



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 2, 2026 – 03:24 AM UTC

PDB ID : 5UK4 / pdb_00005uk4
Title : VESICULAR STOMATITIS VIRUS N PROTEIN IN COMPLEX WITH INHIBITORY NANOBODY 1307
Authors : Hanke, L.; Knockenhauer, K.E.; Ploegh, H.L.; Schwartz, T.U.
Deposited on : 2017-01-19
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

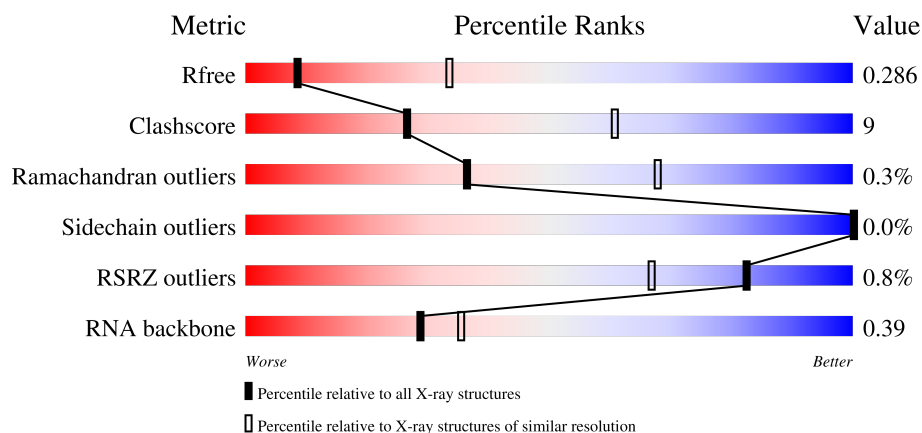
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



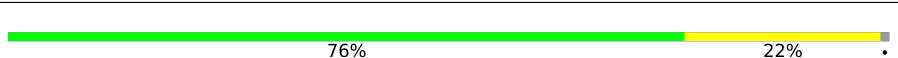
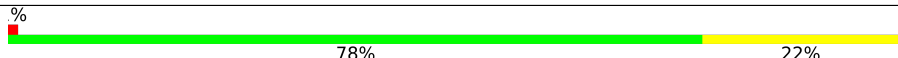
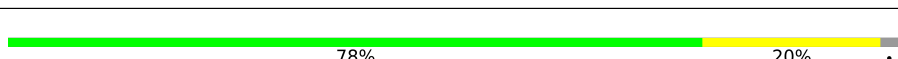
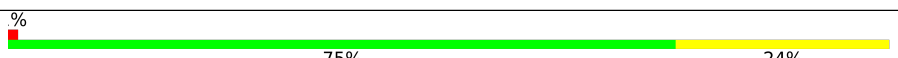
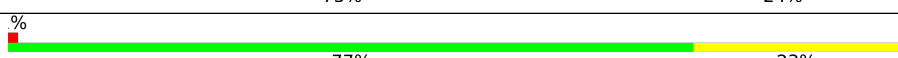
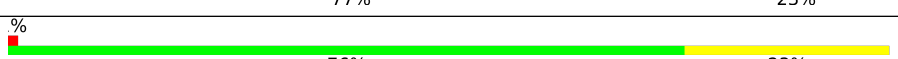
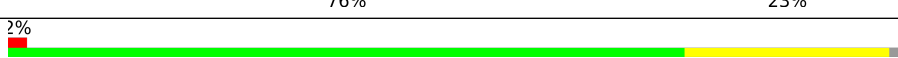
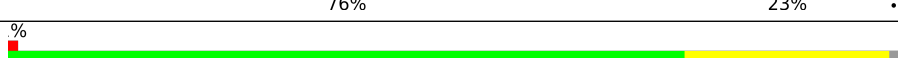
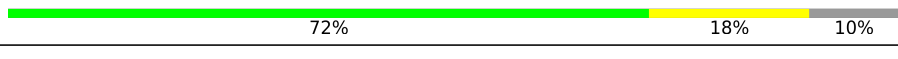
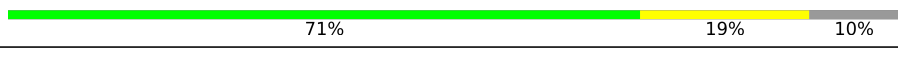
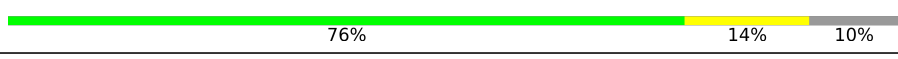
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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	422	
1	B	422	
1	C	422	
1	D	422	

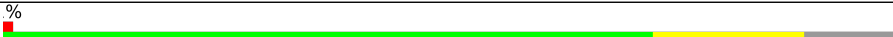
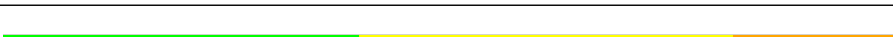
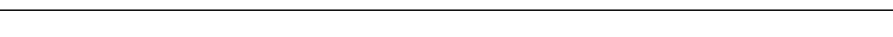
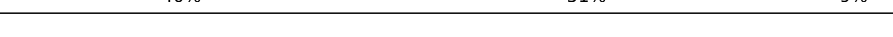
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	E	422		•
1	F	422		
1	G	422		•
1	H	422		
1	I	422		•
1	J	422		
1	K	422		
1	L	422		
1	M	422		•
1	N	422		•
1	O	422		
1	P	422		•
1	Q	422		•
1	R	422		•
1	S	422		
1	T	422		
2	a	139		
2	b	139		
2	c	139		
2	d	139		•
2	e	139		
2	f	139		
2	g	139		
2	h	139		
2	i	139		

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	j	139	
2	k	139	
2	l	139	
2	m	139	
2	n	139	
2	o	139	
2	p	139	
2	q	139	
2	r	139	
2	s	139	
2	t	139	
3	u	45	
3	v	45	
3	w	45	
3	x	45	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 89086 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	414	Total	C	N	O	S	0	0	0
			3281	2090	551	622	18			
1	B	412	Total	C	N	O	S	0	0	0
			3270	2083	548	621	18			
1	Q	419	Total	C	N	O	S	0	0	0
			3316	2111	556	631	18			
1	C	417	Total	C	N	O	S	0	0	0
			3299	2102	554	625	18			
1	R	419	Total	C	N	O	S	0	0	0
			3315	2112	556	629	18			
1	D	418	Total	C	N	O	S	0	0	0
			3305	2106	552	629	18			
1	S	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			
1	E	413	Total	C	N	O	S	0	0	0
			3273	2084	550	621	18			
1	T	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			
1	K	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			
1	L	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			
1	N	418	Total	C	N	O	S	0	0	0
			3305	2106	552	629	18			
1	M	416	Total	C	N	O	S	0	0	0
			3291	2099	550	624	18			
1	F	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			
1	G	416	Total	C	N	O	S	0	0	0
			3295	2099	553	625	18			
1	H	420	Total	C	N	O	S	0	0	0
			3316	2112	554	632	18			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	415	Total	C	N	O	S	0	0	0
			3289	2094	552	625	18			
1	O	420	Total	C	N	O	S	0	0	0
			3323	2116	557	632	18			
1	J	420	Total	C	N	O	S	0	0	0
			3323	2116	557	632	18			
1	A	416	Total	C	N	O	S	0	0	0
			3290	2097	550	625	18			

- Molecule 2 is a protein called Anti-vesicular stomatitis virus N VHH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	p	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	b	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	q	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	c	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	r	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	d	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	s	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	e	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	t	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	k	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	l	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	n	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	m	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	f	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	g	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	h	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	i	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	o	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	j	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			
2	a	125	Total	C	N	O	S	0	0	0
			968	605	171	187	5			

