



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:52 PM UTC

PDB ID : 5ZJU / pdb_00005zju
Title : Crystal structure of in vitro expressed and assembled PCV2 Virus-like Particle
Authors : Yuan, Y.A.; Mo, X.
Deposited on : 2018-03-22
Resolution : 2.80 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

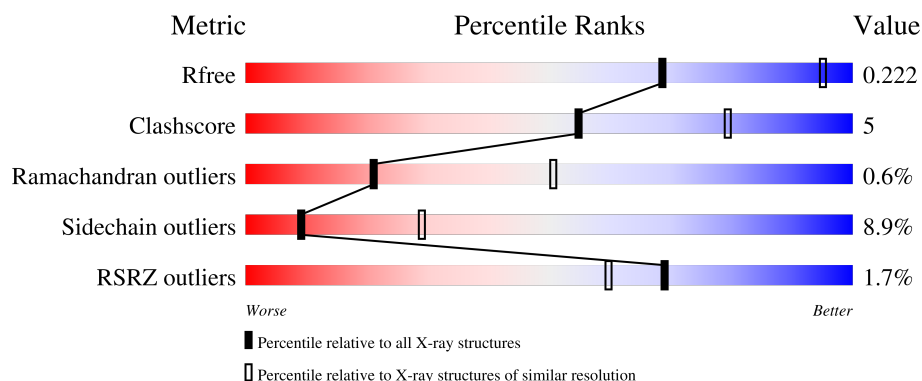
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	1	209	% 73% 14% • 10%
1	2	209	3% 72% 15% • 10%
1	3	209	% 70% 17% •• 10%
1	4	209	% 75% 13% • 10%
1	5	209	% 74% 12% • 10%

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Mol	Chain	Length	Quality of chain
1	6	209	
1	7	209	
1	8	209	
1	9	209	
1	A	209	
1	B	209	
1	C	209	
1	D	209	
1	E	209	
1	F	209	
1	G	209	
1	H	209	
1	I	209	
1	J	209	
1	K	209	
1	L	209	
1	M	209	
1	N	209	
1	O	209	
1	P	209	
1	Q	209	
1	R	209	
1	S	209	
1	T	209	
1	U	209	

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Mol	Chain	Length	Quality of chain
1	V	209	
1	W	209	
1	X	209	
1	Y	209	
1	Z	209	
1	a	209	
1	b	209	
1	c	209	
1	d	209	
1	e	209	
1	f	209	
1	g	209	
1	h	209	
1	i	209	
1	j	209	
1	k	209	
1	l	209	
1	m	209	
1	n	209	
1	o	209	
1	p	209	
1	q	209	
1	r	209	
1	s	209	
1	t	209	

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Mol	Chain	Length	Quality of chain
1	u	209	
1	v	209	
1	w	209	
1	x	209	
1	y	209	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 97686 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	B	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	C	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	D	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	E	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	F	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	G	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	H	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	I	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	J	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	K	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	L	189	Total	C	N	O	S	0	0	0
			1554	996	270	284	4			
1	M	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	N	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	O	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	P	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	R	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	S	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	T	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	U	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	V	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	W	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	X	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	Y	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	Z	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	1	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	2	189	Total 1554	C 996	N 270	O 284	S 4	0	0	0
1	3	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	4	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	5	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	6	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	7	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	8	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	9	189	Total 1554	C 996	N 270	O 284	S 4	0	0	0
1	a	189	Total 1554	C 996	N 270	O 284	S 4	0	0	0
1	b	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	c	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	d	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	e	189	Total 1554	C 996	N 270	O 284	S 4	0	0	0
1	f	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	g	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	h	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	i	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	j	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	k	189	Total 1554	C 996	N 270	O 284	S 4	0	0	0
1	l	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	m	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	n	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	o	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	p	189	Total 1554	C 996	N 270	O 284	S 4	0	0	0
1	q	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	r	189	Total 1554	C 996	N 270	O 284	S 4	0	0	0
1	s	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	t	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	u	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	v	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0
1	w	188	Total 1546	C 990	N 269	O 283	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	x	189	Total	C	N	O	S	0	0	0
			1554	996	270	284	4			
1	y	189	Total	C	N	O	S	0	0	0
			1554	996	270	284	4			

There are 1200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	expression tag	UNP G0Y2B2
A	26	GLY	-	expression tag	UNP G0Y2B2
A	27	SER	-	expression tag	UNP G0Y2B2
A	28	SER	-	expression tag	UNP G0Y2B2
A	29	HIS	-	expression tag	UNP G0Y2B2
A	30	HIS	-	expression tag	UNP G0Y2B2
A	31	HIS	-	expression tag	UNP G0Y2B2
A	32	HIS	-	expression tag	UNP G0Y2B2
A	33	HIS	-	expression tag	UNP G0Y2B2
A	34	HIS	-	expression tag	UNP G0Y2B2
A	35	SER	-	expression tag	UNP G0Y2B2
A	36	SER	-	expression tag	UNP G0Y2B2
A	37	GLY	-	expression tag	UNP G0Y2B2
A	38	LEU	-	expression tag	UNP G0Y2B2
A	39	VAL	-	expression tag	UNP G0Y2B2
A	40	PRO	-	expression tag	UNP G0Y2B2
A	41	ARG	-	expression tag	UNP G0Y2B2
A	42	GLY	-	expression tag	UNP G0Y2B2
A	43	SER	-	expression tag	UNP G0Y2B2
A	44	HIS	-	expression tag	UNP G0Y2B2
