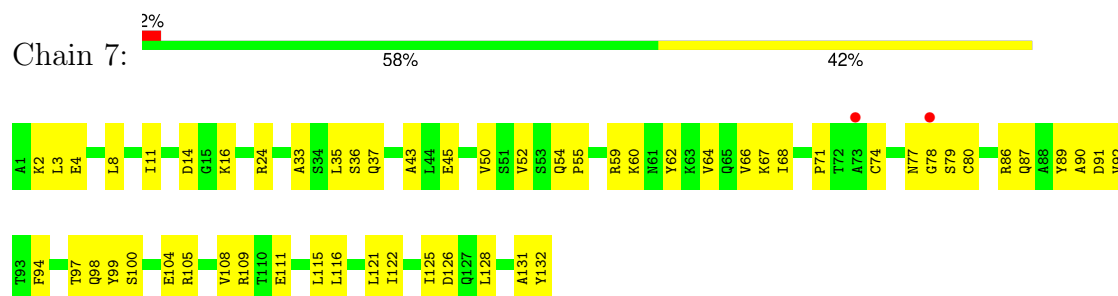


• Molecule 1: Minor capsid protein A1

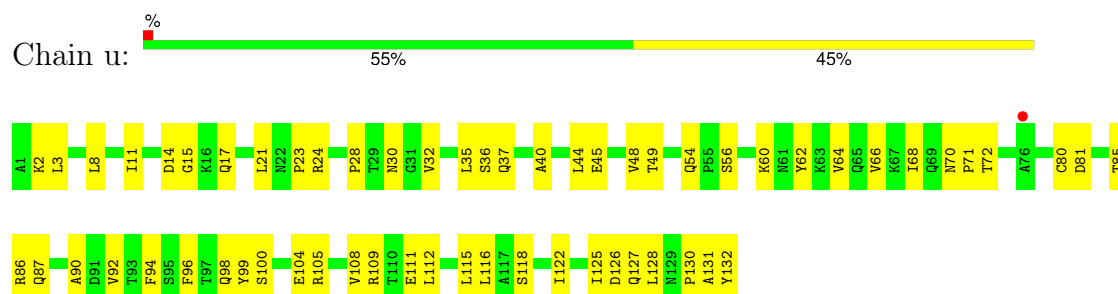
Chain Z:  52% 48%



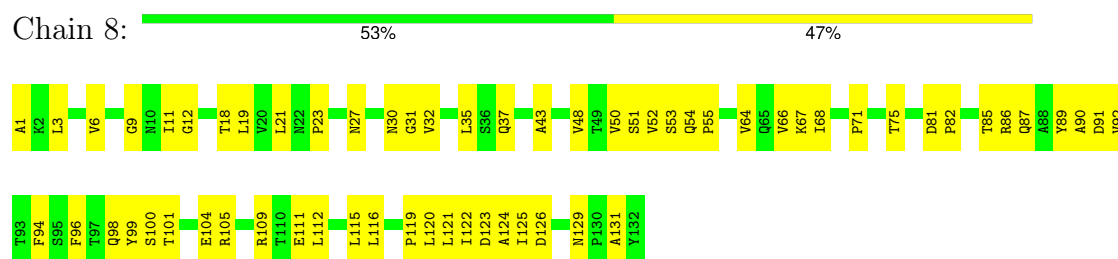
- Molecule 1: Minor capsid protein A1



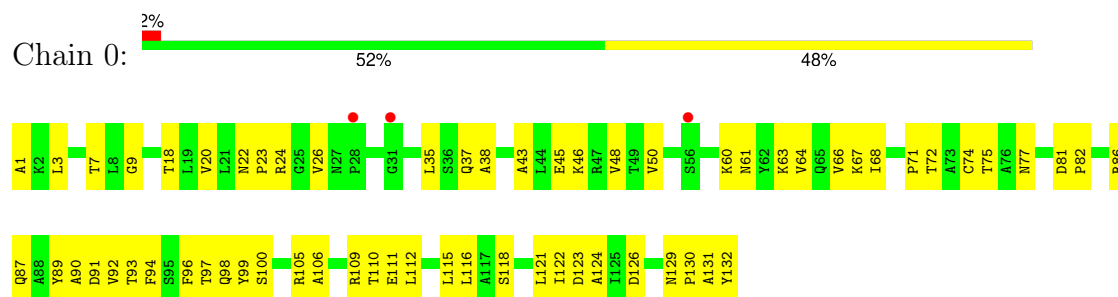
- Molecule 1: Minor capsid protein A1



- Molecule 1: Minor capsid protein A1



- Molecule 1: Minor capsid protein A1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	286.63Å 286.63Å 662.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.56 – 3.54 49.56 – 3.54	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.56-3.54) 100.0 (49.56-3.54)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.278 , 0.328 0.306 , 0.307	Depositor DCC
R_{free} test set	12266 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	100.7	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 111.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.499 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	59580	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.39% 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, 0.333 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	0.26	0/1007	0.56	0/1371
1	1	0.22	0/1007	0.57	0/1371
1	2	0.21	0/1007	0.56	0/1371
1	3	0.28	0/1007	0.62	0/1371
1	4	0.26	0/1007	0.57	0/1371
1	5	0.23	0/1007	0.59	0/1371
1	6	0.33	1/1007 (0.1%)	0.57	0/1371
1	7	0.27	0/1007	0.55	0/1371
1	8	0.23	0/1007	0.54	0/1371
1	9	0.21	0/1007	0.54	0/1371
1	A	0.21	0/1007	0.50	0/1371
1	B	0.22	0/1007	0.54	0/1371
1	C	0.21	0/1007	0.51	0/1371
1	D	0.20	0/1007	0.52	0/1371
1	E	0.20	0/1007	0.50	0/1371
1	F	0.21	0/1007	0.50	0/1371
1	G	0.23	0/1007	0.49	0/1371
1	H	0.23	0/1007	0.55	0/1371
1	I	0.22	0/1007	0.50	0/1371