There are 280 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p	126	GLY	-	expression tag	UNP A0A192B6J6
p	127	GLY	-	expression tag	UNP A0A192B6J6
p	128	LEU	-	expression tag	UNP A0A192B6J6
p	129	PRO	-	expression tag	UNP A0A192B6J6
p	130	GLU	-	expression tag	UNP A0A192B6J6
p	131	THR	-	expression tag	UNP A0A192B6J6
p	132	GLY	-	expression tag	UNP A0A192B6J6
p	133	GLY	-	expression tag	UNP A0A192B6J6
p	134	HIS	-	expression tag	UNP A0A192B6J6
p	135	HIS	-	expression tag	UNP A0A192B6J6
p	136	HIS	-	expression tag	UNP A0A192B6J6
p	137	HIS	-	expression tag	UNP A0A192B6J6
p	138	HIS	-	expression tag	UNP A0A192B6J6
p	139	HIS	-	expression tag	UNP A0A192B6J6
b	126	GLY	-	expression tag	UNP A0A192B6J6
b	127	GLY	-	expression tag	UNP A0A192B6J6
b	128	LEU	-	expression tag	UNP A0A192B6J6
b	129	PRO	-	expression tag	UNP A0A192B6J6
b	130	GLU	-	expression tag	UNP A0A192B6J6
b	131	THR	-	expression tag	UNP A0A192B6J6
b	132	GLY	-	expression tag	UNP A0A192B6J6
b	133	GLY	-	expression tag	UNP A0A192B6J6
b	134	HIS	-	expression tag	UNP A0A192B6J6
b	135	HIS	-	expression tag	UNP A0A192B6J6
b	136	HIS	-	expression tag	UNP A0A192B6J6
b	137	HIS	-	expression tag	UNP A0A192B6J6
b	138	HIS	-	expression tag	UNP A0A192B6J6
b	139	HIS	-	expression tag	UNP A0A192B6J6
q	126	GLY	-	expression tag	UNP A0A192B6J6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
q	127	GLY	-	expression tag	UNP A0A192B6J6
q	128	LEU	-	expression tag	UNP A0A192B6J6
q	129	PRO	-	expression tag	UNP A0A192B6J6
q	130	GLU	-	expression tag	UNP A0A192B6J6
q	131	THR	-	expression tag	UNP A0A192B6J6
q	132	GLY	-	expression tag	UNP A0A192B6J6
q	133	GLY	-	expression tag	UNP A0A192B6J6
q	134	HIS	-	expression tag	UNP A0A192B6J6
q	135	HIS	-	expression tag	UNP A0A192B6J6
q	136	HIS	-	expression tag	UNP A0A192B6J6
q	137	HIS	-	expression tag	UNP A0A192B6J6
q	138	HIS	-	expression tag	UNP A0A192B6J6
q	139	HIS	-	expression tag	UNP A0A192B6J6
c	126	GLY	-	expression tag	UNP A0A192B6J6
c	127	GLY	-	expression tag	UNP A0A192B6J6
c	128	LEU	-	expression tag	UNP A0A192B6J6
c	129	PRO	-	expression tag	UNP A0A192B6J6
c	130	GLU	-	expression tag	UNP A0A192B6J6
c	131	THR	-	expression tag	UNP A0A192B6J6
c	132	GLY	-	expression tag	UNP A0A192B6J6
c	133	GLY	-	expression tag	UNP A0A192B6J6
c	134	HIS	-	expression tag	UNP A0A192B6J6
c	135	HIS	-	expression tag	UNP A0A192B6J6
c	136	HIS	-	expression tag	UNP A0A192B6J6
c	137	HIS	-	expression tag	UNP A0A192B6J6
c	138	HIS	-	expression tag	UNP A0A192B6J6
c	139	HIS	-	expression tag	UNP A0A192B6J6
r	126	GLY	-	expression tag	UNP A0A192B6J6
r	127	GLY	-	expression tag	UNP A0A192B6J6
r	128	LEU	-	expression tag	UNP A0A192B6J6
r	129	PRO	-	expression tag	UNP A0A192B6J6
r	130	GLU	-	expression tag	UNP A0A192B6J6
r	131	THR	-	expression tag	UNP A0A192B6J6
r	132	GLY	-	expression tag	UNP A0A192B6J6
r	133	GLY	-	expression tag	UNP A0A192B6J6
r	134	HIS	-	expression tag	UNP A0A192B6J6
r	135	HIS	-	expression tag	UNP A0A192B6J6
r	136	HIS	-	expression tag	UNP A0A192B6J6
r	137	HIS	-	expression tag	UNP A0A192B6J6
r	138	HIS	-	expression tag	UNP A0A192B6J6
r	139	HIS	-	expression tag	UNP A0A192B6J6
d	126	GLY	-	expression tag	UNP A0A192B6J6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
d	127	GLY	-	expression tag	UNP A0A192B6J6
d	128	LEU	-	expression tag	UNP A0A192B6J6
d	129	PRO	-	expression tag	UNP A0A192B6J6
d	130	GLU	-	expression tag	UNP A0A192B6J6
d	131	THR	-	expression tag	UNP A0A192B6J6
d	132	GLY	-	expression tag	UNP A0A192B6J6
d	133	GLY	-	expression tag	UNP A0A192B6J6
d	134	HIS	-	expression tag	UNP A0A192B6J6
d	135	HIS	-	expression tag	UNP A0A192B6J6
d	136	HIS	-	expression tag	UNP A0A192B6J6
d	137	HIS	-	expression tag	UNP A0A192B6J6
d	138	HIS	-	expression tag	UNP A0A192B6J6
d	139	HIS	-	expression tag	UNP A0A192B6J6
s	126	GLY	-	expression tag	UNP A0A192B6J6
s	127	GLY	-	expression tag	UNP A0A192B6J6
s	128	LEU	-	expression tag	UNP A0A192B6J6
s	129	PRO	-	expression tag	UNP A0A192B6J6
s	130	GLU	-	expression tag	UNP A0A192B6J6
s	131	THR	-	expression tag	UNP A0A192B6J6
s	132	GLY	-	expression tag	UNP A0A192B6J6
s	133	GLY	-	expression tag	UNP A0A192B6J6
s	134	HIS	-	expression tag	UNP A0A192B6J6
s	135	HIS	-	expression tag	UNP A0A192B6J6
s	136	HIS	-	expression tag	UNP A0A192B6J6
s	137	HIS	-	expression tag	UNP A0A192B6J6
s	138	HIS	-	expression tag	UNP A0A192B6J6
s	139	HIS	-	expression tag	UNP A0A192B6J6
e	126	GLY	-	expression tag	UNP A0A192B6J6
e	127	GLY	-	expression tag	UNP A0A192B6J6
e	128	LEU	-	expression tag	UNP A0A192B6J6
e	129	PRO	-	expression tag	UNP A0A192B6J6
e	130	GLU	-	expression tag	UNP A0A192B6J6
e	131	THR	-	expression tag	UNP A0A192B6J6
e	132	GLY	-	expression tag	UNP A0A192B6J6
e	133	GLY	-	expression tag	UNP A0A192B6J6
e	134	HIS	-	expression tag	UNP A0A192B6J6
e	135	HIS	-	expression tag	UNP A0A192B6J6
e	136	HIS	-	expression tag	UNP A0A192B6J6
e	137	HIS	-	expression tag	UNP A0A192B6J6
e	138	HIS	-	expression tag	UNP A0A192B6J6
e	139	HIS	-	expression tag	UNP A0A192B6J6
t	126	GLY	-	expression tag	UNP A0A192B6J6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
t	127	GLY	-	expression tag	UNP A0A192B6J6
t	128	LEU	-	expression tag	UNP A0A192B6J6
t	129	PRO	-	expression tag	UNP A0A192B6J6
t	130	GLU	-	expression tag	UNP A0A192B6J6
t	131	THR	-	expression tag	UNP A0A192B6J6
t	132	GLY	-	expression tag	UNP A0A192B6J6
t	133	GLY	-	expression tag	UNP A0A192B6J6
t	134	HIS	-	expression tag	UNP A0A192B6J6
t	135	HIS	-	expression tag	UNP A0A192B6J6
t	136	HIS	-	expression tag	UNP A0A192B6J6
t	137	HIS	-	expression tag	UNP A0A192B6J6
t	138	HIS	-	expression tag	UNP A0A192B6J6
t	139	HIS	-	expression tag	UNP A0A192B6J6
k	126	GLY	-	expression tag	UNP A0A192B6J6
k	127	GLY	-	expression tag	UNP A0A192B6J6
k	128	LEU	-	expression tag	UNP A0A192B6J6
k	129	PRO	-	expression tag	UNP A0A192B6J6
k	130	GLU	-	expression tag	UNP A0A192B6J6
k	131	THR	-	expression tag	UNP A0A192B6J6
k	132	GLY	-	expression tag	UNP A0A192B6J6
k	133	GLY	-	expression tag	UNP A0A192B6J6
k	134	HIS	-	expression tag	UNP A0A192B6J6
k	135	HIS	-	expression tag	UNP A0A192B6J6
k	136	HIS	-	expression tag	UNP A0A192B6J6
k	137	HIS	-	expression tag	UNP A0A192B6J6
k	138	HIS	-	expression tag	UNP A0A192B6J6
