



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 05:37 PM UTC

PDB ID : 4NIA / pdb_00004nia
Title : Satellite Tobacco Mosaic Virus Refined at room temperature to 1.8 Å Resolution using NCS Restraints
Authors : Larson, S.B.; Day, J.S.; McPherson, A.
Deposited on : 2013-11-05
Resolution : 1.82 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

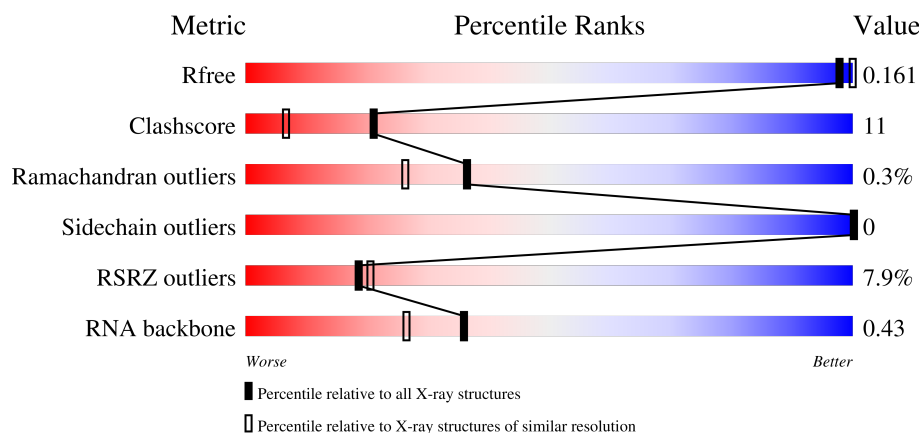
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)
RNA backbone	3983	1006 (2.22-1.42)

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	A	159	82% 9% 9%
1	B	159	86% 5% 9%
1	C	159	82% 8% 9%
1	D	159	75% 15% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	159	% 81% 10% 9%
1	F	159	% 81% 10% 9%
1	G	159	% 84% 6% 9%
1	H	159	% 84% 7% 9%
1	I	159	% 85% 6% 9%
1	J	159	% 79% 11% 9%
1	K	159	% 81% 10% 9%
1	L	159	2% 82% 9% 9%
1	M	159	% 84% 6% 9%
1	N	159	% 85% 6% 9%
1	O	159	3% 84% 7% 9%
2	P	10	40% 30% 60% 10%
2	Q	10	40% 20% 70% 10%
2	R	10	50% 20% 60% 20%
2	S	10	40% 30% 60% 10%
2	T	10	40% 30% 50% 20%
2	U	10	60% 10% 70% 20%
2	V	10	40% 70% 20% 10%
2	W	10	40% 30% 60% 10%
2	X	10	50% 20% 50% 30%
2	Y	10	40% 30% 50% 20%
2	Z	10	50% 30% 40% 30%
2	a	10	40% 60% 30% 10%
2	b	10	40% 30% 60% 10%
2	c	10	40% 40% 50% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	d	10	
3	e	10	
3	f	10	
3	g	10	
3	h	10	
3	i	10	
3	j	10	
3	k	10	
3	l	10	
3	m	10	
3	n	10	
3	o	10	
3	p	10	
3	q	10	
3	r	10	
3	s	10	
4	1	2	
4	2	2	
4	3	2	
4	4	2	
4	5	2	
4	6	2	
4	7	2	
4	8	2	
4	t	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	u	2	100% 50% 50%
4	v	2	100% 50% 50%
4	w	2	100% 50% 50%
4	x	2	100% 50% 50%
4	y	2	100% 50% 50%
4	z	2	100% 50% 50%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 28403 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	144	Total	C	N	O	S	0	19	0
			1224	778	212	226	8			
1	B	144	Total	C	N	O	S	0	17	0
			1201	761	209	222	9			
1	C	144	Total	C	N	O	S	0	19	0
			1226	779	213	225	9			
1	D	144	Total	C	N	O	S	0	22	0
			1244	793	215	228	8			
1	E	144	Total	C	N	O	S	0	19	0
			1215	770	211	226	8			
1	F	144	Total	C	N	O	S	0	19	0
			1225	775	214	228	8			
1	G	144	Total	C	N	O	S	0	18	0
			1208	764	212	224	8			
1	H	144	Total	C	N	O	S	0	20	0
			1222	775	213	225	9			
1	I	144	Total	C	N	O	S	0	16	0
			1196	754	208	225	9			
1	J	144	Total	C	N	O	S	0	19	0
			1216	773	209	225	9			
1	K	144	Total	C	N	O	S	0	20	0
			1221	772	213	227	9			
1	L	144	Total	C	N	O	S	0	18	0
			1206	762	210	225	9			
1	M	144	Total	C	N	O	S	0	15	0
			1186	751	207	220	8			
1	N	144	Total	C	N	O	S	0	19	0
			1220	774	213	224	9			
1	O	144	Total	C	N	O	S	0	20	0
			1221	776	212	224	9			

- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	Q	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	R	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	S	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	T	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	U	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	V	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	W	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	X	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	Y	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	Z	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	a	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	b	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	c	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	d	10	Total 221	C 100	N 50	O 61	P 10	0	10	0

- Molecule 3 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	e	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	f	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	g	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	h	10	Total 201	C 90	N 20	O 81	P 10	0	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	i	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	j	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	k	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	l	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	m	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	n	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	o	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	p	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	q	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	r	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	s	10	Total 201	C 90	N 20	O 81	P 10	0	10	0

- Molecule 4 is a RNA chain called RNA (5'-R(P*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	t	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
4	u	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
4	v	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
4	w	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
4	x	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
4	y	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
4	z	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
4	1	2	Total 26	C 10	N 2	O 12	P 2	0	2	0

Continued on next page...