B	25	MET	-	expression tag	UNP G0Y2B2
B	26	GLY	-	expression tag	UNP G0Y2B2
B	27	SER	-	expression tag	UNP G0Y2B2
B	28	SER	-	expression tag	UNP G0Y2B2
B	29	HIS	-	expression tag	UNP G0Y2B2
B	30	HIS	-	expression tag	UNP G0Y2B2
B	31	HIS	-	expression tag	UNP G0Y2B2
B	32	HIS	-	expression tag	UNP G0Y2B2
B	33	HIS	-	expression tag	UNP G0Y2B2
B	34	HIS	-	expression tag	UNP G0Y2B2
B	35	SER	-	expression tag	UNP G0Y2B2
B	36	SER	-	expression tag	UNP G0Y2B2
B	37	GLY	-	expression tag	UNP G0Y2B2
B	38	LEU	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	39	VAL	-	expression tag	UNP G0Y2B2
B	40	PRO	-	expression tag	UNP G0Y2B2
B	41	ARG	-	expression tag	UNP G0Y2B2
B	42	GLY	-	expression tag	UNP G0Y2B2
B	43	SER	-	expression tag	UNP G0Y2B2
B	44	HIS	-	expression tag	UNP G0Y2B2
C	25	MET	-	expression tag	UNP G0Y2B2
C	26	GLY	-	expression tag	UNP G0Y2B2
C	27	SER	-	expression tag	UNP G0Y2B2
C	28	SER	-	expression tag	UNP G0Y2B2
C	29	HIS	-	expression tag	UNP G0Y2B2
C	30	HIS	-	expression tag	UNP G0Y2B2
C	31	HIS	-	expression tag	UNP G0Y2B2
C	32	HIS	-	expression tag	UNP G0Y2B2
C	33	HIS	-	expression tag	UNP G0Y2B2
C	34	HIS	-	expression tag	UNP G0Y2B2
C	35	SER	-	expression tag	UNP G0Y2B2
C	36	SER	-	expression tag	UNP G0Y2B2
C	37	GLY	-	expression tag	UNP G0Y2B2
C	38	LEU	-	expression tag	UNP G0Y2B2
C	39	VAL	-	expression tag	UNP G0Y2B2
C	40	PRO	-	expression tag	UNP G0Y2B2
C	41	ARG	-	expression tag	UNP G0Y2B2
C	42	GLY	-	expression tag	UNP G0Y2B2
C	43	SER	-	expression tag	UNP G0Y2B2
C	44	HIS	-	expression tag	UNP G0Y2B2
D	25	MET	-	expression tag	UNP G0Y2B2
D	26	GLY	-	expression tag	UNP G0Y2B2
D	27	SER	-	expression tag	UNP G0Y2B2
D	28	SER	-	expression tag	UNP G0Y2B2
D	29	HIS	-	expression tag	UNP G0Y2B2
D	30	HIS	-	expression tag	UNP G0Y2B2
D	31	HIS	-	expression tag	UNP G0Y2B2
D	32	HIS	-	expression tag	UNP G0Y2B2
D	33	HIS	-	expression tag	UNP G0Y2B2
D	34	HIS	-	expression tag	UNP G0Y2B2
D	35	SER	-	expression tag	UNP G0Y2B2
D	36	SER	-	expression tag	UNP G0Y2B2
D	37	GLY	-	expression tag	UNP G0Y2B2
D	38	LEU	-	expression tag	UNP G0Y2B2
D	39	VAL	-	expression tag	UNP G0Y2B2
D	40	PRO	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	41	ARG	-	expression tag	UNP G0Y2B2
D	42	GLY	-	expression tag	UNP G0Y2B2
D	43	SER	-	expression tag	UNP G0Y2B2
D	44	HIS	-	expression tag	UNP G0Y2B2
E	25	MET	-	expression tag	UNP G0Y2B2
E	26	GLY	-	expression tag	UNP G0Y2B2
E	27	SER	-	expression tag	UNP G0Y2B2
E	28	SER	-	expression tag	UNP G0Y2B2
E	29	HIS	-	expression tag	UNP G0Y2B2
E	30	HIS	-	expression tag	UNP G0Y2B2
E	31	HIS	-	expression tag	UNP G0Y2B2
E	32	HIS	-	expression tag	UNP G0Y2B2
E	33	HIS	-	expression tag	UNP G0Y2B2
E	34	HIS	-	expression tag	UNP G0Y2B2
E	35	SER	-	expression tag	UNP G0Y2B2
E	36	SER	-	expression tag	UNP G0Y2B2
E	37	GLY	-	expression tag	UNP G0Y2B2
E	38	LEU	-	expression tag	UNP G0Y2B2
E	39	VAL	-	expression tag	UNP G0Y2B2
E	40	PRO	-	expression tag	UNP G0Y2B2
E	41	ARG	-	expression tag	UNP G0Y2B2
E	42	GLY	-	expression tag	UNP G0Y2B2
E	43	SER	-	expression tag	UNP G0Y2B2
E	44	HIS	-	expression tag	UNP G0Y2B2
F	25	MET	-	expression tag	UNP G0Y2B2
F	26	GLY	-	expression tag	UNP G0Y2B2
F	27	SER	-	expression tag	UNP G0Y2B2
F	28	SER	-	expression tag	UNP G0Y2B2
F	29	HIS	-	expression tag	UNP G0Y2B2
F	30	HIS	-	expression tag	UNP G0Y2B2
F	31	HIS	-	expression tag	UNP G0Y2B2
F	32	HIS	-	expression tag	UNP G0Y2B2
F	33	HIS	-	expression tag	UNP G0Y2B2
F	34	HIS	-	expression tag	UNP G0Y2B2
F	35	SER	-	expression tag	UNP G0Y2B2
F	36	SER	-	expression tag	UNP G0Y2B2
F	37	GLY	-	expression tag	UNP G0Y2B2
F	38	LEU	-	expression tag	UNP G0Y2B2
F	39	VAL	-	expression tag	UNP G0Y2B2
F	40	PRO	-	expression tag	UNP G0Y2B2
F	41	ARG	-	expression tag	UNP G0Y2B2
F	42	GLY	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	43	SER	-	expression tag	UNP G0Y2B2
F	44	HIS	-	expression tag	UNP G0Y2B2
G	25	MET	-	expression tag	UNP G0Y2B2
G	26	GLY	-	expression tag	UNP G0Y2B2
G	27	SER	-	expression tag	UNP G0Y2B2
G	28	SER	-	expression tag	UNP G0Y2B2
G	29	HIS	-	expression tag	UNP G0Y2B2
G	30	HIS	-	expression tag	UNP G0Y2B2
G	31	HIS	-	expression tag	UNP G0Y2B2
G	32	HIS	-	expression tag	UNP G0Y2B2
G	33	HIS	-	expression tag	UNP G0Y2B2
G	34	HIS	-	expression tag	UNP G0Y2B2
G	35	SER	-	expression tag	UNP G0Y2B2
G	36	SER	-	expression tag	UNP G0Y2B2
G	37	GLY	-	expression tag	UNP G0Y2B2
G	38	LEU	-	expression tag	UNP G0Y2B2
G	39	VAL	-	expression tag	UNP G0Y2B2
G	40	PRO	-	expression tag	UNP G0Y2B2
G	41	ARG	-	expression tag	UNP G0Y2B2
G	42	GLY	-	expression tag	UNP G0Y2B2
G	43	SER	-	expression tag	UNP G0Y2B2
G	44	HIS	-	expression tag	UNP G0Y2B2
H	25	MET	-	expression tag	UNP G0Y2B2
H	26	GLY	-	expression tag	UNP G0Y2B2
H	27	SER	-	expression tag	UNP G0Y2B2
H	28	SER	-	expression tag	UNP G0Y2B2
H	29	HIS	-	expression tag	UNP G0Y2B2
H	30	HIS	-	expression tag	UNP G0Y2B2
H	31	HIS	-	expression tag	UNP G0Y2B2
H	32	HIS	-	expression tag	UNP G0Y2B2
H	33	HIS	-	expression tag	UNP G0Y2B2
H	34	HIS	-	expression tag	UNP G0Y2B2
H	35	SER	-	expression tag	UNP G0Y2B2
H	36	SER	-	expression tag	UNP G0Y2B2
H	37	GLY	-	expression tag	UNP G0Y2B2
H	38	LEU	-	expression tag	UNP G0Y2B2
H	39	VAL	-	expression tag	UNP G0Y2B2
H	40	PRO	-	expression tag	UNP G0Y2B2
H	41	ARG	-	expression tag	UNP G0Y2B2
H	42	GLY	-	expression tag	UNP G0Y2B2
H	43	SER	-	expression tag	UNP G0Y2B2
H	44	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	25	MET	-	expression tag	UNP G0Y2B2
I	26	GLY	-	expression tag	UNP G0Y2B2
I	27	SER	-	expression tag	UNP G0Y2B2
I	28	SER	-	expression tag	UNP G0Y2B2
