



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:46 AM UTC

PDB ID : 4V4M / pdb_00004v4m
Title : 1.45 Angstrom Structure of STNV coat protein
Authors : Lane, S.W.; Dennis, C.A.; Lane, C.L.; Trinh, C.H.; Rizkallah, P.J.; Stockley, P.G.; Phillips, S.E.V.
Deposited on : 2011-04-28
Resolution : 1.45 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

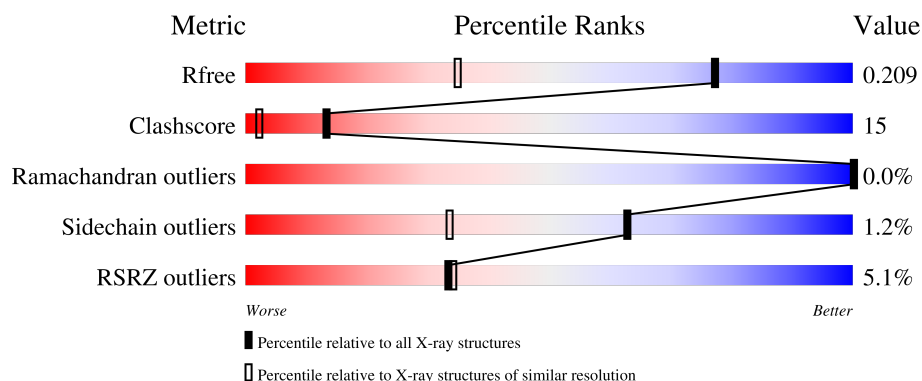
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	196	6% 82% 11% 6%
1	1	196	5% 80% 13% 6%
1	2	196	6% 80% 13% 6%
1	3	196	5% 81% 12% 6%
1	4	196	4% 82% 11% 6%

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Mol	Chain	Length	Quality of chain
1	5	196	
1	6	196	
1	7	196	
1	A	196	
1	B	196	
1	C	196	
1	D	196	
1	E	196	
1	F	196	
1	G	196	
1	H	196	
1	I	196	
1	J	196	
1	K	196	
1	L	196	
1	M	196	
1	N	196	
1	O	196	
1	P	196	
1	Q	196	
1	R	196	
1	S	196	
1	T	196	
1	U	196	
1	V	196	

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Mol	Chain	Length	Quality of chain
1	W	196	
1	X	196	
1	Y	196	
1	Z	196	
1	a	196	
1	b	196	
1	c	196	
1	d	196	
1	e	196	
1	f	196	
1	g	196	
1	h	196	
1	i	196	
1	j	196	
1	k	196	
1	l	196	
1	m	196	
1	n	196	
1	o	196	
1	p	196	
1	q	196	
1	r	196	
1	s	196	
1	t	196	
1	u	196	

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Mol	Chain	Length	Quality of chain
1	v	196	5% 81% 12% 6%
1	w	196	4% 81% 13% 6%
1	x	196	6% 79% 15% 6%
1	y	196	6% 81% 12% 6%
1	z	196	5% 81% 12% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 102135 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	e	184	Total	C	N	O	S	0	2	0
			1439	898	261	273	7			
1	f	184	Total	C	N	O	S	0	4	0
			1450	908	263	272	7			
1	g	184	Total	C	N	O	S	0	2	0
			1437	898	260	272	7			
1	h	184	Total	C	N	O	S	0	4	0
			1451	906	265	274	6			
1	i	184	Total	C	N	O	S	0	3	0
			1448	902	265	274	7			
1	j	184	Total	C	N	O	S	0	2	0
			1441	898	264	273	6			
1	k	184	Total	C	N	O	S	0	2	0
			1440	897	264	273	6			
1	l	184	Total	C	N	O	S	0	1	0
			1432	893	260	272	7			
1	m	184	Total	C	N	O	S	0	2	0
			1440	898	263	272	7			
1	n	184	Total	C	N	O	S	0	4	0
			1450	906	264	273	7			
1	o	184	Total	C	N	O	S	0	1	0
			1433	893	261	273	6			
1	p	184	Total	C	N	O	S	0	1	0
			1432	893	260	272	7			
1	q	184	Total	C	N	O	S	0	1	0
			1432	893	260	272	7			
1	r	184	Total	C	N	O	S	0	3	0
			1448	903	266	272	7			
1	s	184	Total	C	N	O	S	0	2	0
			1436	897	260	272	7			
1	t	184	Total	C	N	O	S	0	7	0
			1472	919	272	274	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	u	184	Total	C	N	O	S	0	2	0
			1440	898	263	272	7			
1	v	184	Total	C	N	O	S	0	2	0
			1440	898	263	272	7			
1	w	184	Total	C	N	O	S	0	3	0
			1444	902	263	272	7			
1	x	184	Total	C	N	O	S	0	3	0
			1445	901	264	273	7			
1	y	184	Total	C	N	O	S	0	2	0
			1436	897	260	272	7			
1	z	184	Total	C	N	O	S	0	4	0
			1451	907	264	273	7			
1	0	184	Total	C	N	O	S	0	2	0
			1440	898	263	272	7			
1	1	184	Total	C	N	O	S	0	3	0
			1446	902	264	273	7			
1	2	184	Total	C	N	O	S	0	4	0
			1452	906	266	273	7			
1	3	184	Total	C	N	O	S	0	4	0
			1454	907	267	273	7			
1	4	184	Total	C	N	O	S	0	3	0
			1443	900	262	274	7			
1	5	184	Total	C	N	O	S	0	1	0
			1432	892	261	273	6			
1	6	184	Total	C	N	O	S	0	3	0
			1448	903	266	272	7			
1	7	184	Total	C	N	O	S	0	2	0
			1438	897	261	273	7			
1	A	184	Total	C	N	O	S	0	6	0
			1460	913	265	275	7			
1	B	184	Total	C	N	O	S	0	6	0
			1464	917	267	273	7			
1	C	184	Total	C	N	O	S	0	4	0
			1454	906	265	276	7			
1	D	184	Total	C	N	O	S	0	4	0
			1445	905	260	273	7			
1	E	184	Total	C	N	O	S	0	2	0
			1437	898	260	272	7			
1	F	184	Total	C	N	O	S	0	2	0
			1438	897	261	273	7			
1	G	184	Total	C	N	O	S	0	4	0
			1450	906	264	273	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	184	Total	C	N	O	S	0	2	0
			1440	898	263	272	7			
1	I	184	Total	C	N	O	S	0	3	0
			1443	902	260	274	7			
1	J	184	Total	C	N	O	S	0	2	0
			1440	898	263	272	7			
1	K	184	Total	C	N	O	S	0	7	0
			1470	919	269	275	7			
1	L	184	Total	C	N	O	S	0	5	0
			1458	913	266	272	7			
1	M	184	Total	C	N	O	S	0	3	0
			1442	901	261	273	7			
1	N	184	Total	C	N	O	S	0	3	0
			1445	901	264	273	7			
1	O	184	Total	C	N	O	S	0	2	0
			1440	898	263	272	7			
1	P	184	Total	C	N	O	S	0	6	0
			1465	917	268	273	7			
1	Q	184	Total	C	N	O	S	0	2	0
			1437	896	261	273	7			
1	R	184	Total	C	N	O	S	0	3	0
			1442	903	260	272	7			
1	S	184	Total	C	N	O	S	0	6	0
			1465	916	268	274	7			
1	T	184	Total	C	N	O	S	0	3	0
			1440	900	260	273	7			
1	U	184	Total	C	N	O	S	0	4	0
			1451	905	265	274	7			
1	V	184	Total	C	N	O	S	0	3	0
			1443	902	260	274	7			
1	W	184	Total	C	N	O	S	0	1	0
			1432	893	260	272	7			
1	X	184	Total	C	N	O	S	0	2	0
			1437	898	260	272	7			
1	Y	184	Total	C	N	O	S	0	3	0
			1445	901	264	273	7			
1	Z	184	Total	C	N	O	S	0	3	0
			1448	903	266	272	7			
1	a	184	Total	C	N	O	S	0	5	0
			1456	910	265	274	7			
1	b	184	Total	C	N	O	S	0	1	0
			1432	893	260	272	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	c	184	Total	C	N	O	S	0	3	0
			1448	903	266	272	7			
1	d	184	Total	C	N	O	S	0	2	0
			1439	898	261	273	7			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	e	1	Total	Ca	0	0
			1	1		
2	f	1	Total	Ca	0	0
			1	1		
2	g	1	Total	Ca	0	0
			1	1		
2	h	1	Total	Ca	0	0
			1	1		
2	i	2	Total	Ca	0	0
			2	2		
2	j	2	Total	Ca	0	0
			2	2		
2	k	1	Total	Ca	0	0
			1	1		
2	l	1	Total	Ca	0	0
			1	1		
2	m	1	Total	Ca	0	0
			1	1		
2	n	2	Total	Ca	0	0
			2	2		
2	o	2	Total	Ca	0	0
			2	2		
2	p	1	Total	Ca	0	0
			1	1		
2	q	2	Total	Ca	0	0
			2	2		
2	r	1	Total	Ca	0	0
			1	1		
2	s	1	Total	Ca	0	0
			1	1		
2	t	1	Total	Ca	0	0
			1	1		
2	u	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	v	1	Total 1	Ca 1	0	0
2	w	1	Total 1	Ca 1	0	0
2	x	1	Total 1	Ca 1	0	0
2	y	1	Total 1	Ca 1	0	0
2	z	1	Total 1	Ca 1	0	0
2	0	2	Total 2	Ca 2	0	0
2	1	3	Total 3	Ca 3	0	0
2	2	2	Total 2	Ca 2	0	0
2	3	2	Total 2	Ca 2	0	0
2	4	2	Total 2	Ca 2	0	0
2	5	2	Total 2	Ca 2	0	0
2	6	2	Total 2	Ca 2	0	0
2	7	1	Total 1	Ca 1	0	0
2	A	2	Total 2	Ca 2	0	0
2	B	3	Total 3	Ca 3	0	0
2	C	1	Total 1	Ca 1	0	0
2	D	1	Total 1	Ca 1	0	0
2	E	3	Total 3	Ca 3	0	0
2	F	1	Total 1	Ca 1	0	0
2	G	3	Total 3	Ca 3	0	0
2	H	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	2	Total 2	Ca 2	0	0
2	J	1	Total 1	Ca 1	0	0
2	K	2	Total 2	Ca 2	0	0
2	L	1	Total 1	Ca 1	0	0
2	M	1	Total 1	Ca 1	0	0
2	N	2	Total 2	Ca 2	0	0
2	O	1	Total 1	Ca 1	0	0
2	P	1	Total 1	Ca 1	0	0
2	Q	2	Total 2	Ca 2	0	0
2	R	2	Total 2	Ca 2	0	0
2	S	2	Total 2	Ca 2	0	0
2	T	2	Total 2	Ca 2	0	0
2	U	3	Total 3	Ca 3	0	0
2	V	2	Total 2	Ca 2	0	0
2	W	1	Total 1	Ca 1	0	0
2	X	1	Total 1	Ca 1	0	0
2	Y	1	Total 1	Ca 1	0	0
2	Z	1	Total 1	Ca 1	0	0
2	a	1	Total 1	Ca 1	0	0
2	b	2	Total 2	Ca 2	0	0
2	c	2	Total 2	Ca 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	d	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	e	258	Total 258	O 258	0	0
3	f	231	Total 231	O 231	0	0
3	g	260	Total 260	O 260	0	0
3	h	281	Total 281	O 281	0	0
3	i	282	Total 282	O 282	0	0
3	j	267	Total 267	O 267	0	0
3	k	256	Total 256	O 256	0	0
3	l	257	Total 257	O 257	0	0
3	m	252	Total 252	O 252	0	0
3	n	251	Total 251	O 251	0	0
3	o	262	Total 262	O 262	0	0
3	p	238	Total 238	O 238	0	0
3	q	258	Total 258	O 258	0	0
3	r	287	Total 287	O 287	0	0
3	s	226	Total 226	O 226	0	0
3	t	236	Total 236	O 236	0	0
3	u	240	Total 240	O 240	0	0
3	v	249	Total 249	O 249	0	0