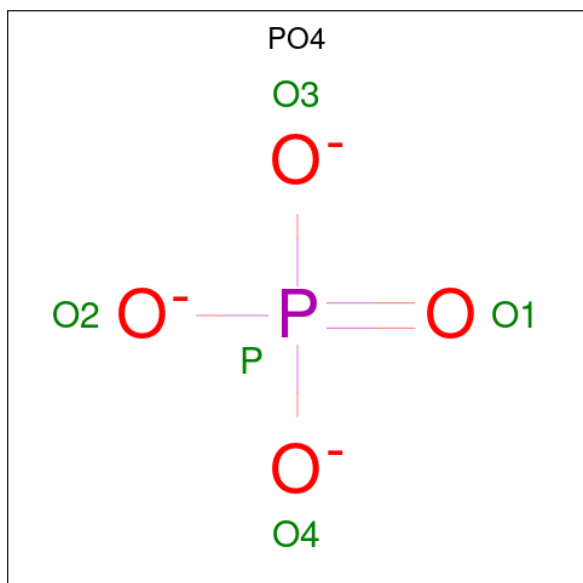
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	2	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	3	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	4	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	5	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	6	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	7	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	8	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

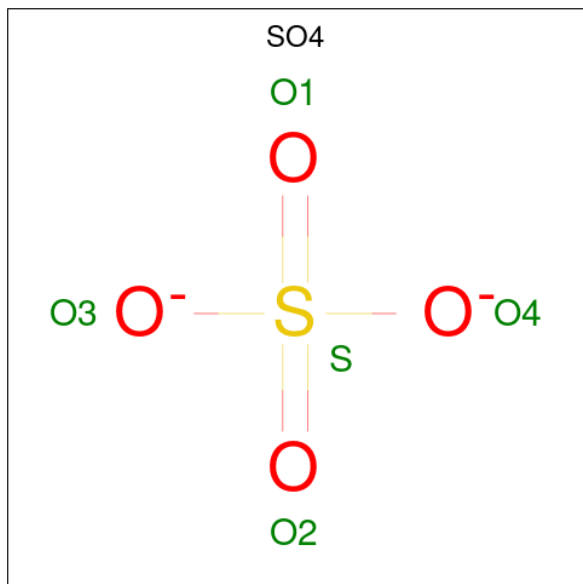
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		
5	K	1	Total	Mg	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	P	0	1
			21	20	1		
6	H	1	Total	O	P	0	1
			21	20	1		
6	K	1	Total	O	P	0	1
			21	20	1		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	224	Total	O	0	33
			224	224		
8	P	8	Total	O	0	0
			8	8		
8	e	9	Total	O	0	1
			9	9		
8	t	1	Total	O	0	0
			1	1		
8	B	205	Total	O	0	36
			205	205		
8	Q	11	Total	O	0	2
			11	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	f	2	Total O 2 2	0	0
8	C	204	Total O 204 204	0	29
8	R	13	Total O 13 13	0	1
8	g	3	Total O 3 3	0	0
8	v	1	Total O 1 1	0	0
8	D	203	Total O 203 203	0	42
8	S	12	Total O 12 12	0	1
8	h	5	Total O 5 5	0	0
8	E	201	Total O 201 201	0	31
8	T	5	Total O 5 5	0	0
8	i	9	Total O 9 9	0	0
8	F	209	Total O 209 209	0	37
8	U	9	Total O 9 9	0	1
8	j	9	Total O 9 9	0	1
8	G	205	Total O 205 205	0	29
8	V	16	Total O 16 16	0	0
8	k	5	Total O 5 5	0	2
8	H	215	Total O 215 215	0	33
8	W	12	Total O 12 12	0	2
8	l	3	Total O 3 3	0	1
8	1	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	I	213	Total O 213 213	0	35
8	X	14	Total O 14 14	0	2
8	m	5	Total O 5 5	0	0
8	J	212	Total O 212 212	0	28
8	Y	8	Total O 8 8	0	1
8	n	5	Total O 5 5	0	0
8	3	1	Total O 1 1	0	0
8	K	192	Total O 192 192	0	36
8	Z	11	Total O 11 11	0	1
8	o	10	Total O 10 10	0	1
8	L	226	Total O 226 226	0	40
8	a	11	Total O 11 11	0	0
8	p	8	Total O 8 8	0	2
8	M	203	Total O 203 203	0	24
8	b	11	Total O 11 11	0	0
8	q	2	Total O 2 2	0	1
8	N	206	Total O 206 206	0	28
8	c	10	Total O 10 10	0	0
8	r	6	Total O 6 6	0	1
8	O	209	Total O 209 209	0	38
8	d	6	Total O 6 6	0	2

Continued on next page...

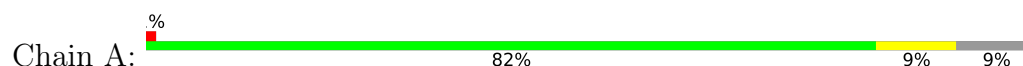
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	s	11	Total 11	O 11	0	1
8	8	1	Total 1	O 1	0	0

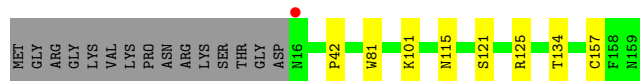
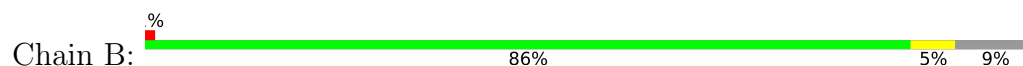
3 Residue-property plots [i](#)

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

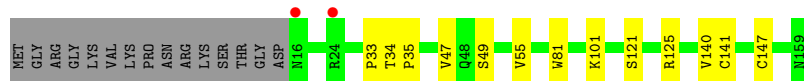
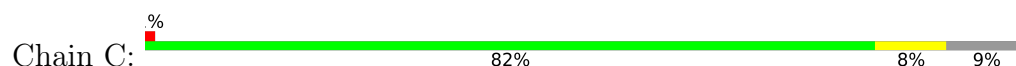
- Molecule 1: Coat protein



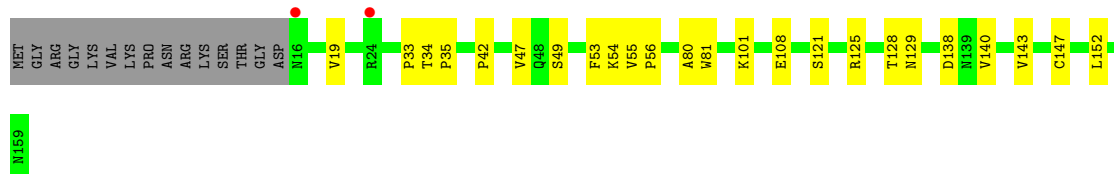
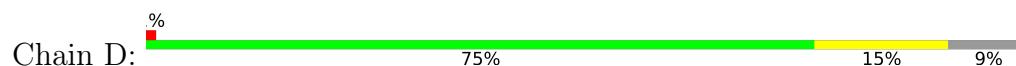
- Molecule 1: Coat protein



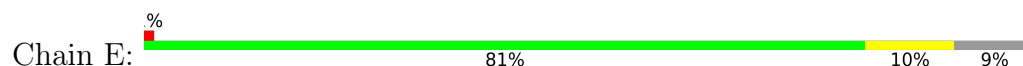
- Molecule 1: Coat protein



- Molecule 1: Coat protein

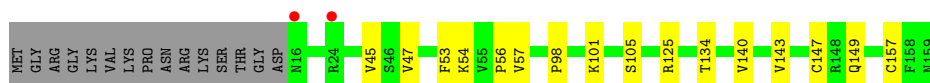
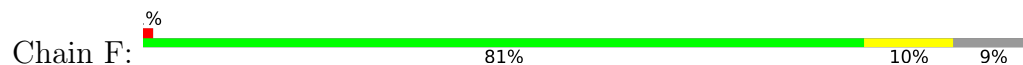