I	29	HIS	-	expression tag	UNP G0Y2B2
I	30	HIS	-	expression tag	UNP G0Y2B2
I	31	HIS	-	expression tag	UNP G0Y2B2
I	32	HIS	-	expression tag	UNP G0Y2B2
I	33	HIS	-	expression tag	UNP G0Y2B2
I	34	HIS	-	expression tag	UNP G0Y2B2
I	35	SER	-	expression tag	UNP G0Y2B2
I	36	SER	-	expression tag	UNP G0Y2B2
I	37	GLY	-	expression tag	UNP G0Y2B2
I	38	LEU	-	expression tag	UNP G0Y2B2
I	39	VAL	-	expression tag	UNP G0Y2B2
I	40	PRO	-	expression tag	UNP G0Y2B2
I	41	ARG	-	expression tag	UNP G0Y2B2
I	42	GLY	-	expression tag	UNP G0Y2B2
I	43	SER	-	expression tag	UNP G0Y2B2
I	44	HIS	-	expression tag	UNP G0Y2B2
J	25	MET	-	expression tag	UNP G0Y2B2
J	26	GLY	-	expression tag	UNP G0Y2B2
J	27	SER	-	expression tag	UNP G0Y2B2
J	28	SER	-	expression tag	UNP G0Y2B2
J	29	HIS	-	expression tag	UNP G0Y2B2
J	30	HIS	-	expression tag	UNP G0Y2B2
J	31	HIS	-	expression tag	UNP G0Y2B2
J	32	HIS	-	expression tag	UNP G0Y2B2
J	33	HIS	-	expression tag	UNP G0Y2B2
J	34	HIS	-	expression tag	UNP G0Y2B2
J	35	SER	-	expression tag	UNP G0Y2B2
J	36	SER	-	expression tag	UNP G0Y2B2
J	37	GLY	-	expression tag	UNP G0Y2B2
J	38	LEU	-	expression tag	UNP G0Y2B2
J	39	VAL	-	expression tag	UNP G0Y2B2
J	40	PRO	-	expression tag	UNP G0Y2B2
J	41	ARG	-	expression tag	UNP G0Y2B2
J	42	GLY	-	expression tag	UNP G0Y2B2
J	43	SER	-	expression tag	UNP G0Y2B2
J	44	HIS	-	expression tag	UNP G0Y2B2
K	25	MET	-	expression tag	UNP G0Y2B2
K	26	GLY	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	27	SER	-	expression tag	UNP G0Y2B2
K	28	SER	-	expression tag	UNP G0Y2B2
K	29	HIS	-	expression tag	UNP G0Y2B2
K	30	HIS	-	expression tag	UNP G0Y2B2
K	31	HIS	-	expression tag	UNP G0Y2B2
K	32	HIS	-	expression tag	UNP G0Y2B2
K	33	HIS	-	expression tag	UNP G0Y2B2
K	34	HIS	-	expression tag	UNP G0Y2B2
K	35	SER	-	expression tag	UNP G0Y2B2
K	36	SER	-	expression tag	UNP G0Y2B2
K	37	GLY	-	expression tag	UNP G0Y2B2
K	38	LEU	-	expression tag	UNP G0Y2B2
K	39	VAL	-	expression tag	UNP G0Y2B2
K	40	PRO	-	expression tag	UNP G0Y2B2
K	41	ARG	-	expression tag	UNP G0Y2B2
K	42	GLY	-	expression tag	UNP G0Y2B2
K	43	SER	-	expression tag	UNP G0Y2B2
K	44	HIS	-	expression tag	UNP G0Y2B2
L	25	MET	-	expression tag	UNP G0Y2B2
L	26	GLY	-	expression tag	UNP G0Y2B2
L	27	SER	-	expression tag	UNP G0Y2B2
L	28	SER	-	expression tag	UNP G0Y2B2
L	29	HIS	-	expression tag	UNP G0Y2B2
L	30	HIS	-	expression tag	UNP G0Y2B2
L	31	HIS	-	expression tag	UNP G0Y2B2
L	32	HIS	-	expression tag	UNP G0Y2B2
L	33	HIS	-	expression tag	UNP G0Y2B2
L	34	HIS	-	expression tag	UNP G0Y2B2
L	35	SER	-	expression tag	UNP G0Y2B2
L	36	SER	-	expression tag	UNP G0Y2B2
L	37	GLY	-	expression tag	UNP G0Y2B2
L	38	LEU	-	expression tag	UNP G0Y2B2
L	39	VAL	-	expression tag	UNP G0Y2B2
L	40	PRO	-	expression tag	UNP G0Y2B2
L	41	ARG	-	expression tag	UNP G0Y2B2
L	42	GLY	-	expression tag	UNP G0Y2B2
L	43	SER	-	expression tag	UNP G0Y2B2
L	44	HIS	-	expression tag	UNP G0Y2B2
M	25	MET	-	expression tag	UNP G0Y2B2
M	26	GLY	-	expression tag	UNP G0Y2B2
M	27	SER	-	expression tag	UNP G0Y2B2
M	28	SER	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
M	29	HIS	-	expression tag	UNP G0Y2B2
M	30	HIS	-	expression tag	UNP G0Y2B2
M	31	HIS	-	expression tag	UNP G0Y2B2
M	32	HIS	-	expression tag	UNP G0Y2B2
M	33	HIS	-	expression tag	UNP G0Y2B2
M	34	HIS	-	expression tag	UNP G0Y2B2
M	35	SER	-	expression tag	UNP G0Y2B2
M	36	SER	-	expression tag	UNP G0Y2B2
M	37	GLY	-	expression tag	UNP G0Y2B2
M	38	LEU	-	expression tag	UNP G0Y2B2
M	39	VAL	-	expression tag	UNP G0Y2B2
M	40	PRO	-	expression tag	UNP G0Y2B2
M	41	ARG	-	expression tag	UNP G0Y2B2
M	42	GLY	-	expression tag	UNP G0Y2B2
M	43	SER	-	expression tag	UNP G0Y2B2
M	44	HIS	-	expression tag	UNP G0Y2B2
N	25	MET	-	expression tag	UNP G0Y2B2
N	26	GLY	-	expression tag	UNP G0Y2B2
N	27	SER	-	expression tag	UNP G0Y2B2
N	28	SER	-	expression tag	UNP G0Y2B2
N	29	HIS	-	expression tag	UNP G0Y2B2
N	30	HIS	-	expression tag	UNP G0Y2B2
N	31	HIS	-	expression tag	UNP G0Y2B2
N	32	HIS	-	expression tag	UNP G0Y2B2
N	33	HIS	-	expression tag	UNP G0Y2B2
N	34	HIS	-	expression tag	UNP G0Y2B2
N	35	SER	-	expression tag	UNP G0Y2B2
N	36	SER	-	expression tag	UNP G0Y2B2
N	37	GLY	-	expression tag	UNP G0Y2B2
N	38	LEU	-	expression tag	UNP G0Y2B2
N	39	VAL	-	expression tag	UNP G0Y2B2
N	40	PRO	-	expression tag	UNP G0Y2B2
N	41	ARG	-	expression tag	UNP G0Y2B2
N	42	GLY	-	expression tag	UNP G0Y2B2
N	43	SER	-	expression tag	UNP G0Y2B2
N	44	HIS	-	expression tag	UNP G0Y2B2
O	25	MET	-	expression tag	UNP G0Y2B2
O	26	GLY	-	expression tag	UNP G0Y2B2
O	27	SER	-	expression tag	UNP G0Y2B2
O	28	SER	-	expression tag	UNP G0Y2B2
O	29	HIS	-	expression tag	UNP G0Y2B2
O	30	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
O	31	HIS	-	expression tag	UNP G0Y2B2
O	32	HIS	-	expression tag	UNP G0Y2B2
O	33	HIS	-	expression tag	UNP G0Y2B2
O	34	HIS	-	expression tag	UNP G0Y2B2
O	35	SER	-	expression tag	UNP G0Y2B2
O	36	SER	-	expression tag	UNP G0Y2B2
O	37	GLY	-	expression tag	UNP G0Y2B2
O	38	LEU	-	expression tag	UNP G0Y2B2
O	39	VAL	-	expression tag	UNP G0Y2B2
O	40	PRO	-	expression tag	UNP G0Y2B2
O	41	ARG	-	expression tag	UNP G0Y2B2
O	42	GLY	-	expression tag	UNP G0Y2B2
O	43	SER	-	expression tag	UNP G0Y2B2
O	44	HIS	-	expression tag	UNP G0Y2B2
P	25	MET	-	expression tag	UNP G0Y2B2
P	26	GLY	-	expression tag	UNP G0Y2B2
P	27	SER	-	expression tag	UNP G0Y2B2
P	28	SER	-	expression tag	UNP G0Y2B2
P	29	HIS	-	expression tag	UNP G0Y2B2
P	30	HIS	-	expression tag	UNP G0Y2B2
P	31	HIS	-	expression tag	UNP G0Y2B2
P	32	HIS	-	expression tag	UNP G0Y2B2