k	139	HIS	-	expression tag	UNP A0A192B6J6
l	126	GLY	-	expression tag	UNP A0A192B6J6
l	127	GLY	-	expression tag	UNP A0A192B6J6
l	128	LEU	-	expression tag	UNP A0A192B6J6
l	129	PRO	-	expression tag	UNP A0A192B6J6
l	130	GLU	-	expression tag	UNP A0A192B6J6
l	131	THR	-	expression tag	UNP A0A192B6J6
l	132	GLY	-	expression tag	UNP A0A192B6J6
l	133	GLY	-	expression tag	UNP A0A192B6J6
l	134	HIS	-	expression tag	UNP A0A192B6J6
l	135	HIS	-	expression tag	UNP A0A192B6J6
l	136	HIS	-	expression tag	UNP A0A192B6J6
l	137	HIS	-	expression tag	UNP A0A192B6J6
l	138	HIS	-	expression tag	UNP A0A192B6J6
l	139	HIS	-	expression tag	UNP A0A192B6J6
n	126	GLY	-	expression tag	UNP A0A192B6J6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
n	127	GLY	-	expression tag	UNP A0A192B6J6
n	128	LEU	-	expression tag	UNP A0A192B6J6
n	129	PRO	-	expression tag	UNP A0A192B6J6
n	130	GLU	-	expression tag	UNP A0A192B6J6
n	131	THR	-	expression tag	UNP A0A192B6J6
n	132	GLY	-	expression tag	UNP A0A192B6J6
n	133	GLY	-	expression tag	UNP A0A192B6J6
n	134	HIS	-	expression tag	UNP A0A192B6J6
n	135	HIS	-	expression tag	UNP A0A192B6J6
n	136	HIS	-	expression tag	UNP A0A192B6J6
n	137	HIS	-	expression tag	UNP A0A192B6J6
n	138	HIS	-	expression tag	UNP A0A192B6J6
n	139	HIS	-	expression tag	UNP A0A192B6J6
m	126	GLY	-	expression tag	UNP A0A192B6J6
m	127	GLY	-	expression tag	UNP A0A192B6J6
m	128	LEU	-	expression tag	UNP A0A192B6J6
m	129	PRO	-	expression tag	UNP A0A192B6J6
m	130	GLU	-	expression tag	UNP A0A192B6J6
m	131	THR	-	expression tag	UNP A0A192B6J6
m	132	GLY	-	expression tag	UNP A0A192B6J6
m	133	GLY	-	expression tag	UNP A0A192B6J6
m	134	HIS	-	expression tag	UNP A0A192B6J6
m	135	HIS	-	expression tag	UNP A0A192B6J6
m	136	HIS	-	expression tag	UNP A0A192B6J6
m	137	HIS	-	expression tag	UNP A0A192B6J6
m	138	HIS	-	expression tag	UNP A0A192B6J6
m	139	HIS	-	expression tag	UNP A0A192B6J6
f	126	GLY	-	expression tag	UNP A0A192B6J6
f	127	GLY	-	expression tag	UNP A0A192B6J6
f	128	LEU	-	expression tag	UNP A0A192B6J6
f	129	PRO	-	expression tag	UNP A0A192B6J6
f	130	GLU	-	expression tag	UNP A0A192B6J6
f	131	THR	-	expression tag	UNP A0A192B6J6
f	132	GLY	-	expression tag	UNP A0A192B6J6
f	133	GLY	-	expression tag	UNP A0A192B6J6
f	134	HIS	-	expression tag	UNP A0A192B6J6
f	135	HIS	-	expression tag	UNP A0A192B6J6
f	136	HIS	-	expression tag	UNP A0A192B6J6
f	137	HIS	-	expression tag	UNP A0A192B6J6
f	138	HIS	-	expression tag	UNP A0A192B6J6
f	139	HIS	-	expression tag	UNP A0A192B6J6
g	126	GLY	-	expression tag	UNP A0A192B6J6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
g	127	GLY	-	expression tag	UNP A0A192B6J6
g	128	LEU	-	expression tag	UNP A0A192B6J6
g	129	PRO	-	expression tag	UNP A0A192B6J6
g	130	GLU	-	expression tag	UNP A0A192B6J6
g	131	THR	-	expression tag	UNP A0A192B6J6
g	132	GLY	-	expression tag	UNP A0A192B6J6
g	133	GLY	-	expression tag	UNP A0A192B6J6
g	134	HIS	-	expression tag	UNP A0A192B6J6
g	135	HIS	-	expression tag	UNP A0A192B6J6
g	136	HIS	-	expression tag	UNP A0A192B6J6
g	137	HIS	-	expression tag	UNP A0A192B6J6
g	138	HIS	-	expression tag	UNP A0A192B6J6
g	139	HIS	-	expression tag	UNP A0A192B6J6
h	126	GLY	-	expression tag	UNP A0A192B6J6
h	127	GLY	-	expression tag	UNP A0A192B6J6
h	128	LEU	-	expression tag	UNP A0A192B6J6
h	129	PRO	-	expression tag	UNP A0A192B6J6
h	130	GLU	-	expression tag	UNP A0A192B6J6
h	131	THR	-	expression tag	UNP A0A192B6J6
h	132	GLY	-	expression tag	UNP A0A192B6J6
h	133	GLY	-	expression tag	UNP A0A192B6J6
h	134	HIS	-	expression tag	UNP A0A192B6J6
h	135	HIS	-	expression tag	UNP A0A192B6J6
h	136	HIS	-	expression tag	UNP A0A192B6J6
h	137	HIS	-	expression tag	UNP A0A192B6J6
h	138	HIS	-	expression tag	UNP A0A192B6J6
h	139	HIS	-	expression tag	UNP A0A192B6J6
i	126	GLY	-	expression tag	UNP A0A192B6J6
i	127	GLY	-	expression tag	UNP A0A192B6J6
i	128	LEU	-	expression tag	UNP A0A192B6J6
i	129	PRO	-	expression tag	UNP A0A192B6J6
i	130	GLU	-	expression tag	UNP A0A192B6J6
i	131	THR	-	expression tag	UNP A0A192B6J6
i	132	GLY	-	expression tag	UNP A0A192B6J6
i	133	GLY	-	expression tag	UNP A0A192B6J6
i	134	HIS	-	expression tag	UNP A0A192B6J6
i	135	HIS	-	expression tag	UNP A0A192B6J6
i	136	HIS	-	expression tag	UNP A0A192B6J6
i	137	HIS	-	expression tag	UNP A0A192B6J6
i	138	HIS	-	expression tag	UNP A0A192B6J6
i	139	HIS	-	expression tag	UNP A0A192B6J6
o	126	GLY	-	expression tag	UNP A0A192B6J6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
o	127	GLY	-	expression tag	UNP A0A192B6J6
o	128	LEU	-	expression tag	UNP A0A192B6J6
o	129	PRO	-	expression tag	UNP A0A192B6J6
o	130	GLU	-	expression tag	UNP A0A192B6J6
o	131	THR	-	expression tag	UNP A0A192B6J6
o	132	GLY	-	expression tag	UNP A0A192B6J6
o	133	GLY	-	expression tag	UNP A0A192B6J6
o	134	HIS	-	expression tag	UNP A0A192B6J6
o	135	HIS	-	expression tag	UNP A0A192B6J6
o	136	HIS	-	expression tag	UNP A0A192B6J6
o	137	HIS	-	expression tag	UNP A0A192B6J6
o	138	HIS	-	expression tag	UNP A0A192B6J6
o	139	HIS	-	expression tag	UNP A0A192B6J6
j	126	GLY	-	expression tag	UNP A0A192B6J6
j	127	GLY	-	expression tag	UNP A0A192B6J6
j	128	LEU	-	expression tag	UNP A0A192B6J6
j	129	PRO	-	expression tag	UNP A0A192B6J6
j	130	GLU	-	expression tag	UNP A0A192B6J6
j	131	THR	-	expression tag	UNP A0A192B6J6
j	132	GLY	-	expression tag	UNP A0A192B6J6
j	133	GLY	-	expression tag	UNP A0A192B6J6
j	134	HIS	-	expression tag	UNP A0A192B6J6
j	135	HIS	-	expression tag	UNP A0A192B6J6
j	136	HIS	-	expression tag	UNP A0A192B6J6
j	137	HIS	-	expression tag	UNP A0A192B6J6
j	138	HIS	-	expression tag	UNP A0A192B6J6
j	139	HIS	-	expression tag	UNP A0A192B6J6
a	126	GLY	-	expression tag	UNP A0A192B6J6
a	127	GLY	-	expression tag	UNP A0A192B6J6
a	128	LEU	-	expression tag	UNP A0A192B6J6
a	129	PRO	-	expression tag	UNP A0A192B6J6
a	130	GLU	-	expression tag	UNP A0A192B6J6
a	131	THR	-	expression tag	UNP A0A192B6J6
a	132	GLY	-	expression tag	UNP A0A192B6J6
a	133	GLY	-	expression tag	UNP A0A192B6J6
a	134	HIS	-	expression tag	UNP A0A192B6J6
a	135	HIS	-	expression tag	UNP A0A192B6J6
a	136	HIS	-	expression tag	UNP A0A192B6J6
a	137	HIS	-	expression tag	UNP A0A192B6J6
a	138	HIS	-	expression tag	UNP A0A192B6J6
a	139	HIS	-	expression tag	UNP A0A192B6J6