- Molecule 1: Coat protein

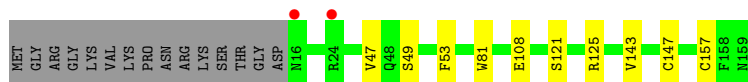
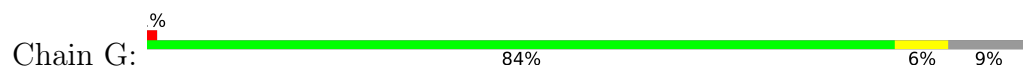




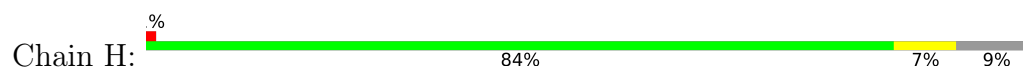
- Molecule 1: Coat protein



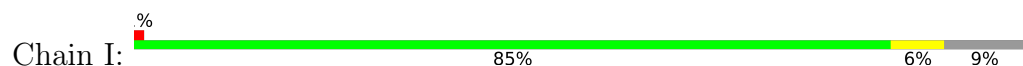
- Molecule 1: Coat protein



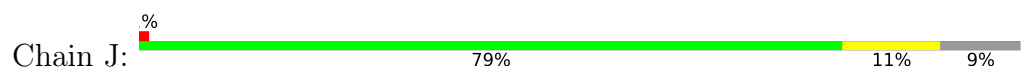
- Molecule 1: Coat protein



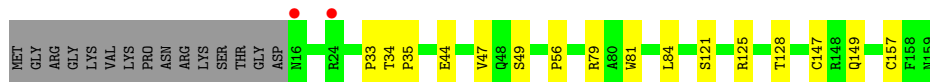
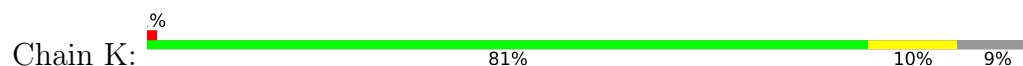
- Molecule 1: Coat protein



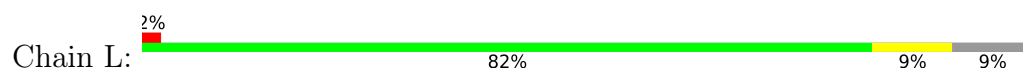
- Molecule 1: Coat protein



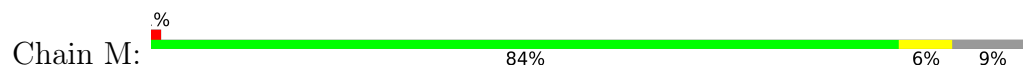
- Molecule 1: Coat protein



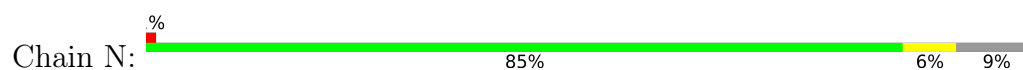
- Molecule 1: Coat protein



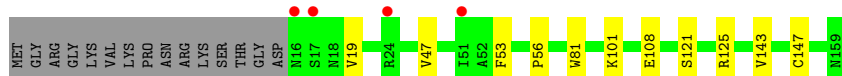
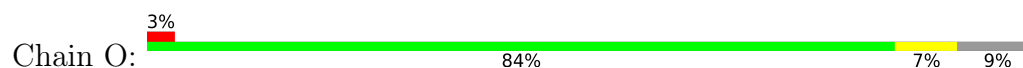
- Molecule 1: Coat protein



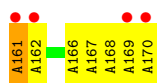
- Molecule 1: Coat protein



- Molecule 1: Coat protein



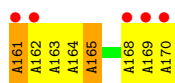
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



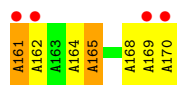
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



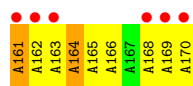
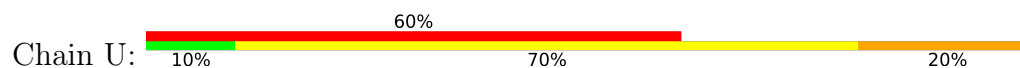
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



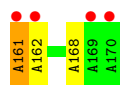
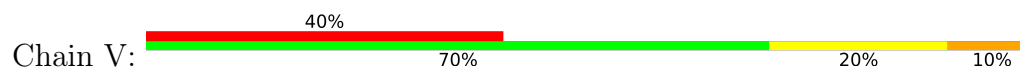
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



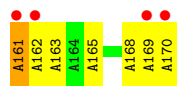
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



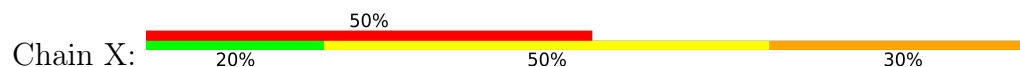
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

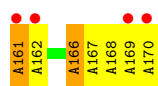


- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

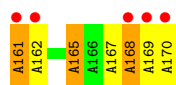


- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

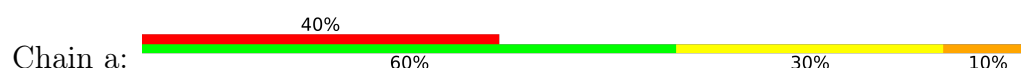




- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



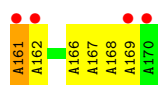
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



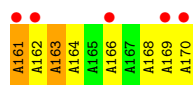
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



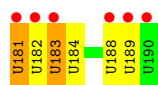
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



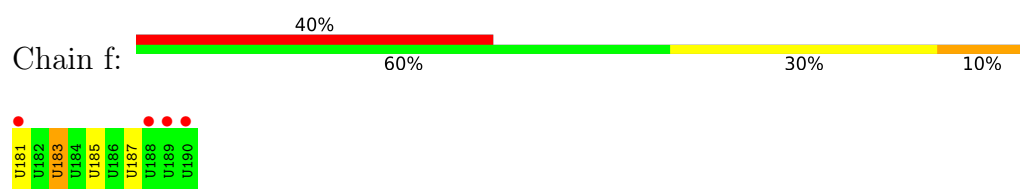
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