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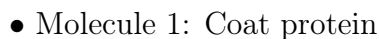
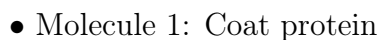
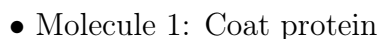
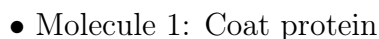
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	w	279	Total 279	O 279	0	0
3	x	260	Total 260	O 260	0	0
3	y	294	Total 294	O 294	0	0
3	z	264	Total 264	O 264	0	0
3	0	242	Total 242	O 242	0	0
3	1	256	Total 256	O 256	0	0
3	2	259	Total 259	O 259	0	0
3	3	245	Total 245	O 245	0	0
3	4	278	Total 278	O 278	0	0
3	5	247	Total 247	O 247	0	0
3	6	264	Total 264	O 264	0	0
3	7	249	Total 249	O 249	0	0
3	A	246	Total 246	O 246	0	0
3	B	235	Total 235	O 235	0	0
3	C	250	Total 250	O 250	0	0
3	D	255	Total 255	O 255	0	0
3	E	229	Total 229	O 229	0	0
3	F	217	Total 217	O 217	0	0
3	G	253	Total 253	O 253	0	0
3	H	248	Total 248	O 248	0	0
3	I	240	Total 240	O 240	0	0

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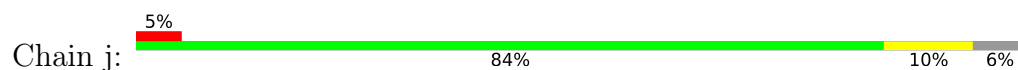
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3	K	273	Total 273	O 273	0	0
3	L	239	Total 239	O 239	0	0
3	M	253	Total 253	O 253	0	0
3	N	256	Total 256	O 256	0	0
3	O	250	Total 250	O 250	0	0
3	P	250	Total 250	O 250	0	0
3	Q	255	Total 255	O 255	0	0
3	R	286	Total 286	O 286	0	0
3	S	237	Total 237	O 237	0	0
3	T	295	Total 295	O 295	0	0
3	U	266	Total 266	O 266	0	0
3	V	258	Total 258	O 258	0	0
3	W	256	Total 256	O 256	0	0
3	X	256	Total 256	O 256	0	0
3	Y	262	Total 262	O 262	0	0
3	Z	285	Total 285	O 285	0	0
3	a	257	Total 257	O 257	0	0
3	b	254	Total 254	O 254	0	0
3	c	269	Total 269	O 269	0	0
3	d	244	Total 244	O 244	0	0

- Molecule 1: Coat protein





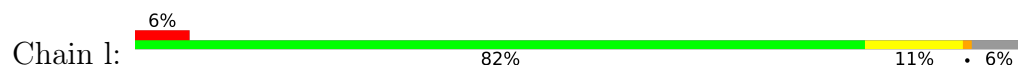
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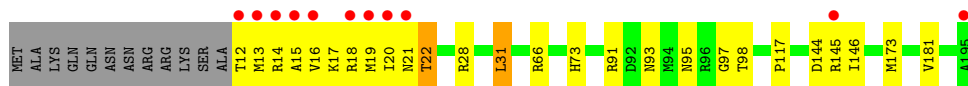
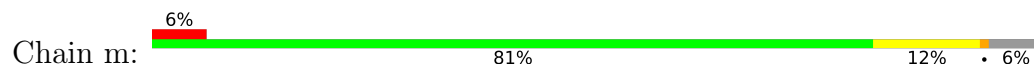
• Molecule 1: Coat protein



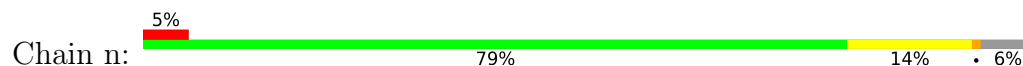
• Molecule 1: Coat protein



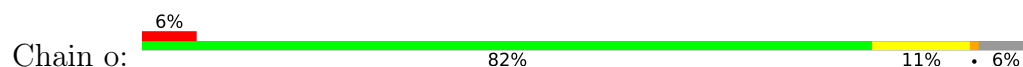
• Molecule 1: Coat protein



• Molecule 1: Coat protein

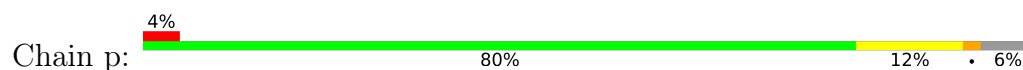


• Molecule 1: Coat protein

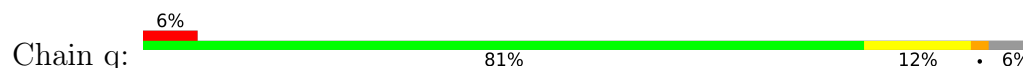




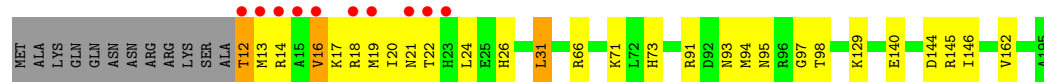
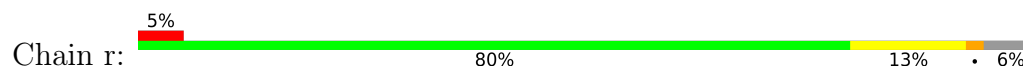
• Molecule 1: Coat protein



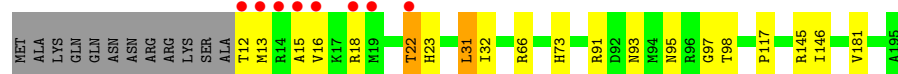
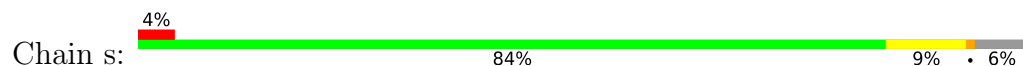
• Molecule 1: Coat protein