P	33	HIS	-	expression tag	UNP G0Y2B2
P	34	HIS	-	expression tag	UNP G0Y2B2
P	35	SER	-	expression tag	UNP G0Y2B2
P	36	SER	-	expression tag	UNP G0Y2B2
P	37	GLY	-	expression tag	UNP G0Y2B2
P	38	LEU	-	expression tag	UNP G0Y2B2
P	39	VAL	-	expression tag	UNP G0Y2B2
P	40	PRO	-	expression tag	UNP G0Y2B2
P	41	ARG	-	expression tag	UNP G0Y2B2
P	42	GLY	-	expression tag	UNP G0Y2B2
P	43	SER	-	expression tag	UNP G0Y2B2
P	44	HIS	-	expression tag	UNP G0Y2B2
Q	25	MET	-	expression tag	UNP G0Y2B2
Q	26	GLY	-	expression tag	UNP G0Y2B2
Q	27	SER	-	expression tag	UNP G0Y2B2
Q	28	SER	-	expression tag	UNP G0Y2B2
Q	29	HIS	-	expression tag	UNP G0Y2B2
Q	30	HIS	-	expression tag	UNP G0Y2B2
Q	31	HIS	-	expression tag	UNP G0Y2B2
Q	32	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	33	HIS	-	expression tag	UNP G0Y2B2
Q	34	HIS	-	expression tag	UNP G0Y2B2
Q	35	SER	-	expression tag	UNP G0Y2B2
Q	36	SER	-	expression tag	UNP G0Y2B2
Q	37	GLY	-	expression tag	UNP G0Y2B2
Q	38	LEU	-	expression tag	UNP G0Y2B2
Q	39	VAL	-	expression tag	UNP G0Y2B2
Q	40	PRO	-	expression tag	UNP G0Y2B2
Q	41	ARG	-	expression tag	UNP G0Y2B2
Q	42	GLY	-	expression tag	UNP G0Y2B2
Q	43	SER	-	expression tag	UNP G0Y2B2
Q	44	HIS	-	expression tag	UNP G0Y2B2
R	25	MET	-	expression tag	UNP G0Y2B2
R	26	GLY	-	expression tag	UNP G0Y2B2
R	27	SER	-	expression tag	UNP G0Y2B2
R	28	SER	-	expression tag	UNP G0Y2B2
R	29	HIS	-	expression tag	UNP G0Y2B2
R	30	HIS	-	expression tag	UNP G0Y2B2
R	31	HIS	-	expression tag	UNP G0Y2B2
R	32	HIS	-	expression tag	UNP G0Y2B2
R	33	HIS	-	expression tag	UNP G0Y2B2
R	34	HIS	-	expression tag	UNP G0Y2B2
R	35	SER	-	expression tag	UNP G0Y2B2
R	36	SER	-	expression tag	UNP G0Y2B2
R	37	GLY	-	expression tag	UNP G0Y2B2
R	38	LEU	-	expression tag	UNP G0Y2B2
R	39	VAL	-	expression tag	UNP G0Y2B2
R	40	PRO	-	expression tag	UNP G0Y2B2
R	41	ARG	-	expression tag	UNP G0Y2B2
R	42	GLY	-	expression tag	UNP G0Y2B2
R	43	SER	-	expression tag	UNP G0Y2B2
R	44	HIS	-	expression tag	UNP G0Y2B2
S	25	MET	-	expression tag	UNP G0Y2B2
S	26	GLY	-	expression tag	UNP G0Y2B2
S	27	SER	-	expression tag	UNP G0Y2B2
S	28	SER	-	expression tag	UNP G0Y2B2
S	29	HIS	-	expression tag	UNP G0Y2B2
S	30	HIS	-	expression tag	UNP G0Y2B2
S	31	HIS	-	expression tag	UNP G0Y2B2
S	32	HIS	-	expression tag	UNP G0Y2B2
S	33	HIS	-	expression tag	UNP G0Y2B2
S	34	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
S	35	SER	-	expression tag	UNP G0Y2B2
S	36	SER	-	expression tag	UNP G0Y2B2
S	37	GLY	-	expression tag	UNP G0Y2B2
S	38	LEU	-	expression tag	UNP G0Y2B2
S	39	VAL	-	expression tag	UNP G0Y2B2
S	40	PRO	-	expression tag	UNP G0Y2B2
S	41	ARG	-	expression tag	UNP G0Y2B2
S	42	GLY	-	expression tag	UNP G0Y2B2
S	43	SER	-	expression tag	UNP G0Y2B2
S	44	HIS	-	expression tag	UNP G0Y2B2
T	25	MET	-	expression tag	UNP G0Y2B2
T	26	GLY	-	expression tag	UNP G0Y2B2
T	27	SER	-	expression tag	UNP G0Y2B2
T	28	SER	-	expression tag	UNP G0Y2B2
T	29	HIS	-	expression tag	UNP G0Y2B2
T	30	HIS	-	expression tag	UNP G0Y2B2
T	31	HIS	-	expression tag	UNP G0Y2B2
T	32	HIS	-	expression tag	UNP G0Y2B2
T	33	HIS	-	expression tag	UNP G0Y2B2
T	34	HIS	-	expression tag	UNP G0Y2B2
T	35	SER	-	expression tag	UNP G0Y2B2
T	36	SER	-	expression tag	UNP G0Y2B2
T	37	GLY	-	expression tag	UNP G0Y2B2
T	38	LEU	-	expression tag	UNP G0Y2B2
T	39	VAL	-	expression tag	UNP G0Y2B2
T	40	PRO	-	expression tag	UNP G0Y2B2
T	41	ARG	-	expression tag	UNP G0Y2B2
T	42	GLY	-	expression tag	UNP G0Y2B2
T	43	SER	-	expression tag	UNP G0Y2B2
T	44	HIS	-	expression tag	UNP G0Y2B2
U	25	MET	-	expression tag	UNP G0Y2B2
U	26	GLY	-	expression tag	UNP G0Y2B2
U	27	SER	-	expression tag	UNP G0Y2B2
U	28	SER	-	expression tag	UNP G0Y2B2
U	29	HIS	-	expression tag	UNP G0Y2B2
U	30	HIS	-	expression tag	UNP G0Y2B2
U	31	HIS	-	expression tag	UNP G0Y2B2
U	32	HIS	-	expression tag	UNP G0Y2B2
U	33	HIS	-	expression tag	UNP G0Y2B2
U	34	HIS	-	expression tag	UNP G0Y2B2
U	35	SER	-	expression tag	UNP G0Y2B2
U	36	SER	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
U	37	GLY	-	expression tag	UNP G0Y2B2
U	38	LEU	-	expression tag	UNP G0Y2B2
U	39	VAL	-	expression tag	UNP G0Y2B2
U	40	PRO	-	expression tag	UNP G0Y2B2
U	41	ARG	-	expression tag	UNP G0Y2B2
U	42	GLY	-	expression tag	UNP G0Y2B2
U	43	SER	-	expression tag	UNP G0Y2B2
U	44	HIS	-	expression tag	UNP G0Y2B2
V	25	MET	-	expression tag	UNP G0Y2B2
V	26	GLY	-	expression tag	UNP G0Y2B2
V	27	SER	-	expression tag	UNP G0Y2B2
V	28	SER	-	expression tag	UNP G0Y2B2
V	29	HIS	-	expression tag	UNP G0Y2B2
V	30	HIS	-	expression tag	UNP G0Y2B2
V	31	HIS	-	expression tag	UNP G0Y2B2
V	32	HIS	-	expression tag	UNP G0Y2B2
V	33	HIS	-	expression tag	UNP G0Y2B2
V	34	HIS	-	expression tag	UNP G0Y2B2
V	35	SER	-	expression tag	UNP G0Y2B2
V	36	SER	-	expression tag	UNP G0Y2B2
V	37	GLY	-	expression tag	UNP G0Y2B2
V	38	LEU	-	expression tag	UNP G0Y2B2
V	39	VAL	-	expression tag	UNP G0Y2B2
V	40	PRO	-	expression tag	UNP G0Y2B2
V	41	ARG	-	expression tag	UNP G0Y2B2
V	42	GLY	-	expression tag	UNP G0Y2B2
V	43	SER	-	expression tag	UNP G0Y2B2
V	44	HIS	-	expression tag	UNP G0Y2B2
W	25	MET	-	expression tag	UNP G0Y2B2
W	26	GLY	-	expression tag	UNP G0Y2B2
W	27	SER	-	expression tag	UNP G0Y2B2
W	28	SER	-	expression tag	UNP G0Y2B2
W	29	HIS	-	expression tag	UNP G0Y2B2
W	30	HIS	-	expression tag	UNP G0Y2B2
W	31	HIS	-	expression tag	UNP G0Y2B2
W	32	HIS	-	expression tag	UNP G0Y2B2
W	33	HIS	-	expression tag	UNP G0Y2B2
W	34	HIS	-	expression tag	UNP G0Y2B2
W	35	SER	-	expression tag	UNP G0Y2B2
W	36	SER	-	expression tag	UNP G0Y2B2