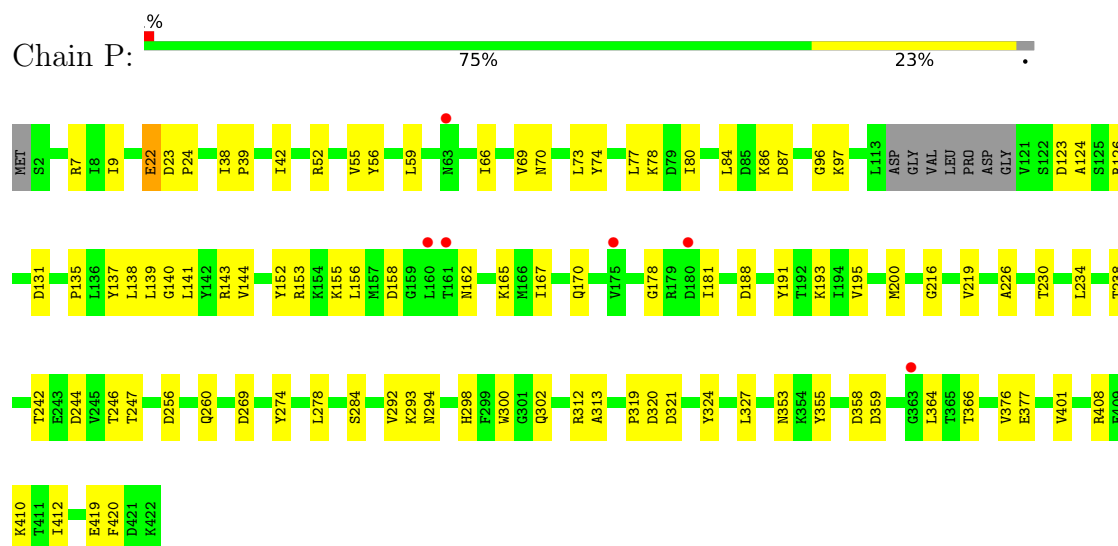
- Molecule 3 is a RNA chain called RNA (45-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	u	45	Total	C	N	O	P	0	0	0
			900	405	90	360	45			
3	v	45	Total	C	N	O	P	0	0	0
			900	405	90	360	45			
3	w	45	Total	C	N	O	P	0	0	0
			900	405	90	360	45			
3	x	45	Total	C	N	O	P	0	0	0
			900	405	90	360	45			

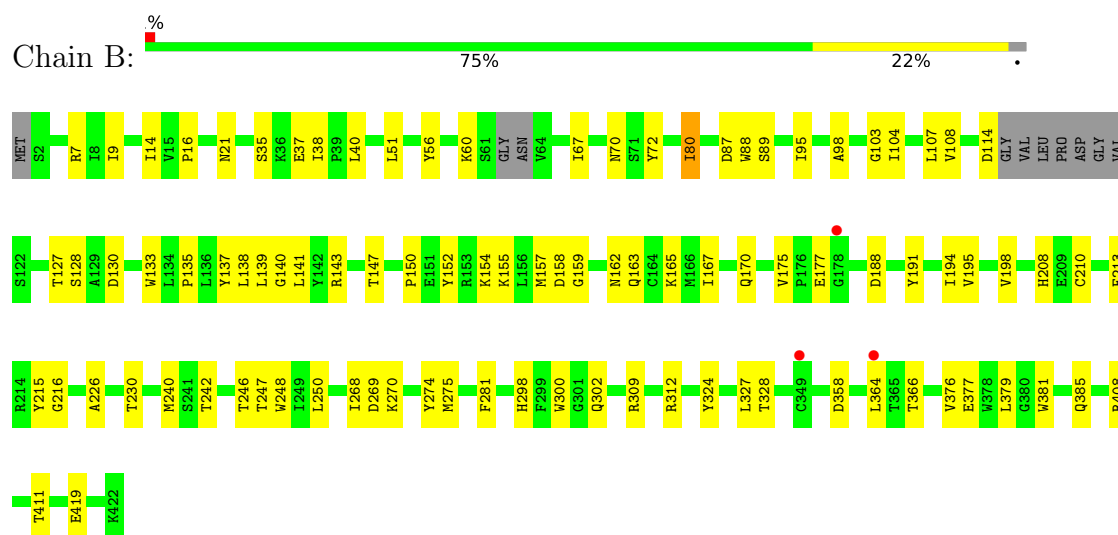
3 Residue-property plots [i](#)

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.