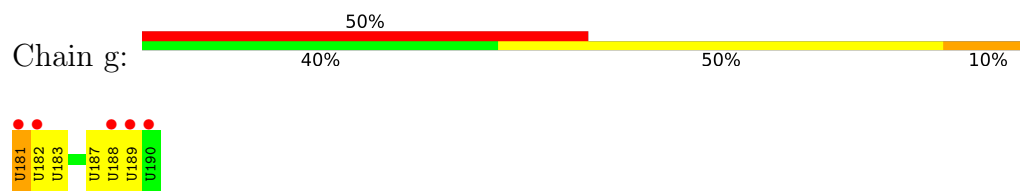
- Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



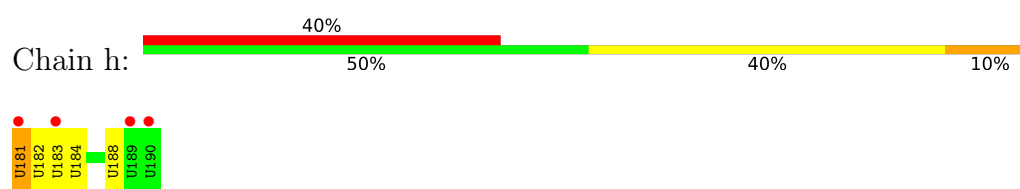
- Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



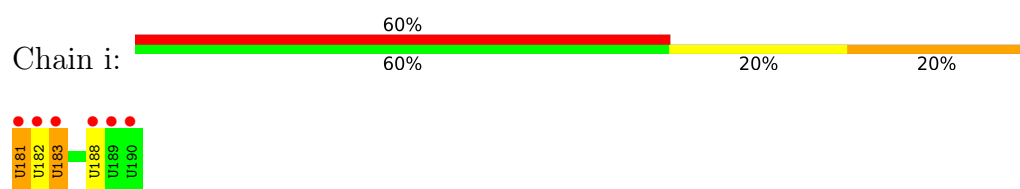
- Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



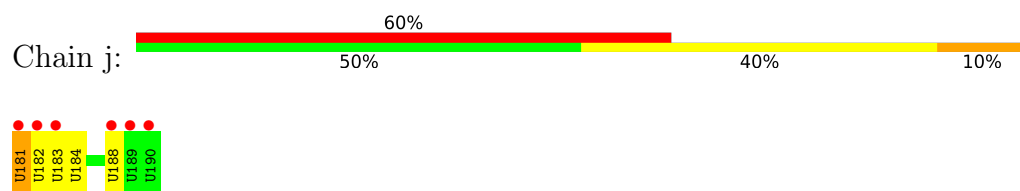
- Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



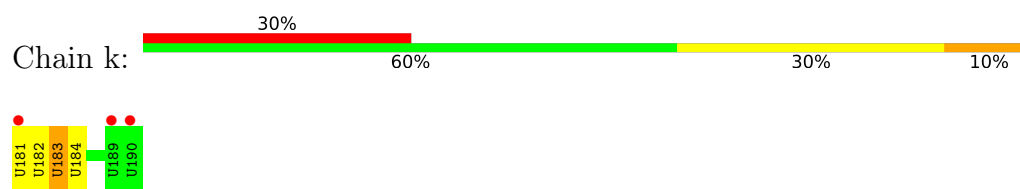
- Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



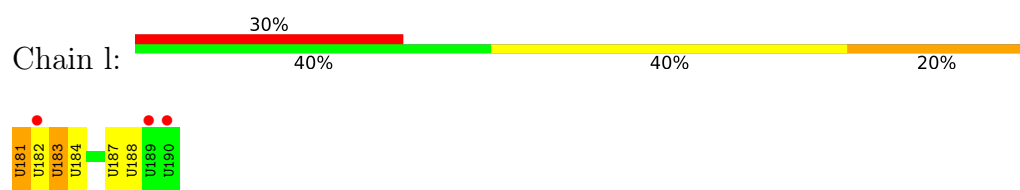
- Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



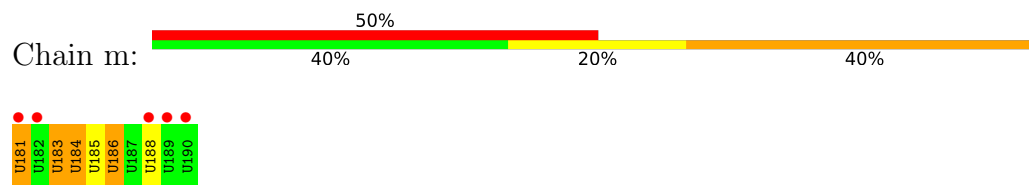
- Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



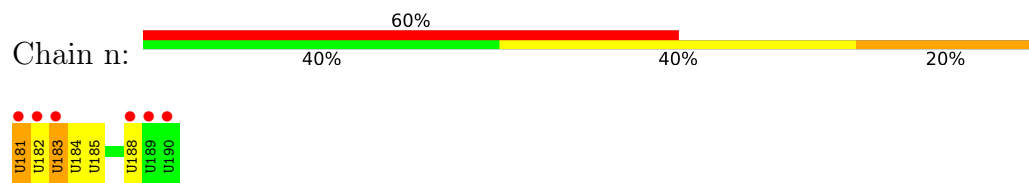
- Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



- Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



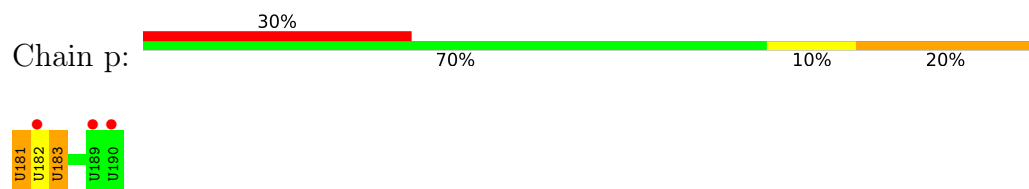
- Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



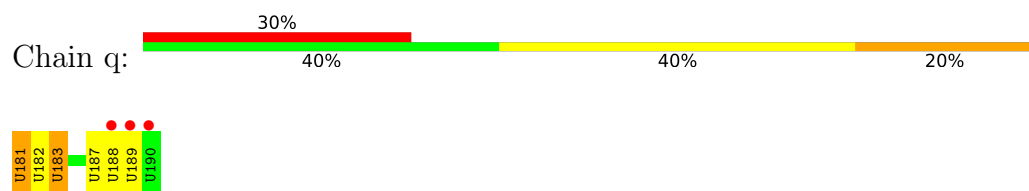
- Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