W	37	GLY	-	expression tag	UNP G0Y2B2
W	38	LEU	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
W	39	VAL	-	expression tag	UNP G0Y2B2
W	40	PRO	-	expression tag	UNP G0Y2B2
W	41	ARG	-	expression tag	UNP G0Y2B2
W	42	GLY	-	expression tag	UNP G0Y2B2
W	43	SER	-	expression tag	UNP G0Y2B2
W	44	HIS	-	expression tag	UNP G0Y2B2
X	25	MET	-	expression tag	UNP G0Y2B2
X	26	GLY	-	expression tag	UNP G0Y2B2
X	27	SER	-	expression tag	UNP G0Y2B2
X	28	SER	-	expression tag	UNP G0Y2B2
X	29	HIS	-	expression tag	UNP G0Y2B2
X	30	HIS	-	expression tag	UNP G0Y2B2
X	31	HIS	-	expression tag	UNP G0Y2B2
X	32	HIS	-	expression tag	UNP G0Y2B2
X	33	HIS	-	expression tag	UNP G0Y2B2
X	34	HIS	-	expression tag	UNP G0Y2B2
X	35	SER	-	expression tag	UNP G0Y2B2
X	36	SER	-	expression tag	UNP G0Y2B2
X	37	GLY	-	expression tag	UNP G0Y2B2
X	38	LEU	-	expression tag	UNP G0Y2B2
X	39	VAL	-	expression tag	UNP G0Y2B2
X	40	PRO	-	expression tag	UNP G0Y2B2
X	41	ARG	-	expression tag	UNP G0Y2B2
X	42	GLY	-	expression tag	UNP G0Y2B2
X	43	SER	-	expression tag	UNP G0Y2B2
X	44	HIS	-	expression tag	UNP G0Y2B2
Y	25	MET	-	expression tag	UNP G0Y2B2
Y	26	GLY	-	expression tag	UNP G0Y2B2
Y	27	SER	-	expression tag	UNP G0Y2B2
Y	28	SER	-	expression tag	UNP G0Y2B2
Y	29	HIS	-	expression tag	UNP G0Y2B2
Y	30	HIS	-	expression tag	UNP G0Y2B2
Y	31	HIS	-	expression tag	UNP G0Y2B2
Y	32	HIS	-	expression tag	UNP G0Y2B2
Y	33	HIS	-	expression tag	UNP G0Y2B2
Y	34	HIS	-	expression tag	UNP G0Y2B2
Y	35	SER	-	expression tag	UNP G0Y2B2
Y	36	SER	-	expression tag	UNP G0Y2B2
Y	37	GLY	-	expression tag	UNP G0Y2B2
Y	38	LEU	-	expression tag	UNP G0Y2B2
Y	39	VAL	-	expression tag	UNP G0Y2B2
Y	40	PRO	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	41	ARG	-	expression tag	UNP G0Y2B2
Y	42	GLY	-	expression tag	UNP G0Y2B2
Y	43	SER	-	expression tag	UNP G0Y2B2
Y	44	HIS	-	expression tag	UNP G0Y2B2
Z	25	MET	-	expression tag	UNP G0Y2B2
Z	26	GLY	-	expression tag	UNP G0Y2B2
Z	27	SER	-	expression tag	UNP G0Y2B2
Z	28	SER	-	expression tag	UNP G0Y2B2
Z	29	HIS	-	expression tag	UNP G0Y2B2
Z	30	HIS	-	expression tag	UNP G0Y2B2
Z	31	HIS	-	expression tag	UNP G0Y2B2
Z	32	HIS	-	expression tag	UNP G0Y2B2
Z	33	HIS	-	expression tag	UNP G0Y2B2
Z	34	HIS	-	expression tag	UNP G0Y2B2
Z	35	SER	-	expression tag	UNP G0Y2B2
Z	36	SER	-	expression tag	UNP G0Y2B2
Z	37	GLY	-	expression tag	UNP G0Y2B2
Z	38	LEU	-	expression tag	UNP G0Y2B2
Z	39	VAL	-	expression tag	UNP G0Y2B2
Z	40	PRO	-	expression tag	UNP G0Y2B2
Z	41	ARG	-	expression tag	UNP G0Y2B2
Z	42	GLY	-	expression tag	UNP G0Y2B2
Z	43	SER	-	expression tag	UNP G0Y2B2
Z	44	HIS	-	expression tag	UNP G0Y2B2
1	25	MET	-	expression tag	UNP G0Y2B2
1	26	GLY	-	expression tag	UNP G0Y2B2
1	27	SER	-	expression tag	UNP G0Y2B2
1	28	SER	-	expression tag	UNP G0Y2B2
1	29	HIS	-	expression tag	UNP G0Y2B2
1	30	HIS	-	expression tag	UNP G0Y2B2
1	31	HIS	-	expression tag	UNP G0Y2B2
1	32	HIS	-	expression tag	UNP G0Y2B2
1	33	HIS	-	expression tag	UNP G0Y2B2
1	34	HIS	-	expression tag	UNP G0Y2B2
1	35	SER	-	expression tag	UNP G0Y2B2
1	36	SER	-	expression tag	UNP G0Y2B2
1	37	GLY	-	expression tag	UNP G0Y2B2
1	38	LEU	-	expression tag	UNP G0Y2B2
1	39	VAL	-	expression tag	UNP G0Y2B2
1	40	PRO	-	expression tag	UNP G0Y2B2
1	41	ARG	-	expression tag	UNP G0Y2B2
1	42	GLY	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
1	43	SER	-	expression tag	UNP G0Y2B2
1	44	HIS	-	expression tag	UNP G0Y2B2
2	25	MET	-	expression tag	UNP G0Y2B2
2	26	GLY	-	expression tag	UNP G0Y2B2
2	27	SER	-	expression tag	UNP G0Y2B2
2	28	SER	-	expression tag	UNP G0Y2B2
2	29	HIS	-	expression tag	UNP G0Y2B2
2	30	HIS	-	expression tag	UNP G0Y2B2
2	31	HIS	-	expression tag	UNP G0Y2B2
2	32	HIS	-	expression tag	UNP G0Y2B2
2	33	HIS	-	expression tag	UNP G0Y2B2
2	34	HIS	-	expression tag	UNP G0Y2B2
2	35	SER	-	expression tag	UNP G0Y2B2
2	36	SER	-	expression tag	UNP G0Y2B2
2	37	GLY	-	expression tag	UNP G0Y2B2
2	38	LEU	-	expression tag	UNP G0Y2B2
2	39	VAL	-	expression tag	UNP G0Y2B2
2	40	PRO	-	expression tag	UNP G0Y2B2
2	41	ARG	-	expression tag	UNP G0Y2B2
2	42	GLY	-	expression tag	UNP G0Y2B2
2	43	SER	-	expression tag	UNP G0Y2B2
2	44	HIS	-	expression tag	UNP G0Y2B2
3	25	MET	-	expression tag	UNP G0Y2B2
3	26	GLY	-	expression tag	UNP G0Y2B2
3	27	SER	-	expression tag	UNP G0Y2B2
3	28	SER	-	expression tag	UNP G0Y2B2
3	29	HIS	-	expression tag	UNP G0Y2B2
3	30	HIS	-	expression tag	UNP G0Y2B2
3	31	HIS	-	expression tag	UNP G0Y2B2
3	32	HIS	-	expression tag	UNP G0Y2B2
3	33	HIS	-	expression tag	UNP G0Y2B2
3	34	HIS	-	expression tag	UNP G0Y2B2
3	35	SER	-	expression tag	UNP G0Y2B2
3	36	SER	-	expression tag	UNP G0Y2B2
3	37	GLY	-	expression tag	UNP G0Y2B2
3	38	LEU	-	expression tag	UNP G0Y2B2
3	39	VAL	-	expression tag	UNP G0Y2B2
3	40	PRO	-	expression tag	UNP G0Y2B2
3	41	ARG	-	expression tag	UNP G0Y2B2
3	42	GLY	-	expression tag	UNP G0Y2B2
3	43	SER	-	expression tag	UNP G0Y2B2
3	44	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
4	25	MET	-	expression tag	UNP G0Y2B2
4	26	GLY	-	expression tag	UNP G0Y2B2
4	27	SER	-	expression tag	UNP G0Y2B2
4	28	SER	-	expression tag	UNP G0Y2B2
4	29	HIS	-	expression tag	UNP G0Y2B2
4	30	HIS	-	expression tag	UNP G0Y2B2
4	31	HIS	-	expression tag	UNP G0Y2B2
4	32	HIS	-	expression tag	UNP G0Y2B2
4	33	HIS	-	expression tag	UNP G0Y2B2
4	34	HIS	-	expression tag	UNP G0Y2B2
4	35	SER	-	expression tag	UNP G0Y2B2
4	36	SER	-	expression tag	UNP G0Y2B2
4	37	GLY	-	expression tag	UNP G0Y2B2
4	38	LEU	-	expression tag	UNP G0Y2B2
4	39	VAL	-	expression tag	UNP G0Y2B2
4	40	PRO	-	expression tag	UNP G0Y2B2