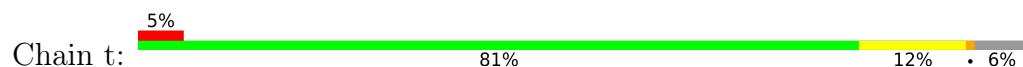
• Molecule 1: Coat protein



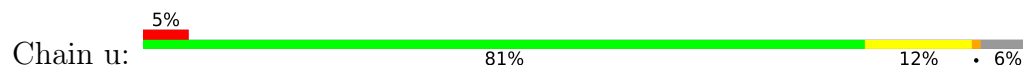
• Molecule 1: Coat protein



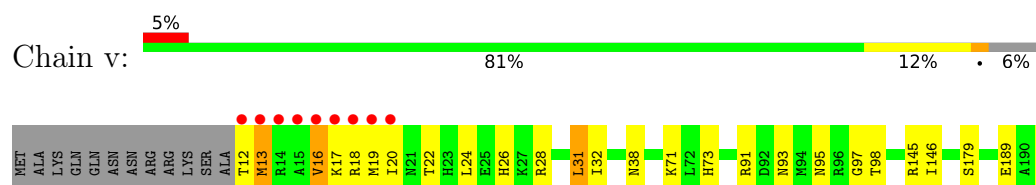
• Molecule 1: Coat protein



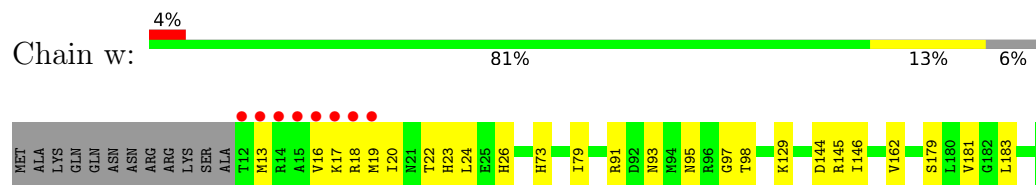
• Molecule 1: Coat protein



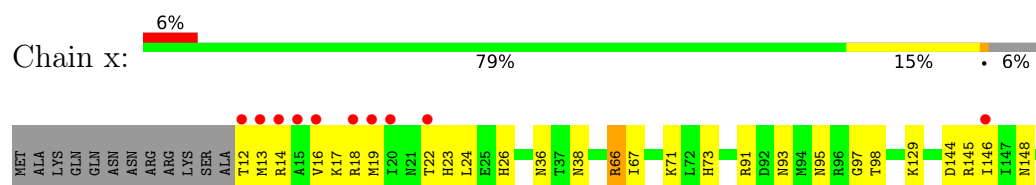
• Molecule 1: Coat protein



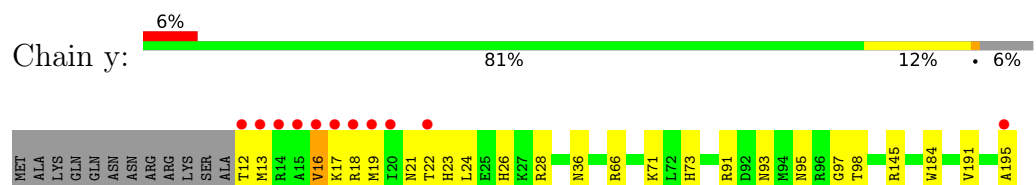
• Molecule 1: Coat protein



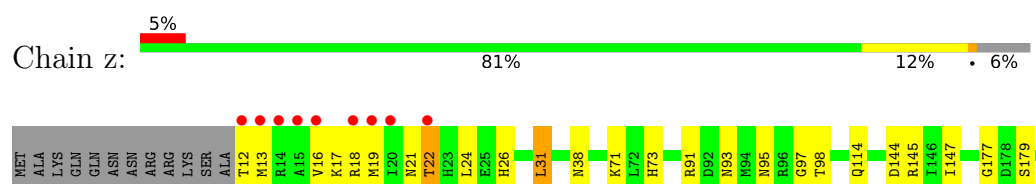
• Molecule 1: Coat protein



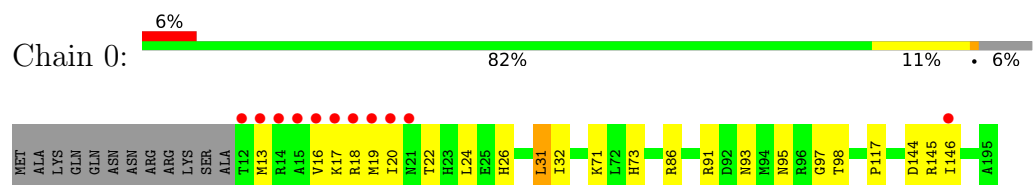
• Molecule 1: Coat protein



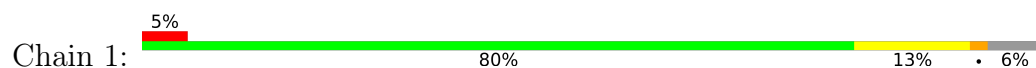
• Molecule 1: Coat protein

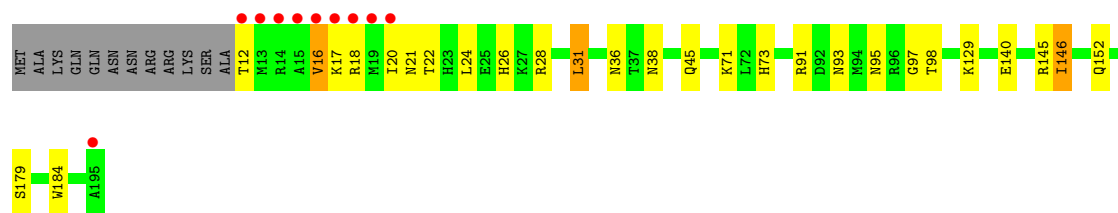


• Molecule 1: Coat protein

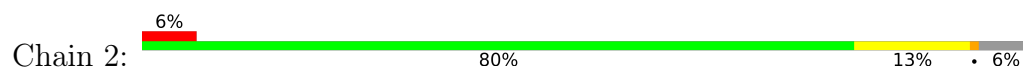


• Molecule 1: Coat protein

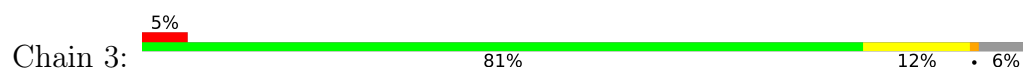




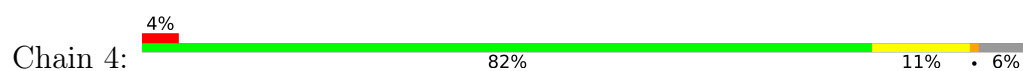
• Molecule 1: Coat protein



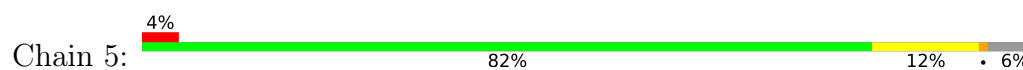
• Molecule 1: Coat protein



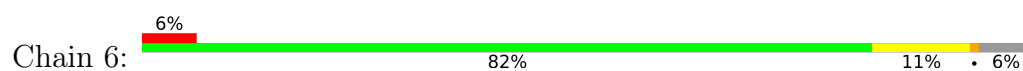
• Molecule 1: Coat protein



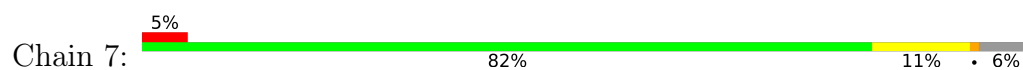
• Molecule 1: Coat protein

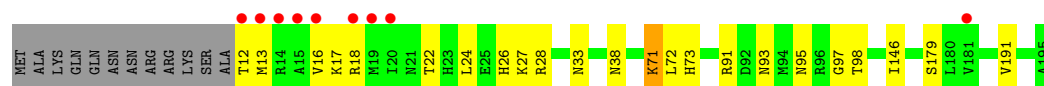


• Molecule 1: Coat protein

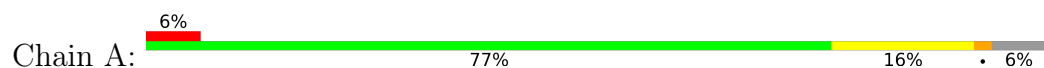


• Molecule 1: Coat protein

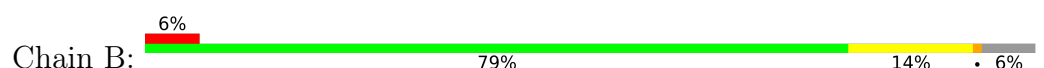




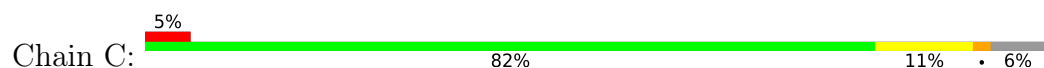
• Molecule 1: Coat protein



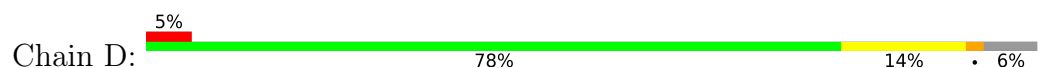
• Molecule 1: Coat protein



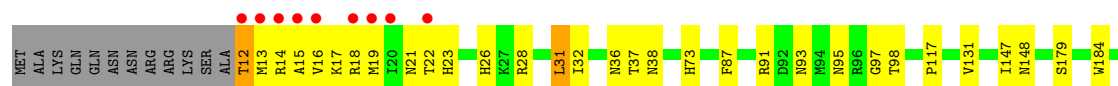
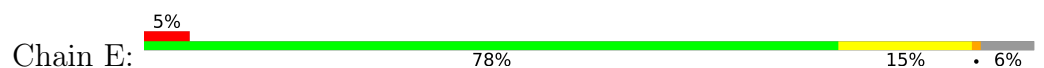
• Molecule 1: Coat protein