1	J	0.22	0/1007	0.52	0/1371
1	K	0.22	0/1007	0.54	0/1371
1	L	0.22	0/1007	0.58	0/1371
1	M	0.24	0/1007	0.54	0/1371
1	N	0.24	0/1007	0.60	1/1371 (0.1%)
1	O	0.21	0/1007	0.50	0/1371
1	P	0.23	0/1007	0.56	0/1371
1	Q	0.23	0/1007	0.53	0/1371
1	R	0.22	0/1007	0.51	0/1371
1	S	0.21	0/1007	0.53	0/1371
1	T	0.22	0/1007	0.52	1/1371 (0.1%)
1	U	0.23	0/1007	0.56	0/1371
1	V	0.21	0/1007	0.54	0/1371
1	W	0.24	0/1007	0.56	0/1371
1	X	0.22	0/1007	0.57	0/1371

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Y	0.22	0/1007	0.60	0/1371
1	Z	0.24	0/1007	0.55	1/1371 (0.1%)
1	a	0.24	0/1007	0.59	1/1371 (0.1%)
1	b	0.30	1/1007 (0.1%)	0.58	0/1371
1	c	0.25	0/1007	0.56	0/1371
1	d	0.20	0/1007	0.50	0/1371
1	e	0.23	0/1007	0.53	0/1371
1	f	0.21	0/1007	0.52	0/1371
1	g	0.21	0/1007	0.54	0/1371
1	h	0.25	0/1007	0.61	0/1371
1	i	0.23	0/1007	0.56	0/1371
1	j	0.21	0/1007	0.54	0/1371
1	k	0.26	0/1007	0.56	0/1371
1	l	0.21	0/1007	0.49	0/1371
1	m	0.24	0/1007	0.53	0/1371
1	n	0.23	0/1007	0.52	0/1371
1	o	0.23	0/1007	0.57	0/1371
1	p	0.24	0/1007	0.58	0/1371
1	q	0.22	0/1007	0.52	0/1371
1	r	0.27	0/1007	0.58	0/1371
1	s	0.26	0/1007	0.54	0/1371
1	t	0.21	0/1007	0.51	0/1371
1	u	0.24	0/1007	0.51	0/1371
1	v	0.25	0/1007	0.62	0/1371
1	w	0.20	0/1007	0.53	0/1371
1	x	0.24	0/1007	0.56	0/1371
All	All	0.23	2/60420 (0.0%)	0.55	4/82260 (0.0%)

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	R	0	1
1	h	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	57	ARG	N-CA	-7.18	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	78	GLY	C-O	-6.38	1.19	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	24	ARG	CA-CB-CG	-7.54	99.03	114.10
1	N	78	GLY	N-CA-C	-6.67	97.36	113.18
1	T	78	GLY	N-CA-C	-6.30	98.25	113.18
1	Z	54	GLN	N-CA-C	5.29	121.51	109.81