4	41	ARG	-	expression tag	UNP G0Y2B2
4	42	GLY	-	expression tag	UNP G0Y2B2
4	43	SER	-	expression tag	UNP G0Y2B2
4	44	HIS	-	expression tag	UNP G0Y2B2
5	25	MET	-	expression tag	UNP G0Y2B2
5	26	GLY	-	expression tag	UNP G0Y2B2
5	27	SER	-	expression tag	UNP G0Y2B2
5	28	SER	-	expression tag	UNP G0Y2B2
5	29	HIS	-	expression tag	UNP G0Y2B2
5	30	HIS	-	expression tag	UNP G0Y2B2
5	31	HIS	-	expression tag	UNP G0Y2B2
5	32	HIS	-	expression tag	UNP G0Y2B2
5	33	HIS	-	expression tag	UNP G0Y2B2
5	34	HIS	-	expression tag	UNP G0Y2B2
5	35	SER	-	expression tag	UNP G0Y2B2
5	36	SER	-	expression tag	UNP G0Y2B2
5	37	GLY	-	expression tag	UNP G0Y2B2
5	38	LEU	-	expression tag	UNP G0Y2B2
5	39	VAL	-	expression tag	UNP G0Y2B2
5	40	PRO	-	expression tag	UNP G0Y2B2
5	41	ARG	-	expression tag	UNP G0Y2B2
5	42	GLY	-	expression tag	UNP G0Y2B2
5	43	SER	-	expression tag	UNP G0Y2B2
5	44	HIS	-	expression tag	UNP G0Y2B2
6	25	MET	-	expression tag	UNP G0Y2B2
6	26	GLY	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
6	27	SER	-	expression tag	UNP G0Y2B2
6	28	SER	-	expression tag	UNP G0Y2B2
6	29	HIS	-	expression tag	UNP G0Y2B2
6	30	HIS	-	expression tag	UNP G0Y2B2
6	31	HIS	-	expression tag	UNP G0Y2B2
6	32	HIS	-	expression tag	UNP G0Y2B2
6	33	HIS	-	expression tag	UNP G0Y2B2
6	34	HIS	-	expression tag	UNP G0Y2B2
6	35	SER	-	expression tag	UNP G0Y2B2
6	36	SER	-	expression tag	UNP G0Y2B2
6	37	GLY	-	expression tag	UNP G0Y2B2
6	38	LEU	-	expression tag	UNP G0Y2B2
6	39	VAL	-	expression tag	UNP G0Y2B2
6	40	PRO	-	expression tag	UNP G0Y2B2
6	41	ARG	-	expression tag	UNP G0Y2B2
6	42	GLY	-	expression tag	UNP G0Y2B2
6	43	SER	-	expression tag	UNP G0Y2B2
6	44	HIS	-	expression tag	UNP G0Y2B2
7	25	MET	-	expression tag	UNP G0Y2B2
7	26	GLY	-	expression tag	UNP G0Y2B2
7	27	SER	-	expression tag	UNP G0Y2B2
7	28	SER	-	expression tag	UNP G0Y2B2
7	29	HIS	-	expression tag	UNP G0Y2B2
7	30	HIS	-	expression tag	UNP G0Y2B2
7	31	HIS	-	expression tag	UNP G0Y2B2
7	32	HIS	-	expression tag	UNP G0Y2B2
7	33	HIS	-	expression tag	UNP G0Y2B2
7	34	HIS	-	expression tag	UNP G0Y2B2
7	35	SER	-	expression tag	UNP G0Y2B2
7	36	SER	-	expression tag	UNP G0Y2B2
7	37	GLY	-	expression tag	UNP G0Y2B2
7	38	LEU	-	expression tag	UNP G0Y2B2
7	39	VAL	-	expression tag	UNP G0Y2B2
7	40	PRO	-	expression tag	UNP G0Y2B2
7	41	ARG	-	expression tag	UNP G0Y2B2
7	42	GLY	-	expression tag	UNP G0Y2B2
7	43	SER	-	expression tag	UNP G0Y2B2
7	44	HIS	-	expression tag	UNP G0Y2B2
8	25	MET	-	expression tag	UNP G0Y2B2
8	26	GLY	-	expression tag	UNP G0Y2B2
8	27	SER	-	expression tag	UNP G0Y2B2
8	28	SER	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
8	29	HIS	-	expression tag	UNP G0Y2B2
8	30	HIS	-	expression tag	UNP G0Y2B2
8	31	HIS	-	expression tag	UNP G0Y2B2
8	32	HIS	-	expression tag	UNP G0Y2B2
8	33	HIS	-	expression tag	UNP G0Y2B2
8	34	HIS	-	expression tag	UNP G0Y2B2
8	35	SER	-	expression tag	UNP G0Y2B2
8	36	SER	-	expression tag	UNP G0Y2B2
8	37	GLY	-	expression tag	UNP G0Y2B2
8	38	LEU	-	expression tag	UNP G0Y2B2
8	39	VAL	-	expression tag	UNP G0Y2B2
8	40	PRO	-	expression tag	UNP G0Y2B2
8	41	ARG	-	expression tag	UNP G0Y2B2
8	42	GLY	-	expression tag	UNP G0Y2B2
8	43	SER	-	expression tag	UNP G0Y2B2
8	44	HIS	-	expression tag	UNP G0Y2B2
9	25	MET	-	expression tag	UNP G0Y2B2
9	26	GLY	-	expression tag	UNP G0Y2B2
9	27	SER	-	expression tag	UNP G0Y2B2
9	28	SER	-	expression tag	UNP G0Y2B2
9	29	HIS	-	expression tag	UNP G0Y2B2
9	30	HIS	-	expression tag	UNP G0Y2B2
9	31	HIS	-	expression tag	UNP G0Y2B2
9	32	HIS	-	expression tag	UNP G0Y2B2
9	33	HIS	-	expression tag	UNP G0Y2B2
9	34	HIS	-	expression tag	UNP G0Y2B2
9	35	SER	-	expression tag	UNP G0Y2B2
9	36	SER	-	expression tag	UNP G0Y2B2
9	37	GLY	-	expression tag	UNP G0Y2B2
9	38	LEU	-	expression tag	UNP G0Y2B2
9	39	VAL	-	expression tag	UNP G0Y2B2
9	40	PRO	-	expression tag	UNP G0Y2B2
9	41	ARG	-	expression tag	UNP G0Y2B2
9	42	GLY	-	expression tag	UNP G0Y2B2
9	43	SER	-	expression tag	UNP G0Y2B2
9	44	HIS	-	expression tag	UNP G0Y2B2
a	25	MET	-	expression tag	UNP G0Y2B2
a	26	GLY	-	expression tag	UNP G0Y2B2
a	27	SER	-	expression tag	UNP G0Y2B2
a	28	SER	-	expression tag	UNP G0Y2B2
a	29	HIS	-	expression tag	UNP G0Y2B2
a	30	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
a	31	HIS	-	expression tag	UNP G0Y2B2
a	32	HIS	-	expression tag	UNP G0Y2B2
a	33	HIS	-	expression tag	UNP G0Y2B2
a	34	HIS	-	expression tag	UNP G0Y2B2
a	35	SER	-	expression tag	UNP G0Y2B2
a	36	SER	-	expression tag	UNP G0Y2B2
a	37	GLY	-	expression tag	UNP G0Y2B2
a	38	LEU	-	expression tag	UNP G0Y2B2
a	39	VAL	-	expression tag	UNP G0Y2B2
a	40	PRO	-	expression tag	UNP G0Y2B2
a	41	ARG	-	expression tag	UNP G0Y2B2
a	42	GLY	-	expression tag	UNP G0Y2B2
a	43	SER	-	expression tag	UNP G0Y2B2
a	44	HIS	-	expression tag	UNP G0Y2B2
b	25	MET	-	expression tag	UNP G0Y2B2
b	26	GLY	-	expression tag	UNP G0Y2B2
b	27	SER	-	expression tag	UNP G0Y2B2
b	28	SER	-	expression tag	UNP G0Y2B2
b	29	HIS	-	expression tag	UNP G0Y2B2
b	30	HIS	-	expression tag	UNP G0Y2B2
b	31	HIS	-	expression tag	UNP G0Y2B2
b	32	HIS	-	expression tag	UNP G0Y2B2
b	33	HIS	-	expression tag	UNP G0Y2B2
b	34	HIS	-	expression tag	UNP G0Y2B2
b	35	SER	-	expression tag	UNP G0Y2B2
b	36	SER	-	expression tag	UNP G0Y2B2
b	37	GLY	-	expression tag	UNP G0Y2B2
b	38	LEU	-	expression tag	UNP G0Y2B2
b	39	VAL	-	expression tag	UNP G0Y2B2
b	40	PRO	-	expression tag	UNP G0Y2B2
b	41	ARG	-	expression tag	UNP G0Y2B2
b	42	GLY	-	expression tag	UNP G0Y2B2
b	43	SER	-	expression tag	UNP G0Y2B2
b	44	HIS	-	expression tag	UNP G0Y2B2