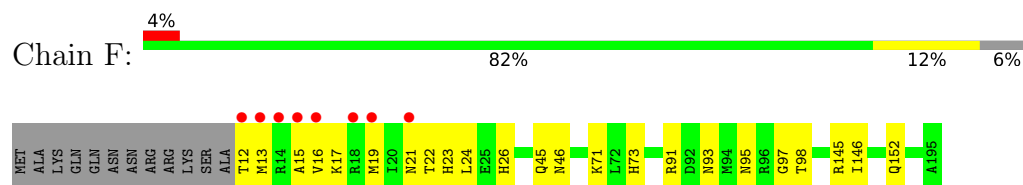
• Molecule 1: Coat protein



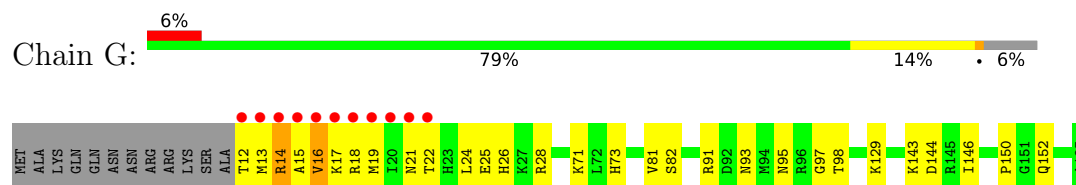
• Molecule 1: Coat protein



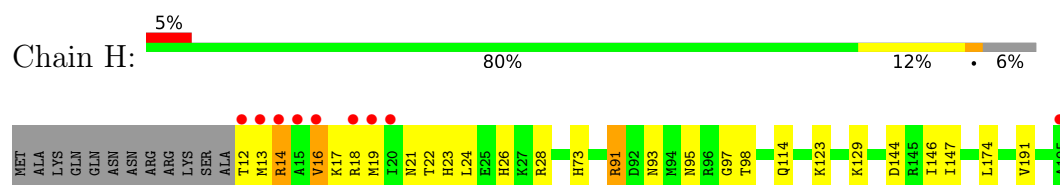
• Molecule 1: Coat protein



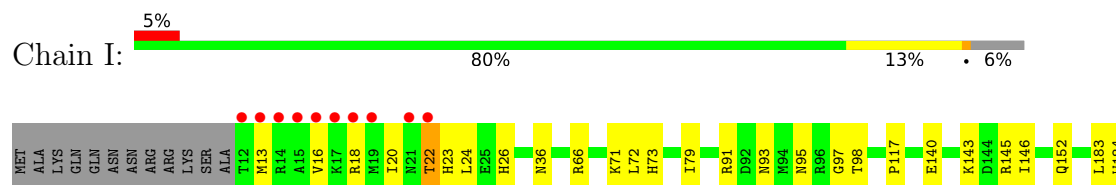
• Molecule 1: Coat protein



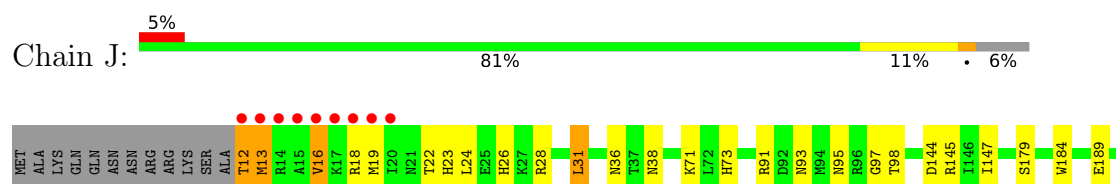
• Molecule 1: Coat protein



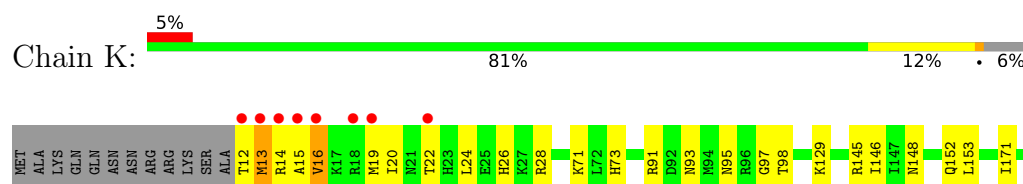
• Molecule 1: Coat protein



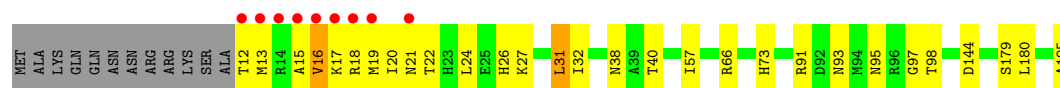
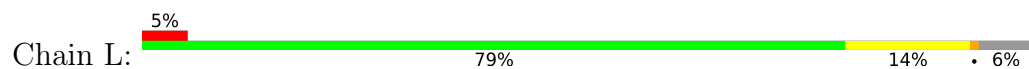
• Molecule 1: Coat protein



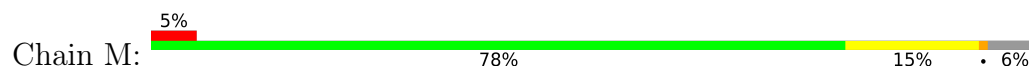
• Molecule 1: Coat protein



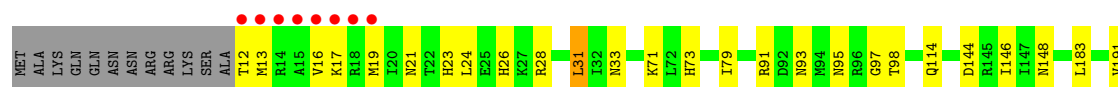
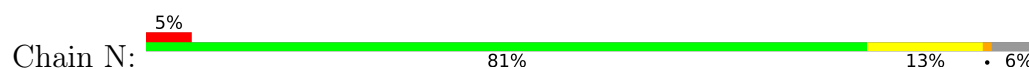
- Molecule 1: Coat protein



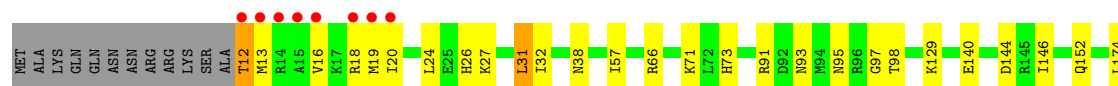
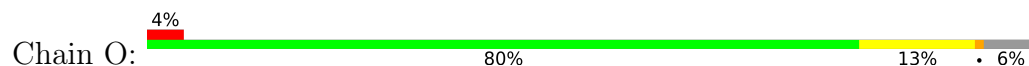
- Molecule 1: Coat protein



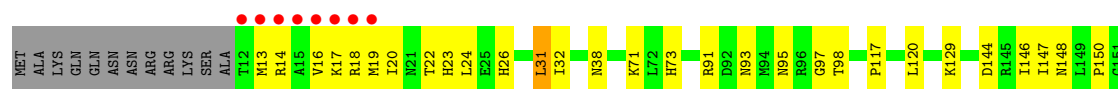
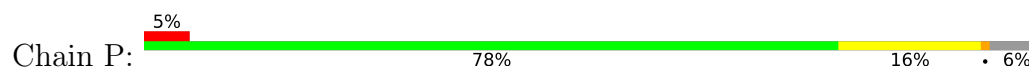
- Molecule 1: Coat protein



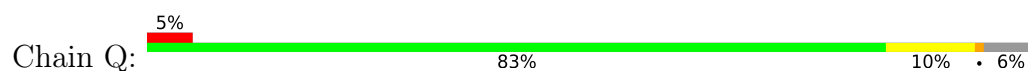
- Molecule 1: Coat protein



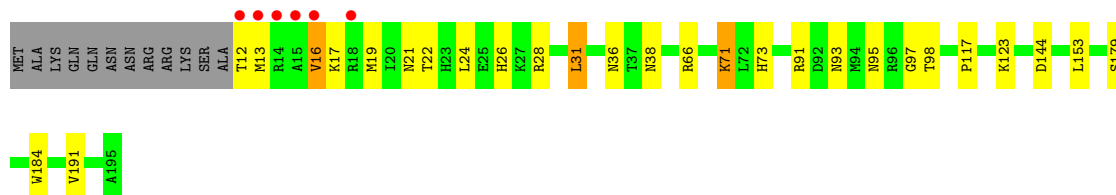
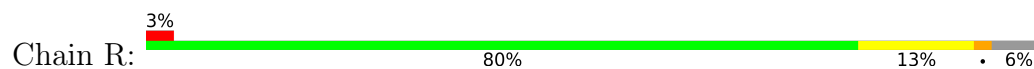
- Molecule 1: Coat protein



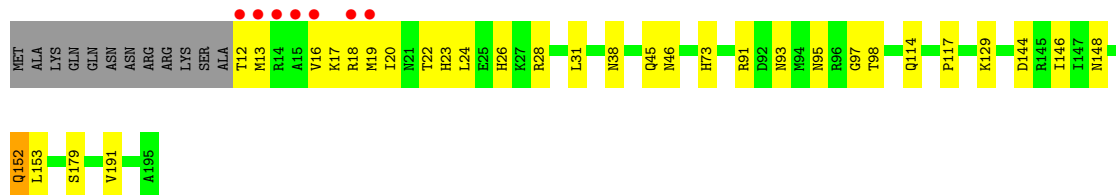
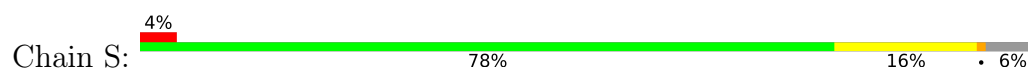
● Molecule 1: Coat protein