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	R	75	THR	Peptide
1	h	80	CYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	993	0	1008	39	30
1	1	993	0	1008	63	0
1	2	993	0	1007	68	0
1	3	993	0	1007	75	0
1	4	993	0	1008	56	21
1	5	993	0	1008	75	0
1	6	993	0	1008	80	0
1	7	993	0	1008	68	7
1	8	993	0	1008	40	28
1	9	993	0	1007	58	9
1	A	993	0	1008	63	1
1	B	993	0	1008	49	3
1	C	993	0	1007	60	0
1	D	993	0	1007	61	0
1	E	993	0	1008	58	0
1	F	993	0	1008	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	993	0	1007	55	0
1	H	993	0	1007	68	5
1	I	993	0	1007	65	2
1	J	993	0	1007	70	0
1	K	993	0	1007	68	0
1	L	993	0	1007	59	5
1	M	993	0	1007	71	0
1	N	993	0	1007	69	2
1	O	993	0	1008	62	0
1	P	993	0	1007	72	3
1	Q	993	0	1006	60	1
1	R	993	0	1006	63	0
1	S	993	0	1006	67	0
1	T	993	0	1007	59	0
1	U	993	0	1007	64	0
1	V	993	0	1007	80	0
1	W	993	0	1007	72	0
1	X	993	0	1008	62	7
1	Y	993	0	1008	73	0
1	Z	993	0	1008	81	0
1	a	993	0	1008	77	15
1	b	993	0	1007	59	2
1	c	993	0	1008	65	0
1	d	993	0	1008	77	0
1	e	993	0	1008	64	0
1	f	993	0	1008	64	0
1	g	993	0	1008	53	4
1	h	993	0	1008	69	23
1	i	993	0	1008	71	13
1	j	993	0	1007	72	0
1	k	993	0	1008	57	15
1	l	993	0	1007	59	8
1	m	993	0	1007	80	0
1	n	993	0	1007	73	0
1	o	993	0	1007	66	0
1	p	993	0	1008	67	0
1	q	993	0	1007	63	0
1	r	993	0	1007	76	0
1	s	993	0	1007	65	0
1	t	993	0	1008	61	0
1	u	993	0	1007	67	22
1	v	993	0	1007	65	12

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	w	993	0	1007	62	17
1	x	993	0	1008	64	1
All	All	59580	0	60444	2866	128

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 24.

The worst 5 of 2866 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)
1:5:60:LYS:HA	1:5:98:GLN:HG2	1.44	0.99
1:W:74:CYS:SG	1:W:77:ASN:ND2	2.38	0.95
1:N:11:ILE:HD11	1:n:111:GLU:HA	1.48	0.95
1:L:92:VAL:HG12	1:l:92:VAL:HG12	1.48	0.95
1:2:68:ILE:HB	1:2:90:ALA:HB3	1.52	0.91

The worst 5 of 128 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:k:80:CYS:SG	1:X:74:CYS:SG[2_655]	1.02	1.18
1:a:24:ARG:NH2	1:v:123:ASP:O[2_655]	1.07	1.13
1:h:80:CYS:CB	1:7:77:ASN:OD1[3_665]	1.10	1.10
1:h:47:ARG:NH2	1:u:56:SER:OG[3_665]	1.21	0.99
1:h:86:ARG:NH2	1:w:81:ASP:OD2[3_665]	1.26	0.94