c	25	MET	-	expression tag	UNP G0Y2B2
c	26	GLY	-	expression tag	UNP G0Y2B2
c	27	SER	-	expression tag	UNP G0Y2B2
c	28	SER	-	expression tag	UNP G0Y2B2
c	29	HIS	-	expression tag	UNP G0Y2B2
c	30	HIS	-	expression tag	UNP G0Y2B2
c	31	HIS	-	expression tag	UNP G0Y2B2
c	32	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
c	33	HIS	-	expression tag	UNP G0Y2B2
c	34	HIS	-	expression tag	UNP G0Y2B2
c	35	SER	-	expression tag	UNP G0Y2B2
c	36	SER	-	expression tag	UNP G0Y2B2
c	37	GLY	-	expression tag	UNP G0Y2B2
c	38	LEU	-	expression tag	UNP G0Y2B2
c	39	VAL	-	expression tag	UNP G0Y2B2
c	40	PRO	-	expression tag	UNP G0Y2B2
c	41	ARG	-	expression tag	UNP G0Y2B2
c	42	GLY	-	expression tag	UNP G0Y2B2
c	43	SER	-	expression tag	UNP G0Y2B2
c	44	HIS	-	expression tag	UNP G0Y2B2
d	25	MET	-	expression tag	UNP G0Y2B2
d	26	GLY	-	expression tag	UNP G0Y2B2
d	27	SER	-	expression tag	UNP G0Y2B2
d	28	SER	-	expression tag	UNP G0Y2B2
d	29	HIS	-	expression tag	UNP G0Y2B2
d	30	HIS	-	expression tag	UNP G0Y2B2
d	31	HIS	-	expression tag	UNP G0Y2B2
d	32	HIS	-	expression tag	UNP G0Y2B2
d	33	HIS	-	expression tag	UNP G0Y2B2
d	34	HIS	-	expression tag	UNP G0Y2B2
d	35	SER	-	expression tag	UNP G0Y2B2
d	36	SER	-	expression tag	UNP G0Y2B2
d	37	GLY	-	expression tag	UNP G0Y2B2
d	38	LEU	-	expression tag	UNP G0Y2B2
d	39	VAL	-	expression tag	UNP G0Y2B2
d	40	PRO	-	expression tag	UNP G0Y2B2
d	41	ARG	-	expression tag	UNP G0Y2B2
d	42	GLY	-	expression tag	UNP G0Y2B2
d	43	SER	-	expression tag	UNP G0Y2B2
d	44	HIS	-	expression tag	UNP G0Y2B2
e	25	MET	-	expression tag	UNP G0Y2B2
e	26	GLY	-	expression tag	UNP G0Y2B2
e	27	SER	-	expression tag	UNP G0Y2B2
e	28	SER	-	expression tag	UNP G0Y2B2
e	29	HIS	-	expression tag	UNP G0Y2B2
e	30	HIS	-	expression tag	UNP G0Y2B2
e	31	HIS	-	expression tag	UNP G0Y2B2
e	32	HIS	-	expression tag	UNP G0Y2B2
e	33	HIS	-	expression tag	UNP G0Y2B2
e	34	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
e	35	SER	-	expression tag	UNP G0Y2B2
e	36	SER	-	expression tag	UNP G0Y2B2
e	37	GLY	-	expression tag	UNP G0Y2B2
e	38	LEU	-	expression tag	UNP G0Y2B2
e	39	VAL	-	expression tag	UNP G0Y2B2
e	40	PRO	-	expression tag	UNP G0Y2B2
e	41	ARG	-	expression tag	UNP G0Y2B2
e	42	GLY	-	expression tag	UNP G0Y2B2
e	43	SER	-	expression tag	UNP G0Y2B2
e	44	HIS	-	expression tag	UNP G0Y2B2
f	25	MET	-	expression tag	UNP G0Y2B2
f	26	GLY	-	expression tag	UNP G0Y2B2
f	27	SER	-	expression tag	UNP G0Y2B2
f	28	SER	-	expression tag	UNP G0Y2B2
f	29	HIS	-	expression tag	UNP G0Y2B2
f	30	HIS	-	expression tag	UNP G0Y2B2
f	31	HIS	-	expression tag	UNP G0Y2B2
f	32	HIS	-	expression tag	UNP G0Y2B2
f	33	HIS	-	expression tag	UNP G0Y2B2
f	34	HIS	-	expression tag	UNP G0Y2B2
f	35	SER	-	expression tag	UNP G0Y2B2
f	36	SER	-	expression tag	UNP G0Y2B2
f	37	GLY	-	expression tag	UNP G0Y2B2
f	38	LEU	-	expression tag	UNP G0Y2B2
f	39	VAL	-	expression tag	UNP G0Y2B2
f	40	PRO	-	expression tag	UNP G0Y2B2
f	41	ARG	-	expression tag	UNP G0Y2B2
f	42	GLY	-	expression tag	UNP G0Y2B2
f	43	SER	-	expression tag	UNP G0Y2B2
f	44	HIS	-	expression tag	UNP G0Y2B2
g	25	MET	-	expression tag	UNP G0Y2B2
g	26	GLY	-	expression tag	UNP G0Y2B2
g	27	SER	-	expression tag	UNP G0Y2B2
g	28	SER	-	expression tag	UNP G0Y2B2
g	29	HIS	-	expression tag	UNP G0Y2B2
g	30	HIS	-	expression tag	UNP G0Y2B2
g	31	HIS	-	expression tag	UNP G0Y2B2
g	32	HIS	-	expression tag	UNP G0Y2B2
g	33	HIS	-	expression tag	UNP G0Y2B2
g	34	HIS	-	expression tag	UNP G0Y2B2
g	35	SER	-	expression tag	UNP G0Y2B2
g	36	SER	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
g	37	GLY	-	expression tag	UNP G0Y2B2
g	38	LEU	-	expression tag	UNP G0Y2B2
g	39	VAL	-	expression tag	UNP G0Y2B2
g	40	PRO	-	expression tag	UNP G0Y2B2
g	41	ARG	-	expression tag	UNP G0Y2B2
g	42	GLY	-	expression tag	UNP G0Y2B2
g	43	SER	-	expression tag	UNP G0Y2B2
g	44	HIS	-	expression tag	UNP G0Y2B2
h	25	MET	-	expression tag	UNP G0Y2B2
h	26	GLY	-	expression tag	UNP G0Y2B2
h	27	SER	-	expression tag	UNP G0Y2B2
h	28	SER	-	expression tag	UNP G0Y2B2
h	29	HIS	-	expression tag	UNP G0Y2B2
h	30	HIS	-	expression tag	UNP G0Y2B2
h	31	HIS	-	expression tag	UNP G0Y2B2
h	32	HIS	-	expression tag	UNP G0Y2B2
h	33	HIS	-	expression tag	UNP G0Y2B2
h	34	HIS	-	expression tag	UNP G0Y2B2
h	35	SER	-	expression tag	UNP G0Y2B2
h	36	SER	-	expression tag	UNP G0Y2B2
h	37	GLY	-	expression tag	UNP G0Y2B2
h	38	LEU	-	expression tag	UNP G0Y2B2
h	39	VAL	-	expression tag	UNP G0Y2B2
h	40	PRO	-	expression tag	UNP G0Y2B2
h	41	ARG	-	expression tag	UNP G0Y2B2
h	42	GLY	-	expression tag	UNP G0Y2B2
h	43	SER	-	expression tag	UNP G0Y2B2
h	44	HIS	-	expression tag	UNP G0Y2B2
i	25	MET	-	expression tag	UNP G0Y2B2
i	26	GLY	-	expression tag	UNP G0Y2B2
i	27	SER	-	expression tag	UNP G0Y2B2
i	28	SER	-	expression tag	UNP G0Y2B2
i	29	HIS	-	expression tag	UNP G0Y2B2
i	30	HIS	-	expression tag	UNP G0Y2B2
i	31	HIS	-	expression tag	UNP G0Y2B2
i	32	HIS	-	expression tag	UNP G0Y2B2
i	33	HIS	-	expression tag	UNP G0Y2B2
i	34	HIS	-	expression tag	UNP G0Y2B2
i	35	SER	-	expression tag	UNP G0Y2B2
i	36	SER	-	expression tag	UNP G0Y2B2
i	37	GLY	-	expression tag	UNP G0Y2B2
i	38	LEU	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
i	39	VAL	-	expression tag	UNP G0Y2B2
i	40	PRO	-	expression tag	UNP G0Y2B2
i	41	ARG	-	expression tag	UNP G0Y2B2
i	42	GLY	-	expression tag	UNP G0Y2B2
i	43	SER	-	expression tag	UNP G0Y2B2
i	44	HIS	-	expression tag	UNP G0Y2B2
j	25	MET	-	expression tag	UNP G0Y2B2
j	26	GLY	-	expression tag	UNP G0Y2B2
j	27	SER	-	expression tag	UNP G0Y2B2
j	28	SER	-	expression tag	UNP G0Y2B2