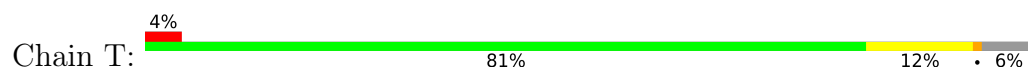
● Molecule 1: Coat protein



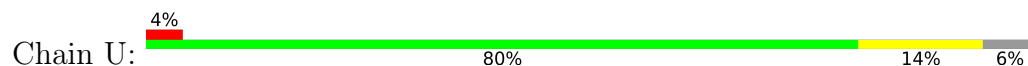
● Molecule 1: Coat protein



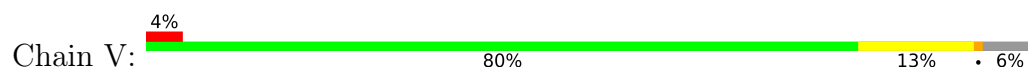
● Molecule 1: Coat protein



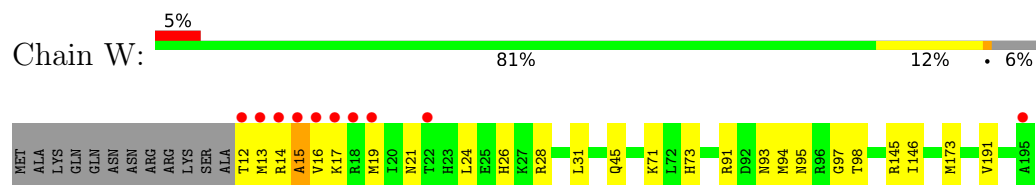
● Molecule 1: Coat protein



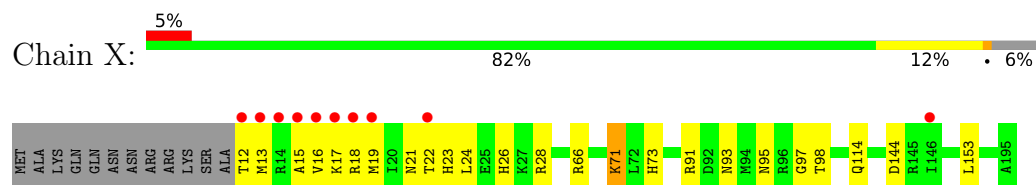
● Molecule 1: Coat protein



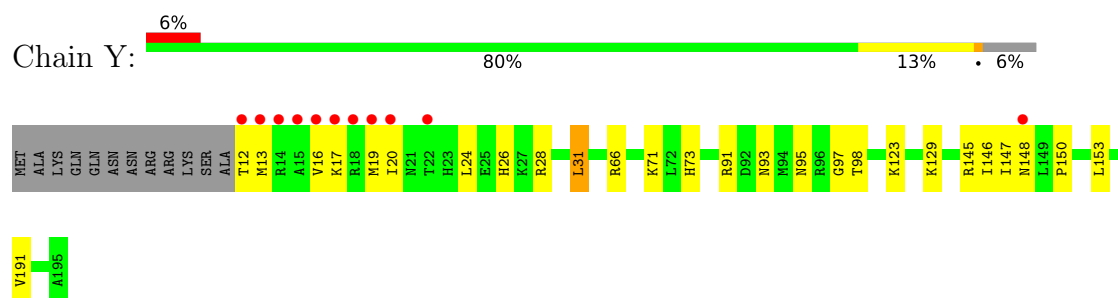
- Molecule 1: Coat protein



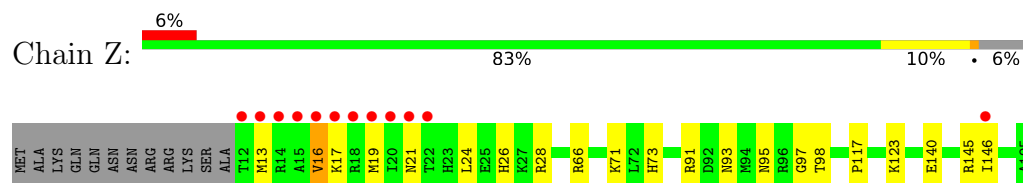
- Molecule 1: Coat protein



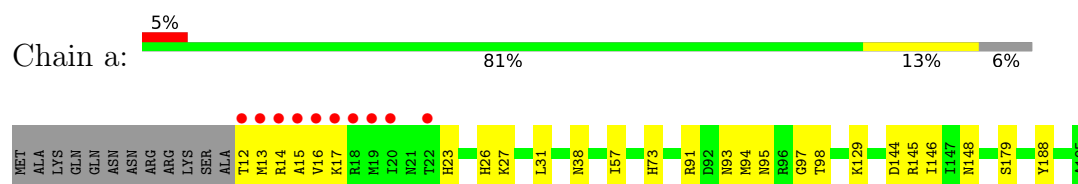
- Molecule 1: Coat protein



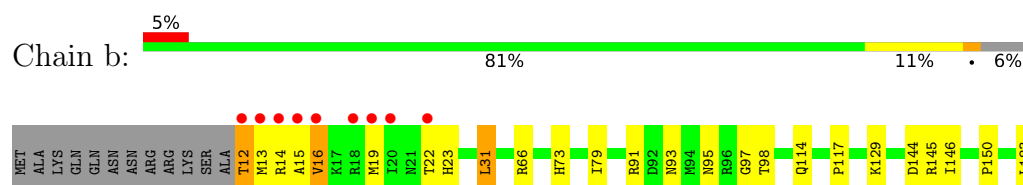
- Molecule 1: Coat protein



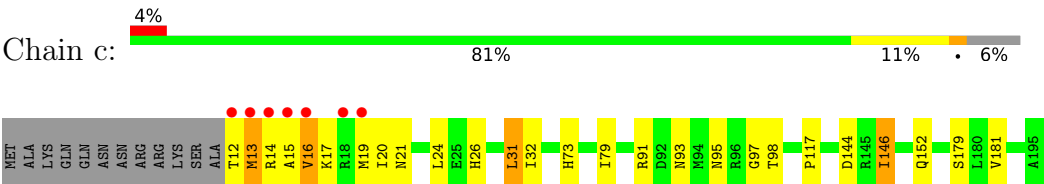
- Molecule 1: Coat protein



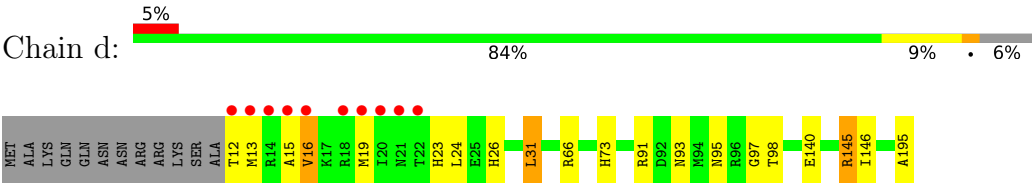
- Molecule 1: Coat protein



- Molecule 1: Coat protein



• Molecule 1: Coat protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	307.58Å 302.26Å 181.92Å 90.00° 92.77° 90.00°	Depositor
Resolution (Å)	12.00 – 1.45 12.00 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (12.00-1.45) 76.1 (12.00-1.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.175 , 0.208 0.185 , 0.209	Depositor DCC
R_{free} test set	111080 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	10.1	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 59.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l 0.009 for -k,-h,-l 0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	102135	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	0.57	0/1468	0.75	0/1988
1	1	0.57	0/1477	0.72	0/2000
1	2	0.56	0/1486	0.74	0/2012
1	3	0.55	0/1488	0.73	0/2014
1	4	0.58	0/1474	0.73	0/1997
1	5	0.55	0/1457	0.74	0/1975
1	6	0.53	0/1479	0.75	0/2002
1	7	0.57	0/1466	0.74	0/1986
1	A	0.56	0/1500	0.75	0/2032
1	B	0.55	0/1504	0.75	0/2036
1	C	0.55	0/1485	0.75	0/2011
1	D	0.57	0/1479	0.72	0/2004
1	E	0.55	0/1465	0.72	0/1985
1	F	0.54	0/1466	0.73	0/1986
1	G	0.52	0/1484	0.76	0/2010
1	H	0.54	0/1468	0.75	0/1988
1	I	0.54	0/1474	0.73	0/1997
1	J	0.56	0/1468	0.75	0/1988
1	K	0.56	0/1513	0.74	0/2048
1	L	0.53	0/1495	0.72	0/2024
1	M	0.57	0/1473	0.72	0/1996
1	N	0.53	0/1476	0.74	0/1999
1	O	0.52	0/1468	0.74	0/1988
1	P	0.55	0/1505	0.74	0/2036
1	Q	0.56	0/1465	0.75	0/1985
1	R	0.57	0/1473	0.73	0/1996
1	S	0.56	0/1505	0.71	0/2037
1	T	0.58	0/1471	0.76	0/1993
1	U	0.56	0/1485	0.73	0/2011
1	V	0.57	0/1474	0.75	0/1997
1	W	0.57	0/1457	0.74	0/1974
1	X	0.56	0/1465	0.74	0/1985

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Y	0.58	0/1476	0.74	0/1999
1	Z	0.59	0/1479	0.75	0/2002
1	a	0.55	0/1493	0.74	0/2022
1	b	0.56	0/1457	0.76	0/1974
1	c	0.58	0/1479	0.73	0/2002
1	d	0.57	0/1464	0.77	0/1984
1	e	0.57	0/1464	0.74	0/1984
1	f	0.54	0/1484	0.72	0/2010
1	g	0.55	0/1465	0.73	0/1985
1	h	0.57	0/1485	0.75	0/2012
1	i	0.55	0/1476	0.73	0/1999
1	j	0.55	0/1469	0.75	0/1990
1	k	0.58	0/1468	0.76	0/1989
1	l	0.56	0/1457	0.73	0/1974
1	m	0.55	0/1468	0.73	0/1988
1	n	0.54	0/1484	0.71	0/2010
1	o	0.57	0/1458	0.76	0/1976
1	p	0.55	0/1457	0.72	0/1974
1	q	0.57	0/1457	0.74	0/1974
1	r	0.57	0/1479	0.77	0/2002
1	s	0.57	0/1464	0.77	0/1984
1	t	0.53	0/1515	0.72	0/2050
1	u	0.56	0/1468	0.75	0/1988
1	v	0.56	0/1468	0.74	0/1988
1	w	0.60	0/1475	0.76	0/1998
1	x	0.55	0/1476	0.74	0/1999
1	y	0.58	0/1464	0.76	0/1984
1	z	0.57	0/1485	0.72	0/2011
All	All	0.56	0/88547	0.74	0/119932