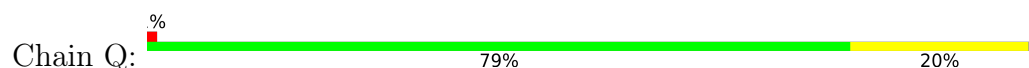
• Molecule 1: Nucleoprotein

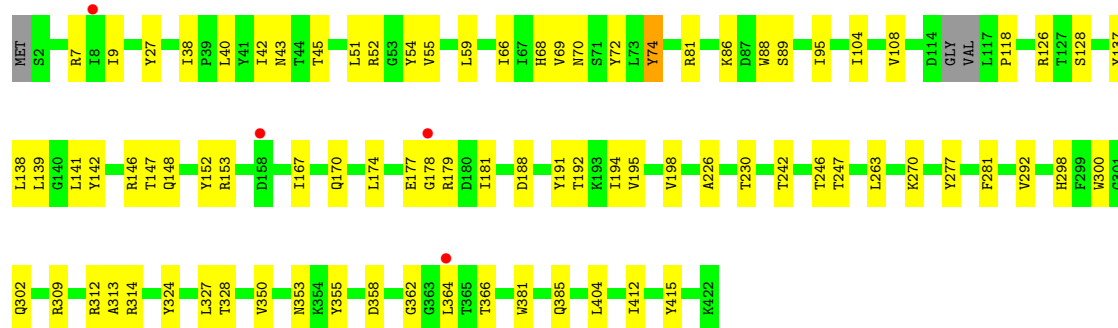


• Molecule 1: Nucleoprotein

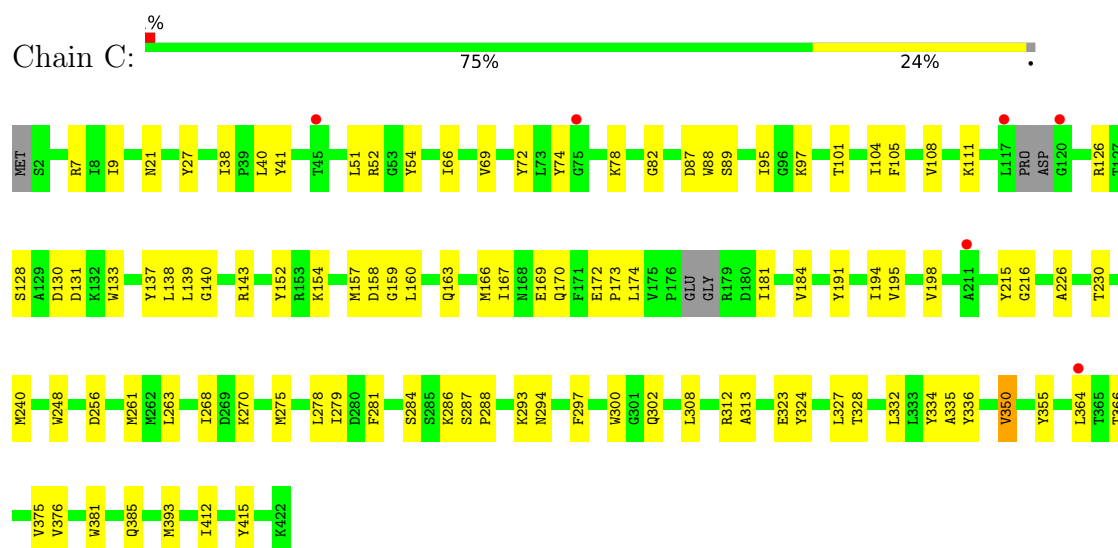


• Molecule 1: Nucleoprotein

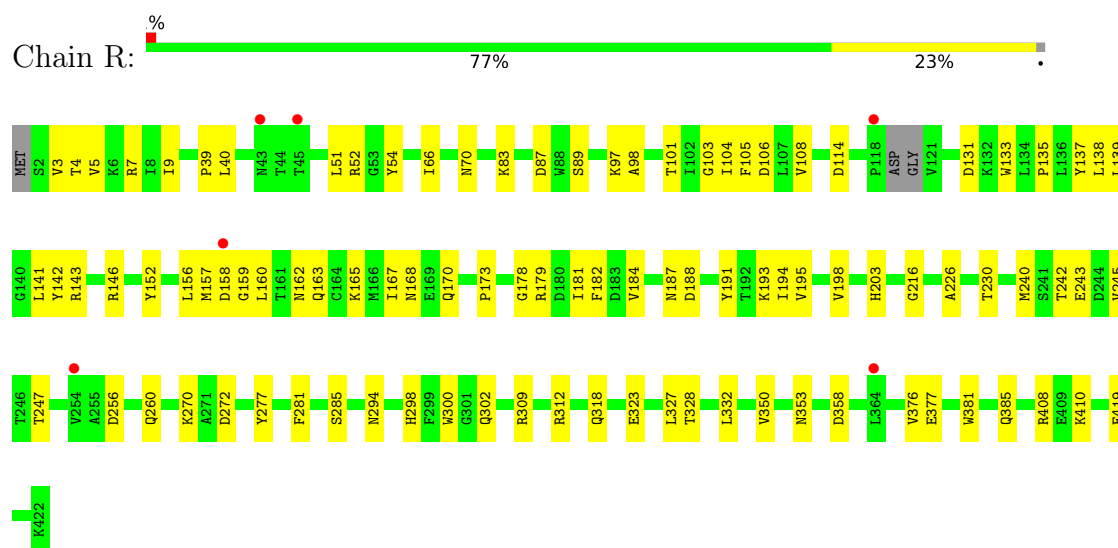




• Molecule 1: Nucleoprotein

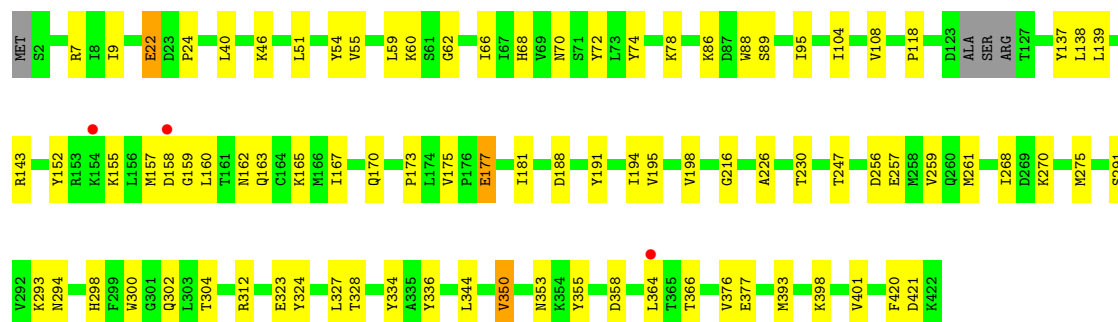


• Molecule 1: Nucleoprotein



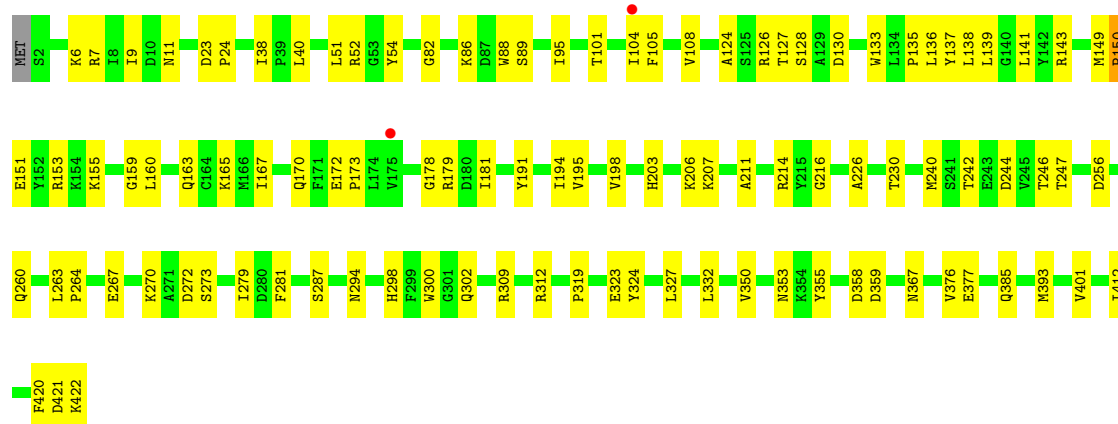
• Molecule 1: Nucleoprotein





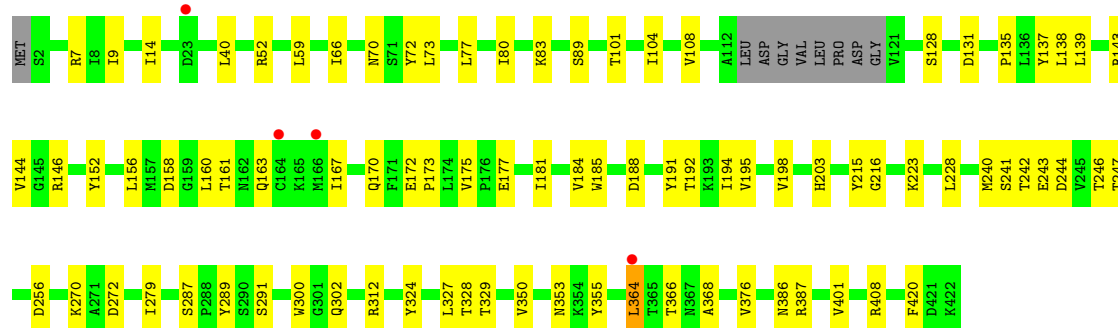
• Molecule 1: Nucleoprotein

Chain S: 75% 24%



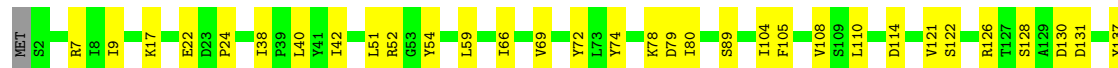
• Molecule 1: Nucleoprotein

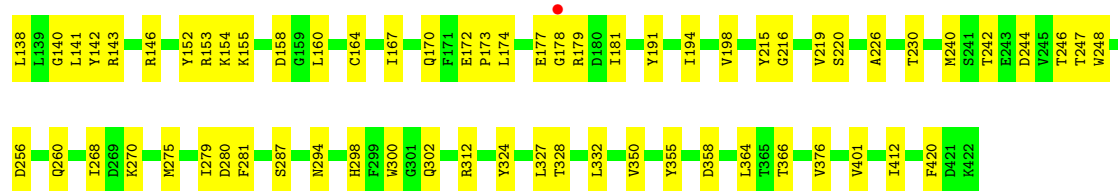
Chain E: 78% 20%



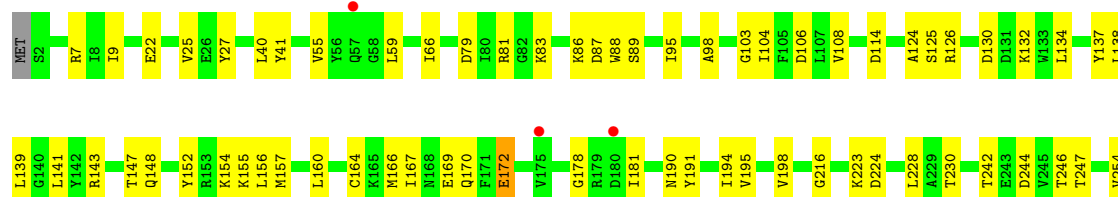
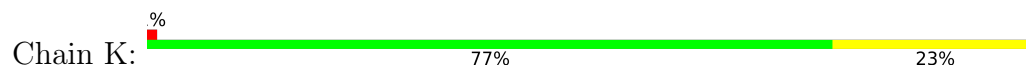
• Molecule 1: Nucleoprotein

Chain T: 77% 23%

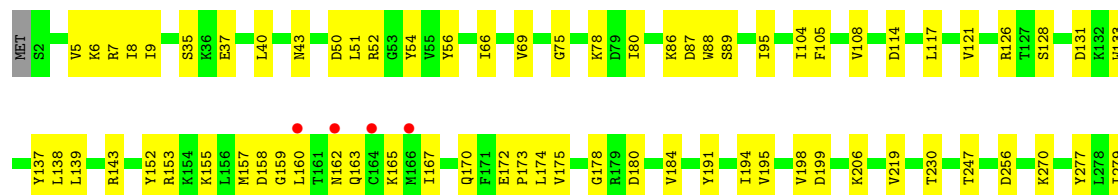
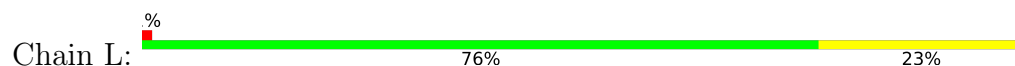




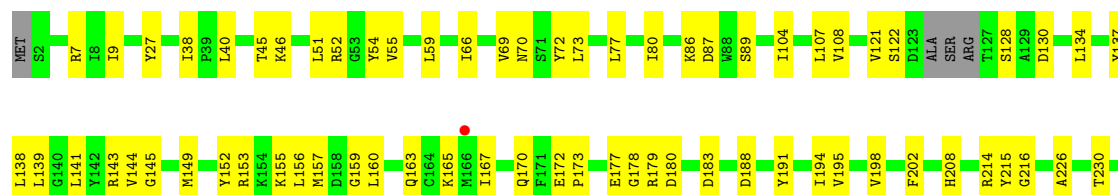
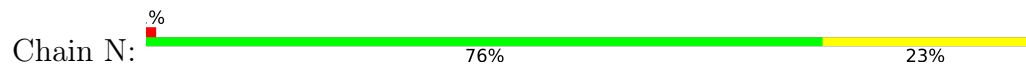
● Molecule 1: Nucleoprotein