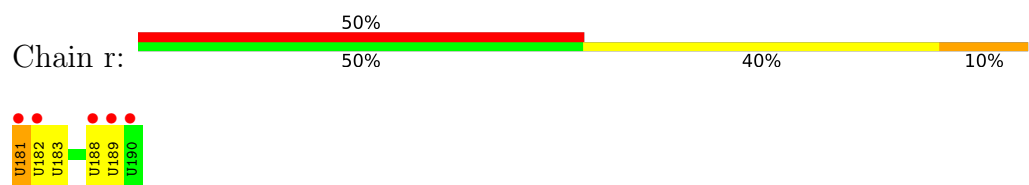
- Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



- Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

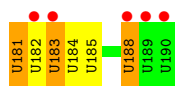


- Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



- Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')





- Molecule 4: RNA (5'-R(P*UP*U)-3')



- Molecule 4: RNA (5'-R(P*UP*U)-3')



- Molecule 4: RNA (5'-R(P*UP*U)-3')



- Molecule 4: RNA (5'-R(P*UP*U)-3')



- Molecule 4: RNA (5'-R(P*UP*U)-3')



- Molecule 4: RNA (5'-R(P*UP*U)-3')



- Molecule 4: RNA (5'-R(P*UP*U)-3')



- Molecule 4: RNA (5'-R(P*UP*U)-3')



- Molecule 4: RNA (5'-R(P*UP*U)-3')



- Molecule 4: RNA (5'-R(P*UP*U)-3')



- Molecule 4: RNA (5'-R(P*UP*U)-3')



- Molecule 4: RNA (5'-R(P*UP*U)-3')



- Molecule 4: RNA (5'-R(P*UP*U)-3')

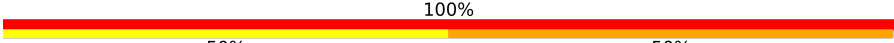


- Molecule 4: RNA (5'-R(P*UP*U)-3')

Chain 7:  100%
50% 50%



- Molecule 4: RNA (5'-R(P*UP*U)-3')

Chain 8:  100%
50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	174.27Å 191.77Å 202.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.04 – 1.82 87.04 – 1.82	Depositor EDS
% Data completeness (in resolution range)	89.5 (87.04-1.82) 89.5 (87.04-1.82)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.123 , 0.156 0.131 , 0.161	Depositor DCC
R_{free} test set	4459 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å ²)	15.1	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	28403	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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: SO4, MG, PO4

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	A	0.67	0/1301	0.76	0/1767
1	B	0.65	0/1269	0.78	0/1725
1	C	0.63	0/1291	0.76	0/1755
1	D	0.63	0/1324	0.74	0/1800
1	E	0.64	0/1282	0.76	0/1745
1	F	0.62	0/1292	0.79	1/1757 (0.1%)
1	G	0.64	0/1276	0.72	0/1735
1	H	0.64	0/1292	0.75	0/1756
1	I	0.73	0/1266	0.79	0/1721
1	J	0.63	0/1288	0.75	0/1752
1	K	0.68	0/1301	0.80	0/1768
1	L	0.64	0/1276	0.75	1/1734 (0.1%)
1	M	0.67	0/1252	0.76	0/1702
1	N	0.65	0/1294	0.77	0/1757
1	O	0.62	0/1299	0.75	0/1766
2	P	0.54	1/250 (0.4%)	0.89	0/386
2	Q	0.56	1/250 (0.4%)	0.90	0/386
2	R	0.54	1/250 (0.4%)	0.86	0/386
2	S	0.53	1/250 (0.4%)	0.82	0/386
2	T	0.53	1/250 (0.4%)	0.87	0/386
2	U	0.53	1/250 (0.4%)	0.85	0/386
2	V	0.52	1/250 (0.4%)	0.88	0/386
2	W	0.55	1/250 (0.4%)	0.91	0/386
2	X	0.53	1/250 (0.4%)	0.81	0/386
2	Y	0.54	1/250 (0.4%)	0.94	0/386
2	Z	0.53	1/250 (0.4%)	0.90	1/386 (0.3%)
2	a	0.54	1/250 (0.4%)	0.88	0/386
2	b	0.57	1/250 (0.4%)	0.92	1/386 (0.3%)
2	c	0.55	1/250 (0.4%)	0.88	0/386
2	d	0.54	1/250 (0.4%)	0.93	0/386
3	e	0.60	1/220 (0.5%)	0.96	0/336
3	f	0.58	1/220 (0.5%)	0.96	2/336 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	g	0.60	1/220 (0.5%)	0.91	0/336
3	h	0.59	1/220 (0.5%)	0.97	0/336
3	i	0.58	1/220 (0.5%)	0.87	0/336
3	j	0.61	1/220 (0.5%)	0.86	0/336
3	k	0.59	1/220 (0.5%)	0.94	0/336
3	l	0.58	1/220 (0.5%)	0.90	0/336
3	m	0.56	1/220 (0.5%)	0.82	0/336
3	n	0.60	1/220 (0.5%)	0.87	0/336
3	o	0.57	1/220 (0.5%)	0.89	0/336
3	p	0.59	1/220 (0.5%)	0.83	0/336
3	q	0.58	1/220 (0.5%)	0.88	0/336
3	r	0.58	1/220 (0.5%)	0.87	0/336
3	s	0.56	1/220 (0.5%)	0.92	0/336
4	1	1.20	1/27 (3.7%)	0.79	0/38
4	2	1.19	1/27 (3.7%)	0.73	0/38
4	3	1.18	1/27 (3.7%)	0.73	0/38
4	4	1.16	1/27 (3.7%)	0.73	0/38
4	5	1.18	1/27 (3.7%)	0.76	0/38
4	6	1.17	1/27 (3.7%)	0.78	0/38
4	7	1.18	1/27 (3.7%)	0.72	0/38
4	8	1.20	1/27 (3.7%)	0.73	0/38
4	t	1.17	1/27 (3.7%)	0.75	0/38
4	u	1.18	1/27 (3.7%)	0.77	0/38
4	v	1.19	1/27 (3.7%)	0.72	0/38
4	w	1.19	1/27 (3.7%)	0.74	0/38
4	x	1.16	1/27 (3.7%)	0.77	0/38
4	y	1.19	1/27 (3.7%)	0.69	0/38
4	z	1.17	1/27 (3.7%)	0.74	0/38
All	All	0.64	45/26758 (0.2%)	0.80	6/37640 (0.0%)

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	f	181[B]	U	OP3-P	6.06	1.60	1.48
2	W	161[B]	A	OP3-P	6.05	1.60	1.48
3	m	181[A]	U	OP3-P	6.05	1.60	1.48
3	e	181[A]	U	OP3-P	6.05	1.60	1.48
2	U	161[B]	A	OP3-P	6.05	1.60	1.48

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	140	VAL	CB-CA-C	-5.74	104.41	111.92
2	b	165[B]	A	C4'-C3'-C2'	-5.63	96.97	102.60
2	Z	168[B]	A	C4'-C3'-C2'	-5.41	97.19	102.60
3	f	185[B]	U	C4'-C3'-C2'	-5.40	97.20	102.60
1	F	140	VAL	CB-CA-C	-5.18	105.13	111.92

There are no chirality outliers.