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1440	0	1449	33	0
1	1	1446	0	1457	48	0
1	2	1452	0	1469	70	0
1	3	1454	0	1470	62	0
1	4	1443	0	1450	55	0
1	5	1432	0	1433	48	0
1	6	1448	0	1462	48	0
1	7	1438	0	1444	37	0
1	A	1460	0	1481	58	0
1	B	1464	0	1492	57	0
1	C	1454	0	1460	41	0
1	D	1445	0	1463	32	0
1	E	1437	0	1447	60	0
1	F	1438	0	1444	45	0
1	G	1450	0	1466	69	0
1	H	1440	0	1449	52	0
1	I	1443	0	1453	41	0
1	J	1440	0	1449	34	0
1	K	1470	0	1495	65	0
1	L	1458	0	1484	44	0
1	M	1442	0	1453	77	0
1	N	1445	0	1455	60	0
1	O	1440	0	1449	62	0
1	P	1465	0	1494	82	0
1	Q	1437	0	1442	50	0
1	R	1442	0	1458	60	0
1	S	1465	0	1487	49	0
1	T	1440	0	1452	51	0
1	U	1451	0	1463	48	0
1	V	1443	0	1453	65	0
1	W	1432	0	1436	45	0
1	X	1437	0	1447	42	0
1	Y	1445	0	1455	57	0
1	Z	1448	0	1462	43	0
1	a	1456	0	1474	36	0
1	b	1432	0	1436	53	0
1	c	1448	0	1462	50	0
1	d	1439	0	1444	37	0
1	e	1439	0	1444	57	0
1	f	1450	0	1471	44	0
1	g	1437	0	1447	34	0
1	h	1451	0	1465	49	0
1	i	1448	0	1454	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	1441	0	1448	41	0
1	k	1440	0	1446	44	0
1	l	1432	0	1436	43	0
1	m	1440	0	1449	51	0
1	n	1450	0	1466	64	0
1	o	1433	0	1435	40	0
1	p	1432	0	1436	58	0
1	q	1432	0	1436	36	0
1	r	1448	0	1462	43	0
1	s	1436	0	1445	39	0
1	t	1472	0	1502	62	0
1	u	1440	0	1449	48	0
1	v	1440	0	1449	48	0
1	w	1444	0	1458	51	0
1	x	1445	0	1455	68	0
1	y	1436	0	1445	42	0
1	z	1451	0	1468	64	0
2	0	2	0	0	0	0
2	1	3	0	0	0	0
2	2	2	0	0	0	0
2	3	2	0	0	0	0
2	4	2	0	0	0	0
2	5	2	0	0	0	0
2	6	2	0	0	0	0
2	7	1	0	0	0	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	3	0	0	0	0
2	F	1	0	0	0	0
2	G	3	0	0	1	0
2	H	1	0	0	0	0
2	I	2	0	0	0	0
2	J	1	0	0	0	0
2	K	2	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	2	0	0	1	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	2	0	0	0	0
2	S	2	0	0	0	0
2	T	2	0	0	0	0
2	U	3	0	0	0	0
2	V	2	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
2	Y	1	0	0	0	0
2	Z	1	0	0	0	0
2	a	1	0	0	0	0
2	b	2	0	0	0	0
2	c	2	0	0	0	0
2	d	1	0	0	0	0
2	e	1	0	0	0	0
2	f	1	0	0	0	0
2	g	1	0	0	0	0
2	h	1	0	0	0	0
2	i	2	0	0	0	0
2	j	2	0	0	0	0
2	k	1	0	0	0	0
2	l	1	0	0	0	0
2	m	1	0	0	0	0
2	n	2	0	0	0	0
2	o	2	0	0	0	0
2	p	1	0	0	0	0
2	q	2	0	0	0	0
2	r	1	0	0	0	0
2	s	1	0	0	0	0
2	t	1	0	0	0	0
2	u	1	0	0	0	0
2	v	1	0	0	0	0
2	w	1	0	0	0	0
2	x	1	0	0	0	0
2	y	1	0	0	0	0
2	z	1	0	0	0	0
3	0	242	0	0	6	0
3	1	256	0	0	10	0
3	2	259	0	0	8	0
3	3	245	0	0	8	0
3	4	278	0	0	16	2
3	5	247	0	0	4	0
3	6	264	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	7	249	0	0	7	0
3	A	246	0	0	14	0
3	B	235	0	0	3	0
3	C	250	0	0	7	0
3	D	255	0	0	6	0
3	E	229	0	0	8	0
3	F	217	0	0	7	0
3	G	253	0	0	9	0
3	H	248	0	0	6	0
3	I	240	0	0	9	0
3	J	245	0	0	2	0
3	K	273	0	0	7	0
3	L	239	0	0	10	0
3	M	253	0	0	7	0
3	N	256	0	0	6	0
3	O	250	0	0	18	0
3	P	250	0	0	8	0
3	Q	255	0	0	9	0
3	R	286	0	0	7	0
3	S	237	0	0	5	0
3	T	295	0	0	11	1
3	U	266	0	0	7	0
3	V	258	0	0	12	0
3	W	256	0	0	6	0
3	X	256	0	0	6	0
3	Y	262	0	0	14	0
3	Z	285	0	0	11	0
3	a	257	0	0	5	0
3	b	254	0	0	14	0
3	c	269	0	0	5	0
3	d	244	0	0	7	0
3	e	258	0	0	10	0
3	f	231	0	0	4	0
3	g	260	0	0	7	0
3	h	281	0	0	9	2
3	i	282	0	0	7	0
3	j	267	0	0	6	0
3	k	256	0	0	13	0
3	l	257	0	0	11	0
3	m	252	0	0	8	0
3	n	251	0	0	9	0
3	o	262	0	0	5	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	p	238	0	0	4	0
3	q	258	0	0	5	0
3	r	287	0	0	6	4
3	s	226	0	0	3	0
3	t	236	0	0	13	0
3	u	240	0	0	8	1
3	v	249	0	0	3	0
3	w	279	0	0	10	0
3	x	260	0	0	8	0
3	y	294	0	0	6	0
3	z	264	0	0	8	0
All	All	102135	0	87405	2577	6

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 15.

The worst 5 of 2577 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:i:19:MET:CE	1:Q:13:MET:CE	1.77	1.60
1:z:13:MET:HE3	1:S:19:MET:CE	1.32	1.56
1:G:19:MET:HE3	1:M:13:MET:CE	1.13	1.56
1:z:19:MET:HE1	1:Y:17:LYS:CB	1.32	1.56
1:G:19:MET:CE	1:M:13:MET:HE3	1.09	1.51

The worst 5 of 6 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)
3:r:405:HOH:O	3:4:419:HOH:O[4_545]	1.23	0.97
3:h:501:HOH:O	3:r:544:HOH:O[4_555]	1.60	0.60
3:h:442:HOH:O	3:r:544:HOH:O[4_555]	1.78	0.42
3:T:434:HOH:O	3:T:585:HOH:O[2_655]	1.94	0.26
3:o:317:HOH:O	3:u:479:HOH:O[2_555]	1.99	0.21

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	1	185/196 (94%)	178 (96%)	7 (4%)	0	100	100
1	2	186/196 (95%)	180 (97%)	6 (3%)	0	100	100
1	3	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
1	4	185/196 (94%)	179 (97%)	6 (3%)	0	100	100
1	5	183/196 (93%)	179 (98%)	4 (2%)	0	100	100
1	6	185/196 (94%)	180 (97%)	5 (3%)	0	100	100
1	7	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	A	188/196 (96%)	183 (97%)	5 (3%)	0	100	100
1	B	188/196 (96%)	183 (97%)	5 (3%)	0	100	100
1	C	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
1	D	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
1	E	184/196 (94%)	176 (96%)	8 (4%)	0	100	100
1	F	184/196 (94%)	176 (96%)	8 (4%)	0	100	100
1	G	186/196 (95%)	178 (96%)	7 (4%)	1 (0%)	24	7
1	H	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	I	185/196 (94%)	180 (97%)	5 (3%)	0	100	100
1	J	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	K	189/196 (96%)	184 (97%)	4 (2%)	1 (0%)	24	7
1	L	187/196 (95%)	182 (97%)	5 (3%)	0	100	100
1	M	185/196 (94%)	178 (96%)	7 (4%)	0	100	100
1	N	185/196 (94%)	180 (97%)	5 (3%)	0	100	100
1	O	184/196 (94%)	180 (98%)	4 (2%)	0	100	100
1	P	188/196 (96%)	182 (97%)	6 (3%)	0	100	100
1	Q	184/196 (94%)	179 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	185/196 (94%)	179 (97%)	6 (3%)	0	100	100
1	S	188/196 (96%)	182 (97%)	6 (3%)	0	100	100
1	T	185/196 (94%)	179 (97%)	6 (3%)	0	100	100
1	U	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
1	V	185/196 (94%)	180 (97%)	5 (3%)	0	100	100
1	W	183/196 (93%)	176 (96%)	6 (3%)	1 (0%)	24	7
1	X	184/196 (94%)	180 (98%)	4 (2%)	0	100	100
1	Y	185/196 (94%)	180 (97%)	5 (3%)	0	100	100
1	Z	185/196 (94%)	179 (97%)	6 (3%)	0	100	100
1	a	187/196 (95%)	182 (97%)	5 (3%)	0	100	100
1	b	183/196 (93%)	179 (98%)	4 (2%)	0	100	100
1	c	185/196 (94%)	179 (97%)	5 (3%)	1 (0%)	24	7
1	d	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	e	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	f	186/196 (95%)	178 (96%)	8 (4%)	0	100	100
1	g	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	h	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
1	i	185/196 (94%)	179 (97%)	5 (3%)	1 (0%)	24	7
1	j	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	k	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	l	183/196 (93%)	178 (97%)	5 (3%)	0	100	100
1	m	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	n	186/196 (95%)	180 (97%)	6 (3%)	0	100	100
1	o	183/196 (93%)	178 (97%)	5 (3%)	0	100	100
1	p	183/196 (93%)	178 (97%)	5 (3%)	0	100	100
1	q	183/196 (93%)	178 (97%)	5 (3%)	0	100	100
1	r	185/196 (94%)	179 (97%)	6 (3%)	0	100	100
1	s	184/196 (94%)	177 (96%)	7 (4%)	0	100	100
1	t	189/196 (96%)	183 (97%)	6 (3%)	0	100	100
1	u	184/196 (94%)	180 (98%)	4 (2%)	0	100	100
1	v	184/196 (94%)	179 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	185/196 (94%)	181 (98%)	4 (2%)	0	100	100
1	x	185/196 (94%)	178 (96%)	7 (4%)	0	100	100
1	y	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	z	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
All	All	11101/11760 (94%)	10766 (97%)	330 (3%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	W	15	ALA
1	G	14	ARG
1	K	13	MET
1	i	14	ARG
1	c	13	MET