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	130/132 (98%)	121 (93%)	9 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	130/132 (98%)	120 (92%)	10 (8%)	0	100	100
1	2	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	3	130/132 (98%)	122 (94%)	7 (5%)	1 (1%)	16	50
1	4	130/132 (98%)	122 (94%)	6 (5%)	2 (2%)	8	37
1	5	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	16	50
1	6	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	16	50
1	7	130/132 (98%)	125 (96%)	4 (3%)	1 (1%)	16	50
1	8	130/132 (98%)	123 (95%)	7 (5%)	0	100	100
1	9	130/132 (98%)	120 (92%)	8 (6%)	2 (2%)	8	37
1	A	130/132 (98%)	122 (94%)	7 (5%)	1 (1%)	16	50
1	B	130/132 (98%)	122 (94%)	7 (5%)	1 (1%)	16	50
1	C	130/132 (98%)	123 (95%)	7 (5%)	0	100	100
1	D	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
1	E	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	16	50
1	F	130/132 (98%)	125 (96%)	4 (3%)	1 (1%)	16	50
1	G	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
1	H	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	I	130/132 (98%)	122 (94%)	7 (5%)	1 (1%)	16	50
1	J	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
1	K	130/132 (98%)	123 (95%)	7 (5%)	0	100	100
1	L	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	16	50
1	M	130/132 (98%)	121 (93%)	7 (5%)	2 (2%)	8	37
1	N	130/132 (98%)	120 (92%)	10 (8%)	0	100	100
1	O	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	16	50
1	P	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	16	50
1	Q	130/132 (98%)	122 (94%)	6 (5%)	2 (2%)	8	37
1	R	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	16	50
1	S	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	T	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	16	50
1	U	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
1	V	130/132 (98%)	122 (94%)	6 (5%)	2 (2%)	8	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	130/132 (98%)	119 (92%)	9 (7%)	2 (2%)	8	37
1	X	130/132 (98%)	122 (94%)	5 (4%)	3 (2%)	5	29
1	Y	130/132 (98%)	120 (92%)	8 (6%)	2 (2%)	8	37
1	Z	130/132 (98%)	120 (92%)	8 (6%)	2 (2%)	8	37
1	a	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
1	b	130/132 (98%)	123 (95%)	7 (5%)	0	100	100
1	c	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	d	130/132 (98%)	121 (93%)	7 (5%)	2 (2%)	8	37
1	e	130/132 (98%)	123 (95%)	7 (5%)	0	100	100
1	f	130/132 (98%)	121 (93%)	7 (5%)	2 (2%)	8	37
1	g	130/132 (98%)	123 (95%)	5 (4%)	2 (2%)	8	37
1	h	130/132 (98%)	123 (95%)	6 (5%)	1 (1%)	16	50
1	i	130/132 (98%)	122 (94%)	7 (5%)	1 (1%)	16	50
1	j	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	16	50
1	k	130/132 (98%)	118 (91%)	9 (7%)	3 (2%)	5	29
1	l	130/132 (98%)	123 (95%)	6 (5%)	1 (1%)	16	50
1	m	130/132 (98%)	122 (94%)	6 (5%)	2 (2%)	8	37
1	n	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	16	50
1	o	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	16	50
1	p	130/132 (98%)	123 (95%)	6 (5%)	1 (1%)	16	50
1	q	130/132 (98%)	122 (94%)	6 (5%)	2 (2%)	8	37
1	r	130/132 (98%)	118 (91%)	9 (7%)	3 (2%)	5	29
1	s	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
1	t	130/132 (98%)	123 (95%)	5 (4%)	2 (2%)	8	37
1	u	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	16	50
1	v	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	16	50
1	w	130/132 (98%)	126 (97%)	4 (3%)	0	100	100
1	x	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
All	All	7800/7920 (98%)	7322 (94%)	418 (5%)	60 (1%)	16	50

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	79	SER
1	F	79	SER
1	f	79	SER
1	i	79	SER
1	j	79	SER