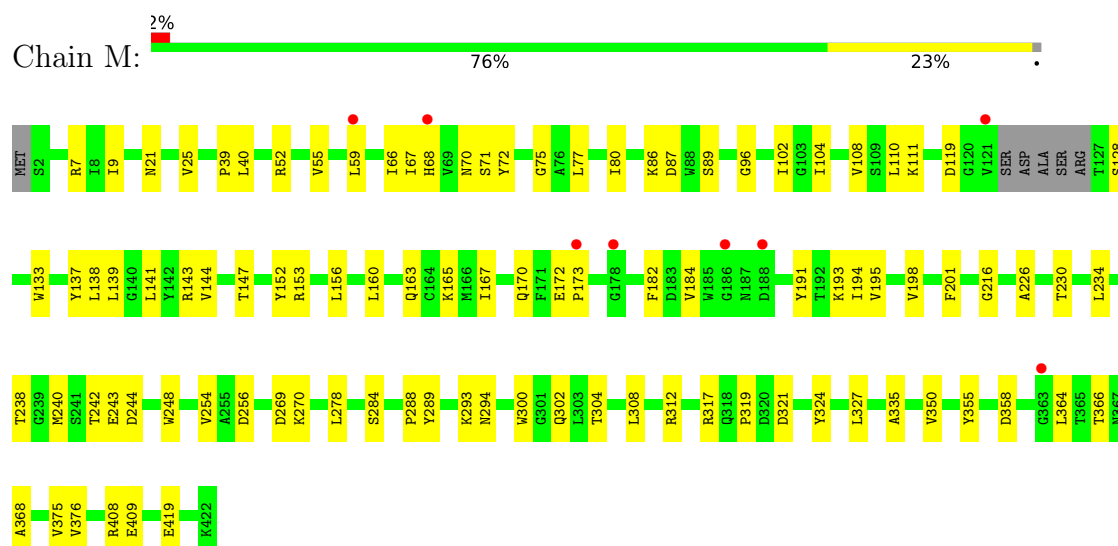
● Molecule 1: Nucleoprotein



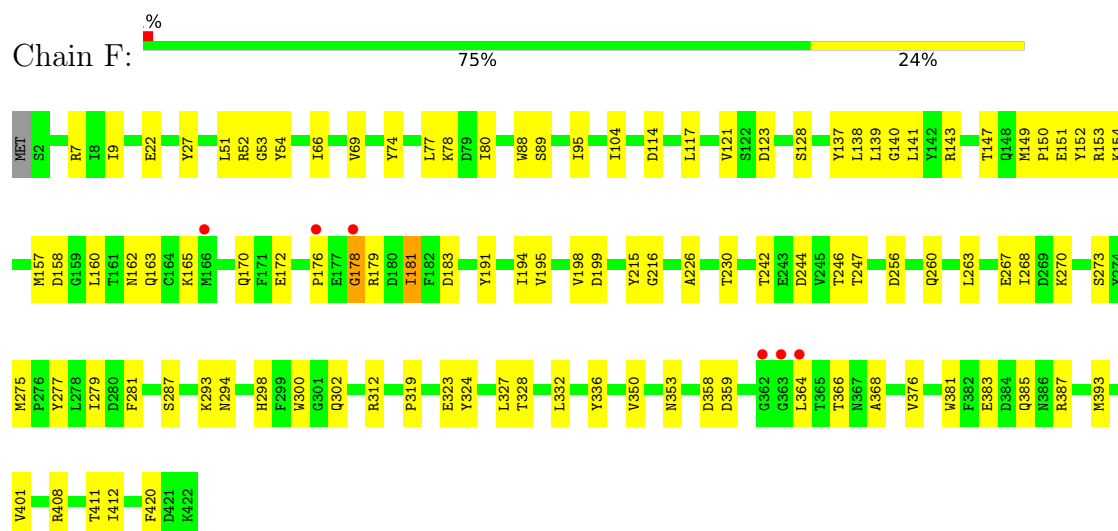
● Molecule 1: Nucleoprotein



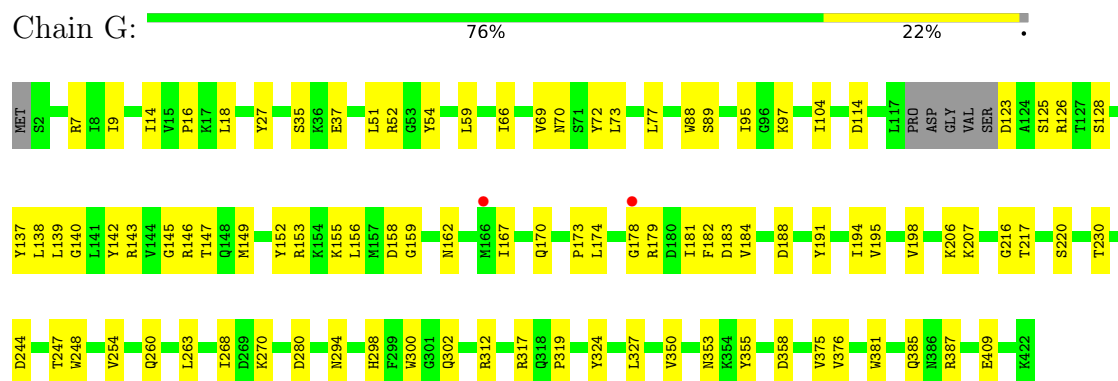
● Molecule 1: Nucleoprotein



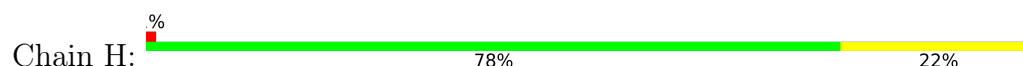
• Molecule 1: Nucleoprotein

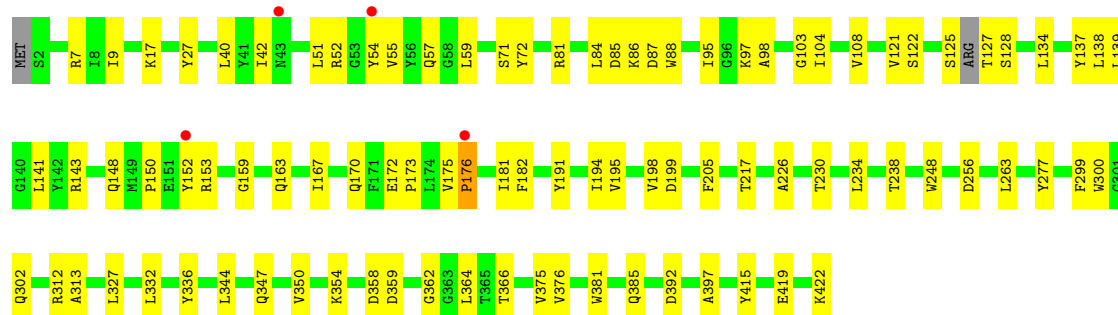


• Molecule 1: Nucleoprotein



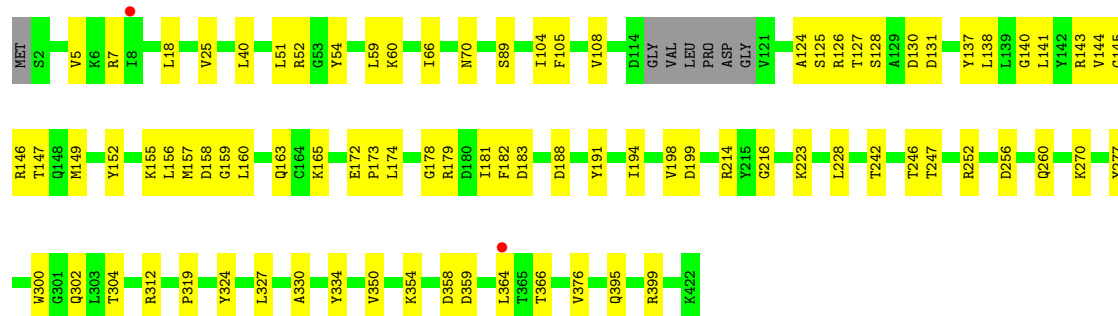
• Molecule 1: Nucleoprotein





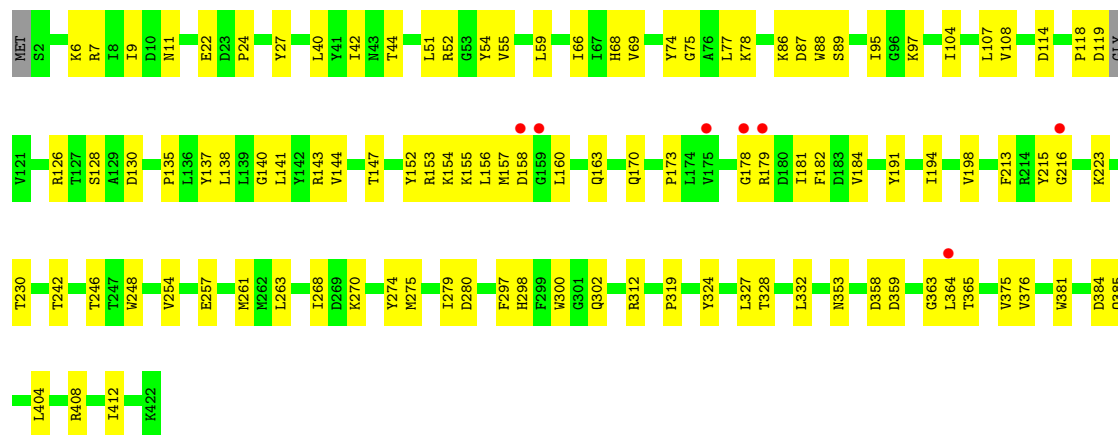
• Molecule 1: Nucleoprotein

Chain I: 78% 20%



• Molecule 1: Nucleoprotein

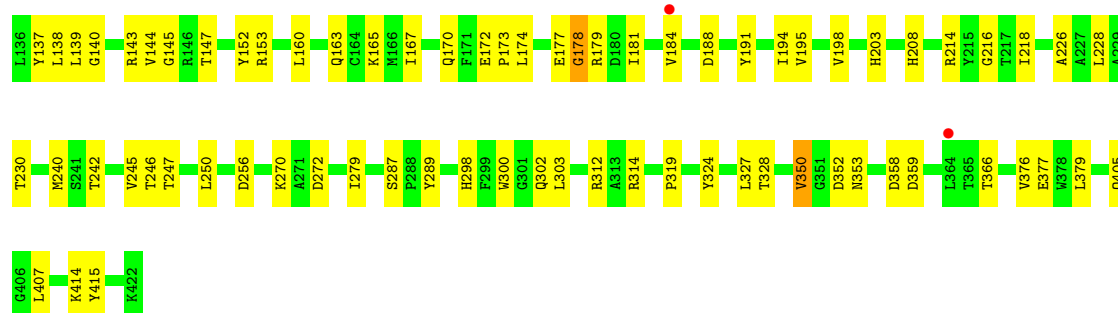
Chain O: 2% 74% 25%



• Molecule 1: Nucleoprotein

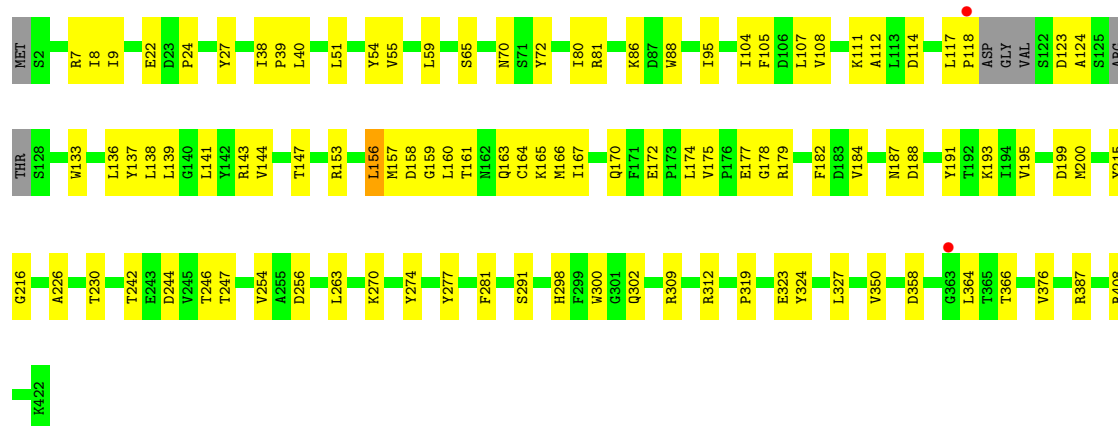
Chain J: 75% 24%





• Molecule 1: Nucleoprotein

Chain A: 75% 24%



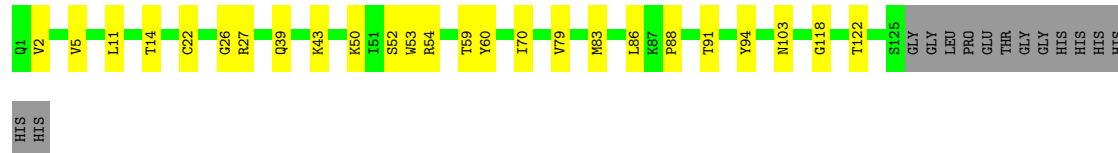
• Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain p: 74% 15% 10%



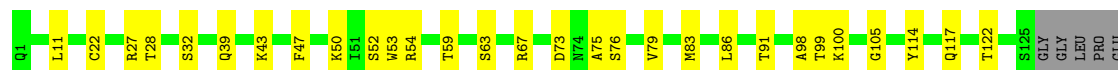
• Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain b: 72% 18% 10%



• Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain q: 69% 21% 10%



THR
GLY
GLY
HIS
HIS
HIS
HIS
HIS
HIS

• Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain c: 71% 19% 10%

Q1 V2 L11 C22 G26 S32 Q39 A40 K43 A49 K50 S51 S52 W53 R54 T59 R67 F68 V79 L82 M83 L86 D90 T91 T99 N103 G104 G105 T122 S125 GLY GLY LEU PRO GLU THR GLY GLY HIS HIS HIS HIS

HIS

• Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain r: 72% 18% 10%

Q1 V2 V5 L11 C22 G26 R27 S32 D46 K50 R54 T59 S63 V79 M83 L86 E89 D90 T91 A98 T99 K100 A101 T102 N103 Y114 V121 T122 S125 GLY GLY LEU PRO GLU THR GLY GLY HIS HIS HIS HIS

HIS

• Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain d: 69% 20% 10%

Q1 V2 L11 L20 S21 C22 S25 G26 R27 S32 I33 A40 K43 A49 K50 I51 S52 W53 T59 S63 R67 V79 Y80 L81 L82 M83 L86 D90 T91 T99 N103 G104 G105 Q117 T122 S125 GLY GLY LEU PRO GLU THR

GLY
GLY
HIS
HIS
HIS
HIS
HIS
HIS

• Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain s: 65% 25% 10%

Q1 V2 V5 V12 S17 C22 G26 R27 S32 I33 N34 F37 A40 K43 E44 R45 K50 I51 S52 W53 R54 T59 R67 R72 D73 N74 N77 M78 V79 M83 L86 D90 T91 T99 K100 N103 G104 G105 V121 T122

V123 S124 S125 GLY GLY LEU PRO THR GLY GLY HIS HIS HIS HIS HIS

• Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain e: 76% 14% 10%

Q1 V2 E6 S21 C22 G26 K50 S51 S52 W53 R54 T59 V79 M83 L86 T91 K100 A101 Y102 F112 W115 T122 S125 GLY GLY LEU PRO GLU THR GLY GLY HIS HIS HIS HIS HIS

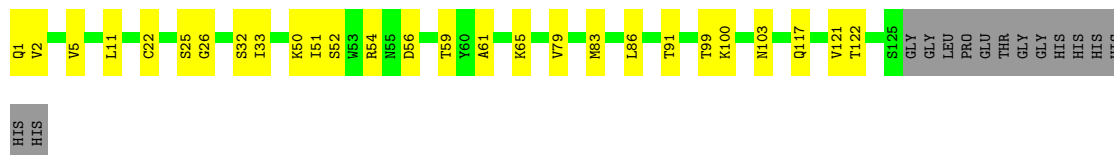
• Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain t: 73% 17% 10%



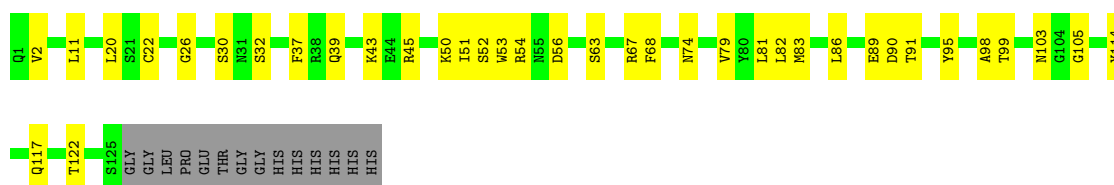
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain k: 71% 19% 10%



- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain l: 63% 27% 10%



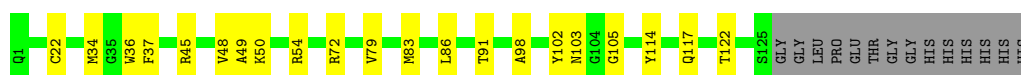
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain n: 65% 25% 10%



- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain m: 75% 15% 10%



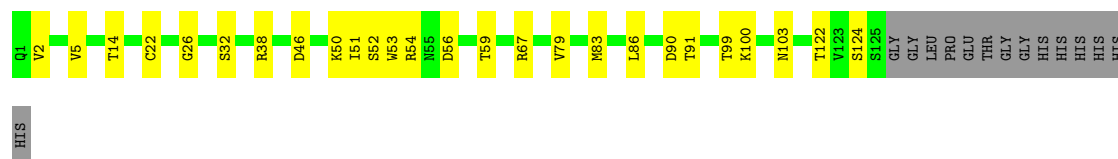
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain f: 73% 17% 10%



- Molecule 2: Anti-vesicular stomatitis virus N VHH

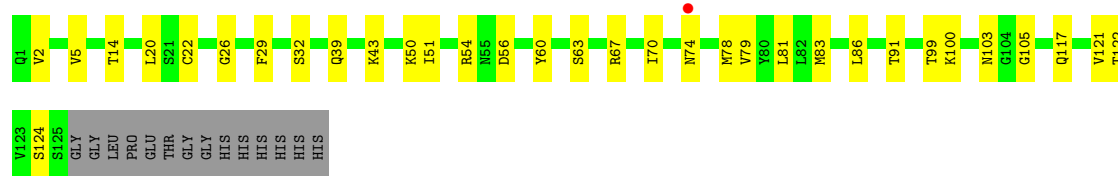
Chain g: 71% 19% 10%



• Molecule 2: Anti-vesicular stomatitis virus N VHH



• Molecule 2: Anti-vesicular stomatitis virus N VHH



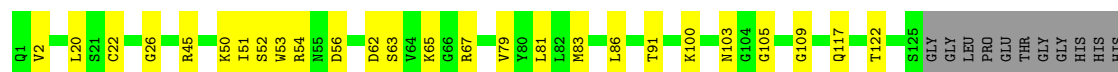
• Molecule 2: Anti-vesicular stomatitis virus N VHH



• Molecule 2: Anti-vesicular stomatitis virus N VHH



• Molecule 2: Anti-vesicular stomatitis virus N VHH



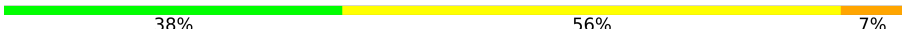
HIS
HIS
HIS

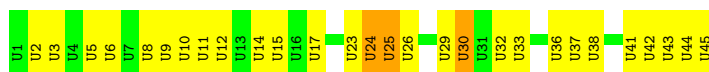
• Molecule 3: RNA (45-MER)

Chain u:  40% 42% 18%

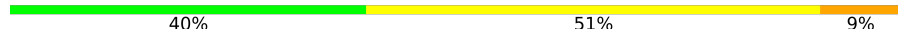


• Molecule 3: RNA (45-MER)

Chain v:  38% 56% 7%

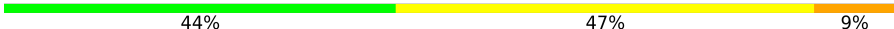


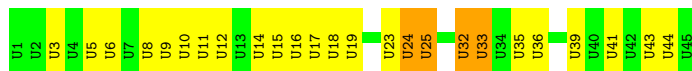
• Molecule 3: RNA (45-MER)

Chain w:  40% 51% 9%



• Molecule 3: RNA (45-MER)

Chain x:  44% 47% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	147.56Å 156.01Å 217.45Å 79.24° 75.66° 62.27°	Depositor
Resolution (Å)	128.35 – 3.20 128.35 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.0 (128.35-3.20) 91.9 (128.35-3.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.236 , 0.288 0.237 , 0.286	Depositor DCC
R_{free} test set	1990 reflections (0.73%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 5.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	89086	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.12	0/3364	0.31	0/4551
1	B	0.11	0/3343	0.31	0/4521
1	C	0.10	0/3372	0.30	0/4561
1	D	0.11	0/3380	0.30	0/4575
1	E	0.11	0/3347	0.32	0/4528
1	F	0.11	0/3403	0.31	0/4607
1	G	0.11	0/3369	0.33	0/4558
1	H	0.13	0/3391	0.33	0/4590
1	I	0.11	0/3363	0.31	0/4550
1	J	0.11	0/3398	0.31	0/4599
1	K	0.11	0/3403	0.32	0/4607
1	L	0.11	0/3403	0.34	1/4607 (0.0%)
1	M	0.12	0/3366	0.30	0/4556
1	N	0.10	0/3380	0.33	0/4575
1	O	0.11	0/3398	0.31	0/4599
1	P	0.11	0/3355	0.31	0/4539
1	Q	0.12	0/3391	0.33	1/4589 (0.0%)
1	R	0.12	0/3390	0.31	0/4588
1	S	0.13	0/3403	0.34	0/4607
1	T	0.11	0/3403	0.31	0/4607
2	a	0.09	0/988	0.30	0/1334
2	b	0.09	0/988	0.31	0/1334
2	c	0.10	0/988	0.31	0/1334
2	d	0.10	0/988	0.33	0/1334
2	e	0.10	0/988	0.32	0/1334
2	f	0.10	0/988	0.30	0/1334
2	g	0.10	0/988	0.30	0/1334
2	h	0.10	0/988	0.31	0/1334
2	i	0.10	0/988	0.32	0/1334
2	j	0.09	0/988	0.31	0/1334
2	k	0.09	0/988	0.31	0/1334
2	l	0.09	0/988	0.30	0/1334
2	m	0.09	0/988	0.29	0/1334
2	n	0.09	0/988	0.30	0/1334

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	o	0.09	0/988	0.30	0/1334
2	p	0.09	0/988	0.30	0/1334
2	q	0.09	0/988	0.30	0/1334
2	r	0.09	0/988	0.32	0/1334
2	s	0.09	0/988	0.31	0/1334
2	t	0.09	0/988	0.33	0/1334
3	u	0.14	0/989	0.42	0/1526
3	v	0.14	0/989	0.42	0/1526
3	w	0.14	0/989	0.42	0/1526
3	x	0.14	0/989	0.44	0/1526
All	All	0.11	0/91338	0.32	2/124298 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	292	VAL	N-CA-C	-6.22	106.74	112.96
1	L	292	VAL	N-CA-C	-6.12	106.84	112.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	152	TYR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3290	0	3249	71	0
1	B	3270	0	3230	64	0
1	C	3299	0	3265	69	0
1	D	3305	0	3263	65	0
1	E	3273	0	3234	58	0
1	F	3327	0	3287	74	0
1	G	3295	0	3258	73	0
1	H	3316	0	3273	60	0
1	I	3289	0	3249	66	0
1	J	3323	0	3283	83	0
1	K	3327	0	3287	65	0
1	L	3327	0	3287	79	1
1	M	3291	0	3254	71	0
1	N	3305	0	3263	71	0
1	O	3323	0	3283	79	0
1	P	3281	0	3245	64	0
1	Q	3316	0	3274	58	1
1	R	3315	0	3279	72	0
1	S	3327	0	3287	77	0
1	T	3327	0	3287	74	0
2	a	968	0	932	16	0
2	b	968	0	932	16	0
2	c	968	0	932	19	0
2	d	968	0	932	20	0
2	e	968	0	932	12	0
2	f	968	0	932	18	0
2	g	968	0	932	17	0
2	h	968	0	932	23	0
2	i	968	0	932	20	0
2	j	968	0	932	19	0
2	k	968	0	932	19	0
2	l	968	0	932	26	0
2	m	968	0	932	14	0
2	n	968	0	932	22	0
2	o	968	0	932	16	0
2	p	968	0	932	15	0
2	q	968	0	932	19	0
2	r	968	0	932	18	0
2	s	968	0	932	26	0
2	t	968	0	932	16	0
3	u	900	0	451	23	0
3	v	900	0	451	17	0
3	w	900	0	451	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	x	900	0	451	17	0
All	All	89086	0	85781	1619	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 1619 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:D:158:ASP:O	1:D:162:ASN:HB2	1.45	1.14
1:M:55:VAL:O	1:M:59:LEU:HD13	1.63	0.97
1:G:158:ASP:O	1:G:162:ASN:HB2	1.66	0.93
1:L:300:TRP:HB2	1:L:327:LEU:HD12	1.51	0.93
1:K:300:TRP:HB2	1:K:327:LEU:HD12	1.51	0.92