There are no planarity outliers.

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	A	1224	0	1272	15	0
1	B	1201	0	1236	7	0
1	C	1226	0	1263	12	0
1	D	1244	0	1290	20	0
1	E	1215	0	1241	16	0
1	F	1225	0	1250	12	0
1	G	1208	0	1241	10	0
1	H	1222	0	1260	12	0
1	I	1196	0	1217	7	0
1	J	1216	0	1251	14	0
1	K	1221	0	1246	15	0
1	L	1206	0	1233	9	0
1	M	1186	0	1220	15	0
1	N	1220	0	1261	10	0
1	O	1221	0	1264	10	0
2	P	221	0	94	20	0
2	Q	221	0	111	6	0
2	R	221	0	111	21	0
2	S	221	0	111	19	0
2	T	221	0	95	21	0
2	U	221	0	93	21	0
2	V	221	0	111	5	0
2	W	221	0	111	21	0
2	X	221	0	111	19	0
2	Y	221	0	94	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	221	0	93	26	0
2	a	221	0	111	3	0
2	b	221	0	111	14	0
2	c	221	0	111	24	0
2	d	221	0	95	20	0
3	e	201	0	83	17	0
3	f	201	0	101	1	0
3	g	201	0	101	19	0
3	h	201	0	101	21	0
3	i	201	0	83	18	0
3	j	201	0	85	16	0
3	k	201	0	101	2	0
3	l	201	0	101	22	0
3	m	201	0	101	24	0
3	n	201	0	85	22	0
3	o	201	0	82	19	0
3	p	201	0	101	7	0
3	q	201	0	101	20	0
3	r	201	0	101	17	0
3	s	201	0	84	18	0
4	1	26	0	10	1	0
4	2	26	0	10	1	0
4	3	26	0	10	2	0
4	4	26	0	10	3	0
4	5	26	0	10	2	0
4	6	26	0	10	5	0
4	7	26	0	10	2	0
4	8	26	0	10	6	0
4	t	26	0	10	3	0
4	u	26	0	10	1	0
4	v	26	0	10	1	0
4	w	26	0	10	1	0
4	x	26	0	10	3	0
4	y	26	0	10	3	0
4	z	26	0	10	2	0
5	A	1	0	0	0	0
5	F	1	0	0	0	0
5	K	1	0	0	0	0
6	C	21	0	0	0	0
6	H	21	0	0	0	0
6	K	21	0	0	0	0
7	E	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	1	1	0	0	0	0
8	3	1	0	0	0	0
8	8	1	0	0	0	0
8	A	224	0	0	2	0
8	B	205	0	0	0	0
8	C	204	0	0	5	0
8	D	203	0	0	6	0
8	E	201	0	0	3	0
8	F	209	0	0	3	0
8	G	205	0	0	6	0
8	H	215	0	0	6	0
8	I	213	0	0	1	0
8	J	212	0	0	4	0
8	K	192	0	0	4	0
8	L	226	0	0	2	0
8	M	203	0	0	6	0
8	N	206	0	0	8	0
8	O	209	0	0	3	0
8	P	8	0	0	0	0
8	Q	11	0	0	0	0
8	R	13	0	0	0	0
8	S	12	0	0	0	0
8	T	5	0	0	0	0
8	U	9	0	0	0	0
8	V	16	0	0	1	0
8	W	12	0	0	0	0
8	X	14	0	0	0	0
8	Y	8	0	0	0	0
8	Z	11	0	0	0	0
8	a	11	0	0	0	0
8	b	11	0	0	0	0
8	c	10	0	0	0	0
8	d	6	0	0	0	0
8	e	9	0	0	0	0
8	f	2	0	0	0	0
8	g	3	0	0	0	0
8	h	5	0	0	0	0
8	i	9	0	0	0	0
8	j	9	0	0	0	0
8	k	5	0	0	2	0
8	l	3	0	0	0	0
8	m	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	n	5	0	0	0	0
8	o	10	0	0	0	0
8	p	8	0	0	0	0
8	q	2	0	0	0	0
8	r	6	0	0	0	0
8	s	11	0	0	0	0
8	t	1	0	0	0	0
8	v	1	0	0	0	0
All	All	28403	0	21869	505	0

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 11.

The worst 5 of 505 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)
2:P:168[A]:A:N6	3:e:182[A]:U:O4	1.61	1.31
2:d:168[B]:A:N6	3:s:182[B]:U:O4	1.67	1.27
2:Z:161[B]:A:O2'	2:Z:162[B]:A:H5'	1.41	1.20
2:c:169[B]:A:N1	3:r:181[B]:U:N3	1.93	1.17
2:T:161[A]:A:O2'	2:T:162[A]:A:H5'	1.46	1.12

There are no symmetry-related clashes.

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	A	163/159 (102%)	158 (97%)	5 (3%)	0	100	100
1	B	159/159 (100%)	154 (97%)	4 (2%)	1 (1%)	21	11
1	C	162/159 (102%)	156 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	166/159 (104%)	161 (97%)	4 (2%)	1 (1%)	21	11
1	E	161/159 (101%)	156 (97%)	5 (3%)	0	100	100
1	F	162/159 (102%)	157 (97%)	5 (3%)	0	100	100
1	G	160/159 (101%)	155 (97%)	5 (3%)	0	100	100
1	H	162/159 (102%)	156 (96%)	6 (4%)	0	100	100
1	I	159/159 (100%)	154 (97%)	5 (3%)	0	100	100
1	J	162/159 (102%)	157 (97%)	4 (2%)	1 (1%)	21	11
1	K	163/159 (102%)	158 (97%)	5 (3%)	0	100	100
1	L	160/159 (101%)	155 (97%)	4 (2%)	1 (1%)	21	11
1	M	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	21	11
1	N	162/159 (102%)	157 (97%)	4 (2%)	1 (1%)	21	11
1	O	163/159 (102%)	157 (96%)	6 (4%)	0	100	100
All	All	2421/2385 (102%)	2342 (97%)	73 (3%)	6 (0%)	36	33

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	42	PRO
1	J	42	PRO
1	N	42	PRO
1	D	42	PRO
1	L	42	PRO