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	110/110 (100%)	110 (100%)	0	100	100
1	1	110/110 (100%)	110 (100%)	0	100	100
1	2	110/110 (100%)	110 (100%)	0	100	100
1	3	110/110 (100%)	109 (99%)	1 (1%)	70	76
1	4	110/110 (100%)	110 (100%)	0	100	100
1	5	110/110 (100%)	110 (100%)	0	100	100
1	6	110/110 (100%)	110 (100%)	0	100	100
1	7	110/110 (100%)	110 (100%)	0	100	100
1	8	110/110 (100%)	110 (100%)	0	100	100
1	9	110/110 (100%)	109 (99%)	1 (1%)	70	76
1	A	110/110 (100%)	110 (100%)	0	100	100
1	B	110/110 (100%)	110 (100%)	0	100	100
1	C	110/110 (100%)	110 (100%)	0	100	100
1	D	110/110 (100%)	110 (100%)	0	100	100
1	E	110/110 (100%)	110 (100%)	0	100	100
1	F	110/110 (100%)	110 (100%)	0	100	100
1	G	110/110 (100%)	110 (100%)	0	100	100
1	H	110/110 (100%)	109 (99%)	1 (1%)	70	76
1	I	110/110 (100%)	110 (100%)	0	100	100
1	J	110/110 (100%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	110/110 (100%)	110 (100%)	0	100	100
1	L	110/110 (100%)	110 (100%)	0	100	100
1	M	110/110 (100%)	109 (99%)	1 (1%)	70	76
1	N	110/110 (100%)	110 (100%)	0	100	100
1	O	110/110 (100%)	110 (100%)	0	100	100
1	P	110/110 (100%)	110 (100%)	0	100	100
1	Q	110/110 (100%)	109 (99%)	1 (1%)	70	76
1	R	110/110 (100%)	109 (99%)	1 (1%)	70	76
1	S	110/110 (100%)	109 (99%)	1 (1%)	70	76
1	T	110/110 (100%)	110 (100%)	0	100	100
1	U	110/110 (100%)	110 (100%)	0	100	100
1	V	110/110 (100%)	110 (100%)	0	100	100
1	W	110/110 (100%)	110 (100%)	0	100	100
1	X	110/110 (100%)	110 (100%)	0	100	100
1	Y	110/110 (100%)	110 (100%)	0	100	100
1	Z	110/110 (100%)	110 (100%)	0	100	100
1	a	110/110 (100%)	110 (100%)	0	100	100
1	b	110/110 (100%)	110 (100%)	0	100	100
1	c	110/110 (100%)	110 (100%)	0	100	100
1	d	110/110 (100%)	109 (99%)	1 (1%)	70	76
1	e	110/110 (100%)	109 (99%)	1 (1%)	70	76
1	f	110/110 (100%)	110 (100%)	0	100	100
1	g	110/110 (100%)	110 (100%)	0	100	100
1	h	110/110 (100%)	110 (100%)	0	100	100
1	i	110/110 (100%)	110 (100%)	0	100	100
1	j	110/110 (100%)	110 (100%)	0	100	100
1	k	110/110 (100%)	110 (100%)	0	100	100
1	l	110/110 (100%)	110 (100%)	0	100	100
1	m	110/110 (100%)	110 (100%)	0	100	100
1	n	110/110 (100%)	109 (99%)	1 (1%)	70	76
1	o	110/110 (100%)	109 (99%)	1 (1%)	70	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	p	110/110 (100%)	110 (100%)	0	100	100
1	q	110/110 (100%)	110 (100%)	0	100	100
1	r	110/110 (100%)	110 (100%)	0	100	100
1	s	110/110 (100%)	109 (99%)	1 (1%)	70	76
1	t	110/110 (100%)	110 (100%)	0	100	100
1	u	110/110 (100%)	110 (100%)	0	100	100
1	v	110/110 (100%)	110 (100%)	0	100	100
1	w	110/110 (100%)	109 (99%)	1 (1%)	70	76
1	x	110/110 (100%)	110 (100%)	0	100	100
All	All	6600/6600 (100%)	6587 (100%)	13 (0%)	87	85