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:81:ARG:NH1	1:L:87:ASP:OD2[1_565]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	410/422 (97%)	388 (95%)	22 (5%)	0	100	100
1	B	406/422 (96%)	372 (92%)	32 (8%)	2 (0%)	24	59
1	C	411/422 (97%)	384 (93%)	26 (6%)	1 (0%)	43	73
1	D	414/422 (98%)	383 (92%)	28 (7%)	3 (1%)	18	52
1	E	409/422 (97%)	379 (93%)	29 (7%)	1 (0%)	43	73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	419/422 (99%)	387 (92%)	27 (6%)	5 (1%)	10	42
1	G	412/422 (98%)	379 (92%)	32 (8%)	1 (0%)	43	73
1	H	416/422 (99%)	384 (92%)	29 (7%)	3 (1%)	18	52
1	I	411/422 (97%)	385 (94%)	26 (6%)	0	100	100
1	J	416/422 (99%)	385 (92%)	28 (7%)	3 (1%)	18	52
1	K	419/422 (99%)	387 (92%)	30 (7%)	2 (0%)	24	59
1	L	419/422 (99%)	388 (93%)	28 (7%)	3 (1%)	18	52
1	M	412/422 (98%)	379 (92%)	33 (8%)	0	100	100
1	N	414/422 (98%)	386 (93%)	26 (6%)	2 (0%)	24	59
1	O	416/422 (99%)	389 (94%)	26 (6%)	1 (0%)	43	73
1	P	410/422 (97%)	388 (95%)	21 (5%)	1 (0%)	43	73
1	Q	415/422 (98%)	394 (95%)	20 (5%)	1 (0%)	43	73
1	R	415/422 (98%)	381 (92%)	34 (8%)	0	100	100
1	S	419/422 (99%)	389 (93%)	29 (7%)	1 (0%)	43	73
1	T	419/422 (99%)	392 (94%)	26 (6%)	1 (0%)	43	73
2	a	123/139 (88%)	115 (94%)	8 (6%)	0	100	100
2	b	123/139 (88%)	120 (98%)	3 (2%)	0	100	100
2	c	123/139 (88%)	119 (97%)	4 (3%)	0	100	100
2	d	123/139 (88%)	118 (96%)	4 (3%)	1 (1%)	16	50
2	e	123/139 (88%)	116 (94%)	7 (6%)	0	100	100
2	f	123/139 (88%)	119 (97%)	4 (3%)	0	100	100
2	g	123/139 (88%)	117 (95%)	6 (5%)	0	100	100
2	h	123/139 (88%)	117 (95%)	6 (5%)	0	100	100
2	i	123/139 (88%)	119 (97%)	4 (3%)	0	100	100
2	j	123/139 (88%)	119 (97%)	4 (3%)	0	100	100
2	k	123/139 (88%)	118 (96%)	5 (4%)	0	100	100
2	l	123/139 (88%)	116 (94%)	7 (6%)	0	100	100
2	m	123/139 (88%)	115 (94%)	8 (6%)	0	100	100
2	n	123/139 (88%)	117 (95%)	6 (5%)	0	100	100
2	o	123/139 (88%)	118 (96%)	5 (4%)	0	100	100
2	p	123/139 (88%)	118 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	q	123/139 (88%)	117 (95%)	6 (5%)	0	100	100
2	r	123/139 (88%)	119 (97%)	4 (3%)	0	100	100
2	s	123/139 (88%)	117 (95%)	6 (5%)	0	100	100
2	t	123/139 (88%)	118 (96%)	5 (4%)	0	100	100
All	All	10742/11220 (96%)	10051 (94%)	659 (6%)	32 (0%)	36	68

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	d	2	VAL
1	L	367	ASN
1	N	121	VAL
1	N	178	GLY
1	F	121	VAL

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	358/363 (99%)	356 (99%)	2 (1%)	78	84
1	B	356/363 (98%)	356 (100%)	0	100	100
1	C	359/363 (99%)	359 (100%)	0	100	100
1	D	360/363 (99%)	360 (100%)	0	100	100
1	E	356/363 (98%)	356 (100%)	0	100	100
1	F	362/363 (100%)	362 (100%)	0	100	100
1	G	358/363 (99%)	358 (100%)	0	100	100
1	H	361/363 (99%)	361 (100%)	0	100	100
1	I	358/363 (99%)	358 (100%)	0	100	100
1	J	362/363 (100%)	362 (100%)	0	100	100
1	K	362/363 (100%)	361 (100%)	1 (0%)	86	88
1	L	362/363 (100%)	362 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	358/363 (99%)	358 (100%)	0	100	100
1	N	360/363 (99%)	360 (100%)	0	100	100
1	O	362/363 (100%)	362 (100%)	0	100	100
1	P	357/363 (98%)	357 (100%)	0	100	100
1	Q	361/363 (99%)	361 (100%)	0	100	100
1	R	361/363 (99%)	361 (100%)	0	100	100
1	S	362/363 (100%)	362 (100%)	0	100	100
1	T	362/363 (100%)	362 (100%)	0	100	100
2	a	101/111 (91%)	101 (100%)	0	100	100
2	b	101/111 (91%)	101 (100%)	0	100	100
2	c	101/111 (91%)	101 (100%)	0	100	100
2	d	101/111 (91%)	101 (100%)	0	100	100
2	e	101/111 (91%)	101 (100%)	0	100	100
2	f	101/111 (91%)	101 (100%)	0	100	100
2	g	101/111 (91%)	101 (100%)	0	100	100
2	h	101/111 (91%)	101 (100%)	0	100	100
2	i	101/111 (91%)	101 (100%)	0	100	100
2	j	101/111 (91%)	101 (100%)	0	100	100
2	k	101/111 (91%)	101 (100%)	0	100	100
2	l	101/111 (91%)	101 (100%)	0	100	100
2	m	101/111 (91%)	101 (100%)	0	100	100
2	n	101/111 (91%)	101 (100%)	0	100	100
2	o	101/111 (91%)	101 (100%)	0	100	100
2	p	101/111 (91%)	100 (99%)	1 (1%)	68	80
2	q	101/111 (91%)	101 (100%)	0	100	100
2	r	101/111 (91%)	101 (100%)	0	100	100
2	s	101/111 (91%)	101 (100%)	0	100	100
2	t	101/111 (91%)	101 (100%)	0	100	100
All	All	9217/9480 (97%)	9213 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	p	79	VAL
1	K	25	VAL
1	A	156	LEU
1	A	160	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	294	ASN
1	H	11	ASN
1	F	162	ASN
1	F	405	GLN
1	I	190	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	u	44/45 (97%)	15 (34%)	0
3	v	44/45 (97%)	14 (31%)	0
3	w	44/45 (97%)	15 (34%)	0
3	x	44/45 (97%)	13 (29%)	0
All	All	176/180 (97%)	57 (32%)	0

5 of 57 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	u	3	U
3	u	5	U
3	u	11	U
3	u	12	U
3	u	14	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	416/422 (98%)	0.03	2 (0%) 87 76	35, 55, 77, 101	0
1	B	412/422 (97%)	0.08	3 (0%) 84 69	36, 64, 85, 93	0
1	C	417/422 (98%)	0.09	6 (1%) 73 54	39, 63, 82, 99	0
1	D	418/422 (99%)	0.06	3 (0%) 84 69	35, 61, 79, 100	0
1	E	413/422 (97%)	0.01	4 (0%) 79 63	34, 56, 77, 89	0
1	F	421/422 (99%)	0.07	6 (1%) 73 54	34, 54, 78, 91	0
1	G	416/422 (98%)	0.04	2 (0%) 87 76	36, 60, 83, 97	0
1	H	420/422 (99%)	0.12	4 (0%) 79 63	34, 64, 85, 93	0
1	I	415/422 (98%)	-0.05	2 (0%) 87 76	35, 56, 76, 100	0
1	J	420/422 (99%)	0.02	3 (0%) 84 69	35, 56, 78, 91	0
1	K	421/422 (99%)	-0.04	4 (0%) 79 63	34, 55, 76, 85	0
1	L	421/422 (99%)	-0.06	4 (0%) 79 63	35, 53, 73, 87	0
1	M	416/422 (98%)	0.21	8 (1%) 66 46	36, 62, 85, 108	0
1	N	418/422 (99%)	-0.00	3 (0%) 84 69	37, 60, 82, 96	0
1	O	420/422 (99%)	0.00	7 (1%) 69 49	34, 51, 74, 94	0
1	P	414/422 (98%)	-0.02	6 (1%) 73 54	35, 57, 77, 99	0
1	Q	419/422 (99%)	0.04	4 (0%) 79 63	35, 57, 75, 94	0
1	R	419/422 (99%)	0.05	6 (1%) 73 54	36, 63, 82, 100	0
1	S	421/422 (99%)	0.06	2 (0%) 87 76	36, 61, 83, 101	0
1	T	421/422 (99%)	-0.05	1 (0%) 91 85	34, 53, 75, 95	0
2	a	125/139 (89%)	-0.07	0 100 100	35, 51, 66, 75	0
2	b	125/139 (89%)	-0.17	0 100 100	40, 53, 69, 78	0
2	c	125/139 (89%)	-0.13	0 100 100	40, 55, 69, 76	0
2	d	125/139 (89%)	-0.13	0 100 100	39, 52, 65, 76	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	e	125/139 (89%)	-0.18	0 100 100	38, 50, 65, 74	0
2	f	125/139 (89%)	-0.13	0 100 100	38, 52, 66, 73	0
2	g	125/139 (89%)	-0.14	0 100 100	40, 53, 67, 75	0
2	h	125/139 (89%)	-0.16	1 (0%) 82 67	38, 50, 68, 74	0
2	i	125/139 (89%)	-0.15	1 (0%) 82 67	37, 48, 67, 78	0
2	j	125/139 (89%)	-0.11	0 100 100	35, 49, 62, 70	0
2	k	125/139 (89%)	-0.25	0 100 100	37, 48, 66, 76	0
2	l	125/139 (89%)	-0.19	0 100 100	38, 51, 65, 79	0
2	m	125/139 (89%)	-0.09	0 100 100	39, 53, 68, 76	0
2	n	125/139 (89%)	-0.20	0 100 100	41, 54, 71, 79	0
2	o	125/139 (89%)	0.01	0 100 100	37, 51, 64, 73	0
2	p	125/139 (89%)	-0.19	0 100 100	37, 51, 68, 76	0
2	q	125/139 (89%)	-0.15	0 100 100	37, 50, 70, 78	0
2	r	125/139 (89%)	-0.18	0 100 100	40, 53, 65, 83	0
2	s	125/139 (89%)	-0.20	1 (0%) 82 67	35, 50, 66, 79	0
2	t	125/139 (89%)	-0.06	1 (0%) 82 67	35, 47, 63, 69	0
3	u	45/45 (100%)	-0.39	0 100 100	44, 56, 68, 74	0
3	v	45/45 (100%)	-0.44	0 100 100	42, 54, 65, 76	0
3	w	45/45 (100%)	-0.42	0 100 100	44, 58, 71, 75	0
3	x	45/45 (100%)	-0.54	0 100 100	45, 52, 65, 71	0
All	All	11038/11400 (96%)	-0.02	84 (0%) 82 67	34, 55, 79, 108	0

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	178	GLY	6.1
1	P	180	ASP	4.9
1	P	160	LEU	4.2
1	K	180	ASP	3.6
1	I	8	ILE	3.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.