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	A	149/140 (106%)	149 (100%)	0	100	100
1	B	145/140 (104%)	145 (100%)	0	100	100
1	C	148/140 (106%)	148 (100%)	0	100	100
1	D	152/140 (109%)	152 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	147/140 (105%)	147 (100%)	0	100	100
1	F	148/140 (106%)	148 (100%)	0	100	100
1	G	146/140 (104%)	146 (100%)	0	100	100
1	H	148/140 (106%)	148 (100%)	0	100	100
1	I	145/140 (104%)	145 (100%)	0	100	100
1	J	148/140 (106%)	148 (100%)	0	100	100
1	K	149/140 (106%)	149 (100%)	0	100	100
1	L	146/140 (104%)	146 (100%)	0	100	100
1	M	143/140 (102%)	143 (100%)	0	100	100
1	N	148/140 (106%)	148 (100%)	0	100	100
1	O	149/140 (106%)	149 (100%)	0	100	100
All	All	2211/2100 (105%)	2211 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	89	ASN
1	L	89	ASN
1	O	89	ASN
1	M	18	ASN
1	E	89	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	P	9/10 (90%)	0	0
2	Q	9/10 (90%)	1 (11%)	0
2	R	9/10 (90%)	1 (11%)	0
2	S	9/10 (90%)	2 (22%)	0
2	T	9/10 (90%)	1 (11%)	0
2	U	9/10 (90%)	1 (11%)	0
2	V	9/10 (90%)	0	0
2	W	9/10 (90%)	1 (11%)	0
2	X	9/10 (90%)	3 (33%)	0
2	Y	9/10 (90%)	1 (11%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Z	9/10 (90%)	2 (22%)	0
2	a	9/10 (90%)	0	0
2	b	9/10 (90%)	1 (11%)	0
2	c	9/10 (90%)	0	0
2	d	9/10 (90%)	2 (22%)	0
3	e	9/10 (90%)	2 (22%)	0
3	f	9/10 (90%)	1 (11%)	0
3	g	9/10 (90%)	1 (11%)	0
3	h	9/10 (90%)	2 (22%)	0
3	i	9/10 (90%)	1 (11%)	0
3	j	9/10 (90%)	1 (11%)	0
3	k	9/10 (90%)	2 (22%)	0
3	l	9/10 (90%)	1 (11%)	0
3	m	9/10 (90%)	3 (33%)	0
3	n	9/10 (90%)	1 (11%)	0
3	o	9/10 (90%)	1 (11%)	0
3	p	9/10 (90%)	1 (11%)	0
3	q	9/10 (90%)	1 (11%)	0
3	r	9/10 (90%)	1 (11%)	0
3	s	9/10 (90%)	2 (22%)	0
4	1	0/2	-	-
4	2	0/2	-	-
4	3	0/2	-	-
4	4	0/2	-	-
4	5	0/2	-	-
4	6	0/2	-	-
4	7	0/2	-	-
4	8	0/2	-	-
4	t	0/2	-	-
4	u	0/2	-	-
4	v	0/2	-	-
4	w	0/2	-	-
4	x	0/2	-	-
4	y	0/2	-	-
4	z	0/2	-	-
All	All	270/330 (81%)	37 (13%)	0

5 of 37 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	e	183[A]	U
3	e	184[A]	U
2	Q	163[A]	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	f	183[B]	U
2	R	165[A]	A

There are no RNA pucker outliers to report.

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 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	PO4	K	201[E]	5	4,4,4	0.95	0	6,6,6	0.48	0
6	PO4	C	201[E]	5	4,4,4	1.01	0	6,6,6	0.44	0
6	PO4	H	201[A]	5	4,4,4	1.00	0	6,6,6	0.55	0
6	PO4	H	201[C]	5	4,4,4	1.05	0	6,6,6	0.27	0
6	PO4	K	201[A]	5	4,4,4	0.91	0	6,6,6	0.63	0
6	PO4	C	201[A]	5	4,4,4	1.00	0	6,6,6	0.51	0
6	PO4	C	201[B]	5	4,4,4	0.95	0	6,6,6	0.33	0
6	PO4	C	201[C]	5	4,4,4	0.99	0	6,6,6	0.73	0
6	PO4	H	201[B]	5	4,4,4	1.02	0	6,6,6	0.53	0
6	PO4	K	201[C]	5	4,4,4	1.02	0	6,6,6	0.33	0
7	SO4	E	201	-	4,4,4	0.25	0	6,6,6	0.07	0
6	PO4	C	201[D]	5	4,4,4	1.01	0	6,6,6	0.45	0
6	PO4	K	201[B]	5	4,4,4	1.07	0	6,6,6	0.42	0
6	PO4	H	201[D]	5	4,4,4	1.06	0	6,6,6	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	PO4	K	201[D]	5	4,4,4	0.95	0	6,6,6	0.56	0
6	PO4	H	201[E]	5	4,4,4	1.07	0	6,6,6	0.38	0