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	159/167 (95%)	158 (99%)	1 (1%)	78	58
1	1	160/167 (96%)	157 (98%)	3 (2%)	50	17
1	2	161/167 (96%)	159 (99%)	2 (1%)	63	33
1	3	161/167 (96%)	159 (99%)	2 (1%)	63	33
1	4	160/167 (96%)	158 (99%)	2 (1%)	61	31
1	5	158/167 (95%)	157 (99%)	1 (1%)	78	58
1	6	160/167 (96%)	159 (99%)	1 (1%)	78	58
1	7	159/167 (95%)	158 (99%)	1 (1%)	78	58
1	A	163/167 (98%)	159 (98%)	4 (2%)	42	11
1	B	163/167 (98%)	160 (98%)	3 (2%)	51	19
1	C	161/167 (96%)	156 (97%)	5 (3%)	35	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	161/167 (96%)	154 (96%)	7 (4%)	26	3
1	E	159/167 (95%)	154 (97%)	5 (3%)	35	7
1	F	159/167 (95%)	159 (100%)	0	100	100
1	G	161/167 (96%)	160 (99%)	1 (1%)	78	58
1	H	159/167 (95%)	155 (98%)	4 (2%)	42	11
1	I	160/167 (96%)	159 (99%)	1 (1%)	78	58
1	J	159/167 (95%)	155 (98%)	4 (2%)	42	11
1	K	164/167 (98%)	163 (99%)	1 (1%)	78	58
1	L	162/167 (97%)	159 (98%)	3 (2%)	50	17
1	M	160/167 (96%)	158 (99%)	2 (1%)	61	31
1	N	160/167 (96%)	159 (99%)	1 (1%)	78	58
1	O	159/167 (95%)	157 (99%)	2 (1%)	61	31
1	P	163/167 (98%)	162 (99%)	1 (1%)	78	58
1	Q	159/167 (95%)	156 (98%)	3 (2%)	50	17
1	R	160/167 (96%)	156 (98%)	4 (2%)	42	11
1	S	163/167 (98%)	161 (99%)	2 (1%)	63	33
1	T	160/167 (96%)	157 (98%)	3 (2%)	50	17
1	U	161/167 (96%)	161 (100%)	0	100	100
1	V	160/167 (96%)	159 (99%)	1 (1%)	78	58
1	W	158/167 (95%)	158 (100%)	0	100	100
1	X	159/167 (95%)	158 (99%)	1 (1%)	78	58
1	Y	160/167 (96%)	159 (99%)	1 (1%)	78	58
1	Z	160/167 (96%)	159 (99%)	1 (1%)	78	58
1	a	162/167 (97%)	162 (100%)	0	100	100
1	b	158/167 (95%)	154 (98%)	4 (2%)	42	11
1	c	160/167 (96%)	157 (98%)	3 (2%)	50	17
1	d	159/167 (95%)	156 (98%)	3 (2%)	50	17
1	e	159/167 (95%)	157 (99%)	2 (1%)	61	31
1	f	161/167 (96%)	159 (99%)	2 (1%)	63	33
1	g	159/167 (95%)	159 (100%)	0	100	100
1	h	161/167 (96%)	160 (99%)	1 (1%)	78	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	i	160/167 (96%)	160 (100%)	0	100	100
1	j	159/167 (95%)	159 (100%)	0	100	100
1	k	159/167 (95%)	157 (99%)	2 (1%)	61	31
1	l	158/167 (95%)	156 (99%)	2 (1%)	61	31
1	m	159/167 (95%)	157 (99%)	2 (1%)	61	31
1	n	161/167 (96%)	159 (99%)	2 (1%)	63	33
1	o	158/167 (95%)	156 (99%)	2 (1%)	61	31
1	p	158/167 (95%)	154 (98%)	4 (2%)	42	11
1	q	158/167 (95%)	155 (98%)	3 (2%)	50	17
1	r	160/167 (96%)	157 (98%)	3 (2%)	50	17
1	s	159/167 (95%)	155 (98%)	4 (2%)	42	11
1	t	164/167 (98%)	162 (99%)	2 (1%)	63	33
1	u	159/167 (95%)	157 (99%)	2 (1%)	61	31
1	v	159/167 (95%)	155 (98%)	4 (2%)	42	11
1	w	160/167 (96%)	160 (100%)	0	100	100
1	x	160/167 (96%)	159 (99%)	1 (1%)	78	58
1	y	159/167 (95%)	158 (99%)	1 (1%)	78	58
1	z	161/167 (96%)	158 (98%)	3 (2%)	50	17
All	All	9601/10020 (96%)	9476 (99%)	125 (1%)	63	31

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	T	71	LYS
1	D	34[B]	SER
1	T	31[B]	LEU
1	b	66	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 587 such sidechains are listed below:

Mol	Chain	Res	Type
1	R	95	ASN
1	c	95	ASN
1	S	148	ASN

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Mol	Chain	Res	Type
1	R	93	ASN
1	X	73	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 92 ligands modelled in this entry, 92 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	184/196 (93%)	-0.21	11 (5%)	27 27	5, 10, 27, 62	2 (1%)
1	1	184/196 (93%)	-0.15	10 (5%)	31 31	6, 10, 26, 63	3 (1%)
1	2	184/196 (93%)	-0.22	11 (5%)	27 27	6, 10, 21, 61	4 (2%)
1	3	184/196 (93%)	-0.17	9 (4%)	35 36	6, 11, 29, 61	4 (2%)
1	4	184/196 (93%)	-0.24	8 (4%)	40 42	6, 10, 25, 58	3 (1%)
1	5	184/196 (93%)	-0.19	8 (4%)	40 42	9, 11, 29, 64	1 (0%)
1	6	184/196 (93%)	-0.15	11 (5%)	27 27	7, 11, 29, 64	3 (1%)
1	7	184/196 (93%)	-0.13	9 (4%)	35 36	7, 11, 28, 61	2 (1%)
1	A	184/196 (93%)	-0.16	11 (5%)	27 27	6, 10, 29, 63	6 (3%)
1	B	184/196 (93%)	-0.13	11 (5%)	27 27	6, 11, 29, 62	6 (3%)
1	C	184/196 (93%)	-0.12	9 (4%)	35 36	7, 12, 28, 61	4 (2%)
1	D	184/196 (93%)	-0.22	9 (4%)	35 36	6, 10, 27, 64	4 (2%)
1	E	184/196 (93%)	-0.07	9 (4%)	35 36	7, 12, 27, 63	2 (1%)
1	F	184/196 (93%)	-0.13	8 (4%)	40 42	7, 12, 28, 63	2 (1%)
1	G	184/196 (93%)	-0.06	11 (5%)	27 27	6, 12, 29, 62	4 (2%)
1	H	184/196 (93%)	-0.13	9 (4%)	35 36	6, 11, 29, 64	2 (1%)
1	I	184/196 (93%)	-0.15	10 (5%)	31 31	7, 11, 29, 62	3 (1%)
1	J	184/196 (93%)	-0.13	9 (4%)	35 36	7, 11, 27, 60	2 (1%)
1	K	184/196 (93%)	-0.26	9 (4%)	35 36	5, 9, 27, 61	7 (3%)
1	L	184/196 (93%)	-0.19	9 (4%)	35 36	6, 10, 28, 62	5 (2%)
1	M	184/196 (93%)	-0.12	10 (5%)	31 31	6, 11, 28, 64	3 (1%)
1	N	184/196 (93%)	-0.02	9 (4%)	35 36	6, 12, 29, 63	3 (1%)
1	O	184/196 (93%)	-0.12	8 (4%)	40 42	7, 11, 29, 62	2 (1%)
1	P	184/196 (93%)	-0.14	9 (4%)	35 36	5, 11, 28, 62	6 (3%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Q	184/196 (93%)	-0.10	10 (5%) 31 31	7, 11, 28, 62	2 (1%)
1	R	184/196 (93%)	-0.21	6 (3%) 49 52	6, 10, 27, 61	3 (1%)
1	S	184/196 (93%)	-0.19	7 (3%) 44 47	6, 10, 27, 62	6 (3%)
1	T	184/196 (93%)	-0.30	7 (3%) 44 47	6, 9, 27, 63	3 (1%)
1	U	184/196 (93%)	-0.24	8 (4%) 40 42	5, 9, 27, 64	4 (2%)
1	V	184/196 (93%)	-0.26	7 (3%) 44 47	6, 10, 26, 59	3 (1%)
1	W	184/196 (93%)	-0.07	10 (5%) 31 31	6, 11, 29, 65	1 (0%)
1	X	184/196 (93%)	-0.19	10 (5%) 31 31	6, 10, 28, 60	2 (1%)
1	Y	184/196 (93%)	-0.24	11 (5%) 27 27	6, 10, 28, 61	3 (1%)
1	Z	184/196 (93%)	-0.27	12 (6%) 25 24	5, 9, 28, 64	3 (1%)
1	a	184/196 (93%)	-0.18	10 (5%) 31 31	7, 11, 28, 59	5 (2%)
1	b	184/196 (93%)	-0.19	10 (5%) 31 31	6, 10, 27, 58	1 (0%)
1	c	184/196 (93%)	-0.21	7 (3%) 44 47	5, 10, 27, 64	3 (1%)
1	d	184/196 (93%)	-0.26	10 (5%) 31 31	5, 9, 27, 62	2 (1%)
1	e	184/196 (93%)	-0.12	11 (5%) 27 27	6, 10, 27, 63	2 (1%)
1	f	184/196 (93%)	-0.12	9 (4%) 35 36	7, 12, 29, 60	4 (2%)
1	g	184/196 (93%)	-0.12	11 (5%) 27 27	7, 11, 28, 63	2 (1%)
1	h	184/196 (93%)	-0.16	8 (4%) 40 42	5, 10, 25, 61	4 (2%)
1	i	184/196 (93%)	-0.15	9 (4%) 35 36	5, 10, 28, 60	3 (1%)
1	j	184/196 (93%)	-0.14	9 (4%) 35 36	7, 11, 26, 62	2 (1%)
1	k	184/196 (93%)	-0.21	8 (4%) 40 42	7, 10, 27, 61	2 (1%)
1	l	184/196 (93%)	-0.19	11 (5%) 27 27	7, 10, 27, 61	1 (0%)
1	m	184/196 (93%)	-0.06	11 (5%) 27 27	7, 12, 29, 64	2 (1%)
1	n	184/196 (93%)	0.02	10 (5%) 31 31	7, 12, 30, 63	4 (2%)
1	o	184/196 (93%)	-0.19	11 (5%) 27 27	7, 11, 29, 64	1 (0%)
1	p	184/196 (93%)	-0.16	7 (3%) 44 47	6, 11, 26, 61	1 (0%)
1	q	184/196 (93%)	-0.22	11 (5%) 27 27	6, 10, 26, 61	1 (0%)
1	r	184/196 (93%)	-0.22	10 (5%) 31 31	6, 9, 27, 62	3 (1%)
1	s	184/196 (93%)	-0.14	8 (4%) 40 42	6, 11, 28, 61	2 (1%)
1	t	184/196 (93%)	-0.15	10 (5%) 31 31	6, 11, 29, 61	7 (3%)
1	u	184/196 (93%)	-0.17	9 (4%) 35 36	6, 10, 29, 60	2 (1%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	v	184/196 (93%)	-0.19	10 (5%) 31 31	6, 10, 27, 61	2 (1%)
1	w	184/196 (93%)	-0.24	8 (4%) 40 42	5, 9, 25, 60	3 (1%)
1	x	184/196 (93%)	-0.24	11 (5%) 27 27	5, 10, 27, 62	3 (1%)
1	y	184/196 (93%)	-0.20	11 (5%) 27 27	6, 9, 26, 58	2 (1%)
1	z	184/196 (93%)	-0.13	9 (4%) 35 36	6, 11, 27, 61	4 (2%)
All	All	11040/11760 (93%)	-0.17	564 (5%) 33 34	5, 11, 34, 65	181 (1%)

The worst 5 of 564 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	h	12	THR	7.7
1	e	12	THR	7.5
1	7	16	VAL	7.0
1	A	12	THR	6.9
1	S	12	THR	6.8

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	N	202	1/1	0.97	0.05	10,10,10,10	0
2	CA	E	202	1/1	0.98	0.04	9,9,9,9	0
2	CA	N	201	1/1	0.98	0.03	11,11,11,11	0
2	CA	A	202	1/1	0.98	0.06	9,9,9,9	0
2	CA	n	202	1/1	0.99	0.03	11,11,11,11	0
2	CA	q	202	1/1	0.99	0.03	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	x	201	1/1	0.99	0.01	8,8,8,8	0
2	CA	z	201	1/1	0.99	0.02	9,9,9,9	0
2	CA	0	201	1/1	0.99	0.04	8,8,8,8	0
2	CA	0	202	1/1	0.99	0.02	8,8,8,8	0
2	CA	1	202	1/1	0.99	0.05	8,8,8,8	0
2	CA	2	202	1/1	0.99	0.02	9,9,9,9	0
2	CA	3	202	1/1	0.99	0.04	9,9,9,9	0
2	CA	4	202	1/1	0.99	0.04	8,8,8,8	0
2	CA	5	201	1/1	0.99	0.02	10,10,10,10	0
2	CA	5	202	1/1	0.99	0.04	9,9,9,9	0
2	CA	6	202	1/1	0.99	0.06	9,9,9,9	0
2	CA	g	201	1/1	0.99	0.02	8,8,8,8	0
2	CA	B	203	1/1	0.99	0.07	9,9,9,9	0
2	CA	i	201	1/1	0.99	0.01	8,8,8,8	0
2	CA	E	203	1/1	0.99	0.03	11,11,11,11	0
2	CA	G	201	1/1	0.99	0.02	10,10,10,10	0
2	CA	G	202	1/1	0.99	0.04	12,12,12,12	0
2	CA	G	203	1/1	0.99	0.04	9,9,9,9	0
2	CA	I	201	1/1	0.99	0.06	10,10,10,10	0
2	CA	K	201	1/1	0.99	0.02	9,9,9,9	0
2	CA	M	201	1/1	0.99	0.02	9,9,9,9	0
2	CA	i	202	1/1	0.99	0.02	11,11,11,11	0
2	CA	m	201	1/1	0.99	0.02	11,11,11,11	0
2	CA	P	201	1/1	0.99	0.03	10,10,10,10	0
2	CA	Q	202	1/1	0.99	0.04	8,8,8,8	0
2	CA	R	201	1/1	0.99	0.03	8,8,8,8	0
2	CA	S	201	1/1	0.99	0.01	9,9,9,9	0
2	CA	S	202	1/1	0.99	0.07	8,8,8,8	0
2	CA	T	202	1/1	0.99	0.06	7,7,7,7	0
2	CA	U	203	1/1	0.99	0.07	8,8,8,8	0
2	CA	V	201	1/1	0.99	0.03	6,6,6,6	0
2	CA	W	201	1/1	0.99	0.02	10,10,10,10	0
2	CA	Z	201	1/1	0.99	0.02	8,8,8,8	0
2	CA	b	201	1/1	0.99	0.02	9,9,9,9	0
2	CA	b	202	1/1	0.99	0.04	8,8,8,8	0
2	CA	q	201	1/1	1.00	0.01	7,7,7,7	0
2	CA	7	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	A	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	e	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	B	201	1/1	1.00	0.01	10,10,10,10	0
2	CA	B	202	1/1	1.00	0.03	10,10,10,10	0
2	CA	r	201	1/1	1.00	0.01	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	C	201	1/1	1.00	0.02	10,10,10,10	0
2	CA	D	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	E	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	s	201	1/1	1.00	0.02	8,8,8,8	0
2	CA	t	201	1/1	1.00	0.01	10,10,10,10	0
2	CA	F	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	u	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	v	201	1/1	1.00	0.01	8,8,8,8	0
2	CA	w	201	1/1	1.00	0.01	8,8,8,8	0
2	CA	H	201	1/1	1.00	0.01	10,10,10,10	0
2	CA	j	201	1/1	1.00	0.01	8,8,8,8	0
2	CA	I	202	1/1	1.00	0.01	10,10,10,10	0
2	CA	J	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	y	201	1/1	1.00	0.01	8,8,8,8	0
2	CA	K	202	1/1	1.00	0.01	9,9,9,9	0
2	CA	L	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	j	202	1/1	1.00	0.05	8,8,8,8	0
2	CA	k	201	1/1	1.00	0.01	8,8,8,8	0
2	CA	l	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	O	201	1/1	1.00	0.01	10,10,10,10	0
2	CA	1	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	Q	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	h	201	1/1	1.00	0.01	8,8,8,8	0
2	CA	1	203	1/1	1.00	0.03	10,10,10,10	0
2	CA	R	202	1/1	1.00	0.01	8,8,8,8	0
2	CA	2	201	1/1	1.00	0.04	10,10,10,10	0
2	CA	n	201	1/1	1.00	0.03	11,11,11,11	0
2	CA	T	201	1/1	1.00	0.01	8,8,8,8	0
2	CA	3	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	U	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	U	202	1/1	1.00	0.01	8,8,8,8	0
2	CA	f	201	1/1	1.00	0.01	10,10,10,10	0
2	CA	4	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	V	202	1/1	1.00	0.01	8,8,8,8	0
2	CA	o	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	X	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	Y	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	o	202	1/1	1.00	0.03	12,12,12,12	0
2	CA	a	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	p	201	1/1	1.00	0.01	9,9,9,9	0
2	CA	6	201	1/1	1.00	0.02	9,9,9,9	0
2	CA	c	201	1/1	1.00	0.01	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	c	202	1/1	1.00	0.02	10,10,10,10	0
2	CA	d	201	1/1	1.00	0.02	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.