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	74	CYS
1	R	80	CYS
1	3	80	CYS
1	s	80	CYS
1	w	74	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
1	q	129	ASN
1	V	70	ASN
1	r	37	GLN
1	t	61	ASN
1	4	129	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	132/132 (100%)	-0.77	3 (2%) 61 34	69, 97, 152, 179	0
1	1	132/132 (100%)	-0.64	1 (0%) 82 57	81, 107, 161, 179	0
1	2	132/132 (100%)	-0.86	1 (0%) 82 57	74, 104, 163, 180	0
1	3	132/132 (100%)	-0.89	1 (0%) 82 57	79, 103, 164, 182	0
1	4	132/132 (100%)	-0.77	1 (0%) 82 57	73, 100, 149, 179	0
1	5	132/132 (100%)	-0.93	0 100 100	66, 102, 164, 181	0
1	6	132/132 (100%)	-0.78	0 100 100	72, 102, 162, 182	0
1	7	132/132 (100%)	-0.66	2 (1%) 72 43	78, 109, 167, 183	0
1	8	132/132 (100%)	-0.80	0 100 100	70, 97, 165, 191	0
1	9	132/132 (100%)	-0.89	1 (0%) 82 57	72, 103, 166, 175	0
1	A	132/132 (100%)	-0.84	0 100 100	68, 100, 157, 175	0
1	B	132/132 (100%)	-0.70	0 100 100	70, 101, 156, 172	0
1	C	132/132 (100%)	-0.77	0 100 100	80, 102, 156, 175	0
1	D	132/132 (100%)	-0.74	1 (0%) 82 57	83, 106, 160, 182	0
1	E	132/132 (100%)	-0.87	0 100 100	71, 102, 157, 176	0
1	F	132/132 (100%)	-0.87	0 100 100	71, 102, 155, 179	0
1	G	132/132 (100%)	-0.89	0 100 100	74, 101, 148, 180	0
1	H	132/132 (100%)	-0.90	0 100 100	74, 101, 150, 170	0
1	I	132/132 (100%)	-0.79	1 (0%) 82 57	76, 103, 155, 174	0
1	J	132/132 (100%)	-0.76	0 100 100	82, 106, 151, 177	0
1	K	132/132 (100%)	-0.77	0 100 100	69, 97, 151, 181	0
1	L	132/132 (100%)	-0.76	0 100 100	69, 98, 152, 178	0
1	M	132/132 (100%)	-0.81	2 (1%) 72 43	71, 96, 159, 178	0
1	N	132/132 (100%)	-0.82	0 100 100	70, 95, 151, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	O	132/132 (100%)	-0.87	0 100 100	70, 100, 150, 175	0
1	P	132/132 (100%)	-0.77	1 (0%) 82 57	65, 95, 151, 178	0
1	Q	132/132 (100%)	-0.77	1 (0%) 82 57	71, 96, 153, 200	0
1	R	132/132 (100%)	-0.77	0 100 100	70, 95, 151, 194	0
1	S	132/132 (100%)	-0.78	1 (0%) 82 57	70, 98, 149, 185	0
1	T	132/132 (100%)	-0.79	1 (0%) 82 57	70, 100, 150, 179	0
1	U	132/132 (100%)	-0.73	2 (1%) 72 43	79, 107, 156, 184	0
1	V	132/132 (100%)	-0.84	0 100 100	80, 102, 159, 179	0
1	W	132/132 (100%)	-0.80	0 100 100	75, 104, 165, 184	0
1	X	132/132 (100%)	-0.85	0 100 100	77, 103, 162, 186	0
1	Y	132/132 (100%)	-0.86	0 100 100	74, 103, 162, 179	0
1	Z	132/132 (100%)	-0.69	1 (0%) 82 57	66, 102, 166, 181	0
1	a	132/132 (100%)	-0.66	0 100 100	74, 103, 153, 188	0
1	b	132/132 (100%)	-0.69	1 (0%) 82 57	72, 105, 166, 189	0
1	c	132/132 (100%)	-0.67	0 100 100	79, 104, 163, 182	0
1	d	132/132 (100%)	-0.61	3 (2%) 61 34	78, 107, 165, 188	0
1	e	132/132 (100%)	-0.65	3 (2%) 61 34	70, 102, 159, 178	0
1	f	132/132 (100%)	-0.71	1 (0%) 82 57	72, 102, 163, 186	0
1	g	132/132 (100%)	-0.82	0 100 100	75, 103, 154, 190	0
1	h	132/132 (100%)	-0.76	1 (0%) 82 57	73, 106, 165, 190	0
1	i	132/132 (100%)	-0.72	0 100 100	75, 103, 156, 187	0
1	j	132/132 (100%)	-0.72	0 100 100	76, 105, 159, 186	0
1	k	132/132 (100%)	-0.86	0 100 100	69, 96, 157, 178	0
1	l	132/132 (100%)	-0.85	1 (0%) 82 57	70, 101, 154, 175	0
1	m	132/132 (100%)	-0.81	1 (0%) 82 57	71, 95, 154, 180	0
1	n	132/132 (100%)	-0.59	0 100 100	68, 102, 156, 178	0
1	o	132/132 (100%)	-0.76	2 (1%) 72 43	72, 101, 159, 184	0
1	p	132/132 (100%)	-0.74	2 (1%) 72 43	67, 96, 152, 179	0
1	q	132/132 (100%)	-0.82	0 100 100	72, 98, 159, 183	0
1	r	132/132 (100%)	-0.78	1 (0%) 82 57	70, 97, 162, 181	0
1	s	132/132 (100%)	-0.55	2 (1%) 72 43	67, 102, 159, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	t	132/132 (100%)	-0.76	1 (0%) 82 57	71, 101, 158, 187	0
1	u	132/132 (100%)	-0.73	1 (0%) 82 57	82, 109, 163, 176	0
1	v	132/132 (100%)	-0.76	0 100 100	77, 106, 162, 189	0
1	w	132/132 (100%)	-0.78	0 100 100	72, 104, 163, 179	0
1	x	132/132 (100%)	-0.77	0 100 100	77, 104, 163, 186	0
All	All	7920/7920 (100%)	-0.77	41 (0%) 87 66	65, 102, 162, 200	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	77	ASN	3.6
1	P	77	ASN	3.5
1	D	40	ALA	3.5
1	h	58	ASN	3.5
1	7	78	GLY	3.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.