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	A	144/159 (90%)	-0.55	2 (1%) 73 79	9, 18, 30, 78	19 (13%)
1	B	144/159 (90%)	-0.50	1 (0%) 84 88	10, 19, 34, 79	17 (11%)
1	C	144/159 (90%)	-0.47	2 (1%) 73 79	9, 19, 33, 77	19 (13%)
1	D	144/159 (90%)	-0.45	2 (1%) 73 79	8, 18, 30, 78	22 (15%)
1	E	144/159 (90%)	-0.46	2 (1%) 73 79	10, 18, 32, 77	19 (13%)
1	F	144/159 (90%)	-0.46	2 (1%) 73 79	9, 18, 32, 77	19 (13%)
1	G	144/159 (90%)	-0.46	2 (1%) 73 79	10, 19, 30, 77	18 (12%)
1	H	144/159 (90%)	-0.49	2 (1%) 73 79	10, 18, 30, 77	20 (13%)
1	I	144/159 (90%)	-0.53	2 (1%) 73 79	9, 18, 31, 77	16 (11%)
1	J	144/159 (90%)	-0.52	2 (1%) 73 79	10, 18, 32, 77	19 (13%)
1	K	144/159 (90%)	-0.48	2 (1%) 73 79	9, 17, 31, 79	20 (13%)
1	L	144/159 (90%)	-0.49	3 (2%) 63 70	10, 19, 30, 77	18 (12%)
1	M	144/159 (90%)	-0.47	2 (1%) 73 79	10, 19, 30, 78	15 (10%)
1	N	144/159 (90%)	-0.48	2 (1%) 73 79	10, 18, 30, 78	19 (13%)
1	O	144/159 (90%)	-0.49	4 (2%) 55 60	10, 19, 29, 77	20 (13%)
2	P	10/10 (100%)	1.66	4 (40%) 1 0	15, 23, 92, 108	10 (100%)
2	Q	10/10 (100%)	1.66	4 (40%) 1 0	16, 23, 93, 97	10 (100%)
2	R	10/10 (100%)	1.84	5 (50%) 0 0	21, 29, 95, 97	10 (100%)
2	S	10/10 (100%)	1.59	4 (40%) 1 0	21, 27, 95, 97	10 (100%)
2	T	10/10 (100%)	1.90	4 (40%) 1 0	21, 26, 90, 94	10 (100%)
2	U	10/10 (100%)	2.37	6 (60%) 0 0	26, 35, 102, 107	10 (100%)
2	V	10/10 (100%)	1.70	4 (40%) 1 0	20, 25, 98, 108	10 (100%)
2	W	10/10 (100%)	1.31	4 (40%) 1 0	17, 24, 92, 93	10 (100%)
2	X	10/10 (100%)	1.91	5 (50%) 0 0	22, 30, 98, 99	10 (100%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
2	Y	10/10 (100%)	1.71	4 (40%)	1	0	15, 24, 87, 92	10 (100%)
2	Z	10/10 (100%)	2.14	5 (50%)	0	0	20, 32, 102, 107	10 (100%)
2	a	10/10 (100%)	1.43	4 (40%)	1	0	12, 23, 91, 104	10 (100%)
2	b	10/10 (100%)	1.52	4 (40%)	1	0	12, 25, 94, 95	10 (100%)
2	c	10/10 (100%)	1.57	4 (40%)	1	0	14, 24, 88, 96	10 (100%)
2	d	10/10 (100%)	2.34	5 (50%)	0	0	25, 34, 102, 109	10 (100%)
3	e	10/10 (100%)	1.52	6 (60%)	0	0	9, 53, 104, 111	10 (100%)
3	f	10/10 (100%)	1.27	4 (40%)	1	0	9, 65, 107, 109	10 (100%)
3	g	10/10 (100%)	1.37	5 (50%)	0	0	10, 55, 113, 122	10 (100%)
3	h	10/10 (100%)	1.04	4 (40%)	1	0	8, 54, 108, 114	10 (100%)
3	i	10/10 (100%)	1.48	6 (60%)	0	0	7, 51, 104, 111	10 (100%)
3	j	10/10 (100%)	1.44	6 (60%)	0	0	8, 60, 101, 107	10 (100%)
3	k	10/10 (100%)	1.17	3 (30%)	1	1	10, 60, 97, 103	10 (100%)
3	l	10/10 (100%)	1.15	3 (30%)	1	1	8, 63, 109, 114	10 (100%)
3	m	10/10 (100%)	1.52	5 (50%)	0	0	21, 67, 116, 128	10 (100%)
3	n	10/10 (100%)	1.65	6 (60%)	0	0	9, 51, 103, 111	10 (100%)
3	o	10/10 (100%)	1.58	5 (50%)	0	0	9, 64, 107, 108	10 (100%)
3	p	10/10 (100%)	1.17	3 (30%)	1	1	10, 69, 116, 116	10 (100%)
3	q	10/10 (100%)	1.23	3 (30%)	1	1	8, 63, 105, 113	10 (100%)
3	r	10/10 (100%)	1.28	5 (50%)	0	0	10, 64, 114, 116	10 (100%)
3	s	10/10 (100%)	1.69	5 (50%)	0	0	9, 68, 104, 122	10 (100%)
4	1	2/2 (100%)	4.46	2 (100%)	0	0	29, 29, 29, 48	2 (100%)
4	2	2/2 (100%)	4.31	2 (100%)	0	0	30, 30, 30, 51	2 (100%)
4	3	2/2 (100%)	3.88	2 (100%)	0	0	29, 29, 29, 45	2 (100%)
4	4	2/2 (100%)	4.51	2 (100%)	0	0	30, 30, 30, 48	2 (100%)
4	5	2/2 (100%)	4.62	2 (100%)	0	0	29, 29, 29, 49	2 (100%)
4	6	2/2 (100%)	4.51	2 (100%)	0	0	29, 29, 29, 46	2 (100%)
4	7	2/2 (100%)	4.16	2 (100%)	0	0	27, 27, 27, 48	2 (100%)
4	8	2/2 (100%)	3.94	2 (100%)	0	0	30, 30, 30, 50	2 (100%)
4	t	2/2 (100%)	4.56	2 (100%)	0	0	30, 30, 30, 47	2 (100%)
4	u	2/2 (100%)	4.88	2 (100%)	0	0	30, 30, 30, 47	2 (100%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
4	v	2/2 (100%)	4.72	2 (100%)	0	0	33, 33, 33, 50	2 (100%)
4	w	2/2 (100%)	4.64	2 (100%)	0	0	30, 30, 30, 45	2 (100%)
4	x	2/2 (100%)	4.16	2 (100%)	0	0	31, 31, 31, 50	2 (100%)
4	y	2/2 (100%)	4.37	2 (100%)	0	0	33, 33, 33, 47	2 (100%)
4	z	2/2 (100%)	4.40	2 (100%)	0	0	31, 31, 31, 49	2 (100%)
All	All	2490/2715 (91%)	-0.18	197 (7%)	18	20	7, 19, 74, 128	610 (24%)

The worst 5 of 197 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	4	195[A]	U	6.0
4	v	195[B]	U	5.7
4	u	195[A]	U	5.7
4	5	195[A]	U	5.7
4	6	195[A]	U	5.4

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](#)

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
7	SO4	E	201	5/5	0.71	0.20	144,152,154,157	0
5	MG	A	201	1/1	0.83	0.25	63,63,63,63	0
5	MG	K	202	1/1	0.87	0.25	64,64,64,64	0
5	MG	F	201	1/1	0.89	0.22	57,57,57,57	0
6	PO4	C	201[B]	5/5	1.00	0.02	7,10,15,23	4
6	PO4	C	201[C]	5/5	1.00	0.02	8,12,13,15	4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PO4	C	201[D]	5/5	1.00	0.02	4,10,21,23	4
6	PO4	C	201[E]	5/5	1.00	0.02	12,15,17,30	4
6	PO4	H	201[A]	5/5	1.00	0.03	6,11,14,19	4
6	PO4	H	201[B]	5/5	1.00	0.03	8,9,16,26	4
6	PO4	H	201[C]	5/5	1.00	0.03	4,10,15,19	4
6	PO4	H	201[D]	5/5	1.00	0.03	7,12,14,18	4
6	PO4	H	201[E]	5/5	1.00	0.03	6,12,14,19	4
6	PO4	K	201[A]	5/5	1.00	0.03	7,10,13,18	4
6	PO4	K	201[B]	5/5	1.00	0.03	4,9,16,18	4
6	PO4	K	201[C]	5/5	1.00	0.03	6,13,14,29	4
6	PO4	K	201[D]	5/5	1.00	0.03	10,11,15,30	4
6	PO4	K	201[E]	5/5	1.00	0.03	4,6,13,19	4
6	PO4	C	201[A]	5/5	1.00	0.02	4,9,21,23	4

6.5 Other polymers [i](#)

There are no such residues in this entry.