j	29	HIS	-	expression tag	UNP G0Y2B2
j	30	HIS	-	expression tag	UNP G0Y2B2
j	31	HIS	-	expression tag	UNP G0Y2B2
j	32	HIS	-	expression tag	UNP G0Y2B2
j	33	HIS	-	expression tag	UNP G0Y2B2
j	34	HIS	-	expression tag	UNP G0Y2B2
j	35	SER	-	expression tag	UNP G0Y2B2
j	36	SER	-	expression tag	UNP G0Y2B2
j	37	GLY	-	expression tag	UNP G0Y2B2
j	38	LEU	-	expression tag	UNP G0Y2B2
j	39	VAL	-	expression tag	UNP G0Y2B2
j	40	PRO	-	expression tag	UNP G0Y2B2
j	41	ARG	-	expression tag	UNP G0Y2B2
j	42	GLY	-	expression tag	UNP G0Y2B2
j	43	SER	-	expression tag	UNP G0Y2B2
j	44	HIS	-	expression tag	UNP G0Y2B2
k	25	MET	-	expression tag	UNP G0Y2B2
k	26	GLY	-	expression tag	UNP G0Y2B2
k	27	SER	-	expression tag	UNP G0Y2B2
k	28	SER	-	expression tag	UNP G0Y2B2
k	29	HIS	-	expression tag	UNP G0Y2B2
k	30	HIS	-	expression tag	UNP G0Y2B2
k	31	HIS	-	expression tag	UNP G0Y2B2
k	32	HIS	-	expression tag	UNP G0Y2B2
k	33	HIS	-	expression tag	UNP G0Y2B2
k	34	HIS	-	expression tag	UNP G0Y2B2
k	35	SER	-	expression tag	UNP G0Y2B2
k	36	SER	-	expression tag	UNP G0Y2B2
k	37	GLY	-	expression tag	UNP G0Y2B2
k	38	LEU	-	expression tag	UNP G0Y2B2
k	39	VAL	-	expression tag	UNP G0Y2B2
k	40	PRO	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
k	41	ARG	-	expression tag	UNP G0Y2B2
k	42	GLY	-	expression tag	UNP G0Y2B2
k	43	SER	-	expression tag	UNP G0Y2B2
k	44	HIS	-	expression tag	UNP G0Y2B2
l	25	MET	-	expression tag	UNP G0Y2B2
l	26	GLY	-	expression tag	UNP G0Y2B2
l	27	SER	-	expression tag	UNP G0Y2B2
l	28	SER	-	expression tag	UNP G0Y2B2
l	29	HIS	-	expression tag	UNP G0Y2B2
l	30	HIS	-	expression tag	UNP G0Y2B2
l	31	HIS	-	expression tag	UNP G0Y2B2
l	32	HIS	-	expression tag	UNP G0Y2B2
l	33	HIS	-	expression tag	UNP G0Y2B2
l	34	HIS	-	expression tag	UNP G0Y2B2
l	35	SER	-	expression tag	UNP G0Y2B2
l	36	SER	-	expression tag	UNP G0Y2B2
l	37	GLY	-	expression tag	UNP G0Y2B2
l	38	LEU	-	expression tag	UNP G0Y2B2
l	39	VAL	-	expression tag	UNP G0Y2B2
l	40	PRO	-	expression tag	UNP G0Y2B2
l	41	ARG	-	expression tag	UNP G0Y2B2
l	42	GLY	-	expression tag	UNP G0Y2B2
l	43	SER	-	expression tag	UNP G0Y2B2
l	44	HIS	-	expression tag	UNP G0Y2B2
m	25	MET	-	expression tag	UNP G0Y2B2
m	26	GLY	-	expression tag	UNP G0Y2B2
m	27	SER	-	expression tag	UNP G0Y2B2
m	28	SER	-	expression tag	UNP G0Y2B2
m	29	HIS	-	expression tag	UNP G0Y2B2
m	30	HIS	-	expression tag	UNP G0Y2B2
m	31	HIS	-	expression tag	UNP G0Y2B2
m	32	HIS	-	expression tag	UNP G0Y2B2
m	33	HIS	-	expression tag	UNP G0Y2B2
m	34	HIS	-	expression tag	UNP G0Y2B2
m	35	SER	-	expression tag	UNP G0Y2B2
m	36	SER	-	expression tag	UNP G0Y2B2
m	37	GLY	-	expression tag	UNP G0Y2B2
m	38	LEU	-	expression tag	UNP G0Y2B2
m	39	VAL	-	expression tag	UNP G0Y2B2
m	40	PRO	-	expression tag	UNP G0Y2B2
m	41	ARG	-	expression tag	UNP G0Y2B2
m	42	GLY	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
m	43	SER	-	expression tag	UNP G0Y2B2
m	44	HIS	-	expression tag	UNP G0Y2B2
n	25	MET	-	expression tag	UNP G0Y2B2
n	26	GLY	-	expression tag	UNP G0Y2B2
n	27	SER	-	expression tag	UNP G0Y2B2
n	28	SER	-	expression tag	UNP G0Y2B2
n	29	HIS	-	expression tag	UNP G0Y2B2
n	30	HIS	-	expression tag	UNP G0Y2B2
n	31	HIS	-	expression tag	UNP G0Y2B2
n	32	HIS	-	expression tag	UNP G0Y2B2
n	33	HIS	-	expression tag	UNP G0Y2B2
n	34	HIS	-	expression tag	UNP G0Y2B2
n	35	SER	-	expression tag	UNP G0Y2B2
n	36	SER	-	expression tag	UNP G0Y2B2
n	37	GLY	-	expression tag	UNP G0Y2B2
n	38	LEU	-	expression tag	UNP G0Y2B2
n	39	VAL	-	expression tag	UNP G0Y2B2
n	40	PRO	-	expression tag	UNP G0Y2B2
n	41	ARG	-	expression tag	UNP G0Y2B2
n	42	GLY	-	expression tag	UNP G0Y2B2
n	43	SER	-	expression tag	UNP G0Y2B2
n	44	HIS	-	expression tag	UNP G0Y2B2
o	25	MET	-	expression tag	UNP G0Y2B2
o	26	GLY	-	expression tag	UNP G0Y2B2
o	27	SER	-	expression tag	UNP G0Y2B2
o	28	SER	-	expression tag	UNP G0Y2B2
o	29	HIS	-	expression tag	UNP G0Y2B2
o	30	HIS	-	expression tag	UNP G0Y2B2
o	31	HIS	-	expression tag	UNP G0Y2B2
o	32	HIS	-	expression tag	UNP G0Y2B2
o	33	HIS	-	expression tag	UNP G0Y2B2
o	34	HIS	-	expression tag	UNP G0Y2B2
o	35	SER	-	expression tag	UNP G0Y2B2
o	36	SER	-	expression tag	UNP G0Y2B2
o	37	GLY	-	expression tag	UNP G0Y2B2
o	38	LEU	-	expression tag	UNP G0Y2B2
o	39	VAL	-	expression tag	UNP G0Y2B2
o	40	PRO	-	expression tag	UNP G0Y2B2
o	41	ARG	-	expression tag	UNP G0Y2B2
o	42	GLY	-	expression tag	UNP G0Y2B2
o	43	SER	-	expression tag	UNP G0Y2B2
o	44	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
p	25	MET	-	expression tag	UNP G0Y2B2
p	26	GLY	-	expression tag	UNP G0Y2B2
p	27	SER	-	expression tag	UNP G0Y2B2
p	28	SER	-	expression tag	UNP G0Y2B2
p	29	HIS	-	expression tag	UNP G0Y2B2
p	30	HIS	-	expression tag	UNP G0Y2B2
p	31	HIS	-	expression tag	UNP G0Y2B2
p	32	HIS	-	expression tag	UNP G0Y2B2
p	33	HIS	-	expression tag	UNP G0Y2B2
p	34	HIS	-	expression tag	UNP G0Y2B2
p	35	SER	-	expression tag	UNP G0Y2B2
p	36	SER	-	expression tag	UNP G0Y2B2
p	37	GLY	-	expression tag	UNP G0Y2B2
p	38	LEU	-	expression tag	UNP G0Y2B2
p	39	VAL	-	expression tag	UNP G0Y2B2
p	40	PRO	-	expression tag	UNP G0Y2B2
p	41	ARG	-	expression tag	UNP G0Y2B2
p	42	GLY	-	expression tag	UNP G0Y2B2
p	43	SER	-	expression tag	UNP G0Y2B2
p	44	HIS	-	expression tag	UNP G0Y2B2
q	25	MET	-	expression tag	UNP G0Y2B2
q	26	GLY	-	expression tag	UNP G0Y2B2
q	27	SER	-	expression tag	UNP G0Y2B2
q	28	SER	-	expression tag	UNP G0Y2B2
q	29	HIS	-	expression tag	UNP G0Y2B2
q	30	HIS	-	expression tag	UNP G0Y2B2
q	31	HIS	-	expression tag	UNP G0Y2B2
q	32	HIS	-	expression tag	UNP G0Y2B2
q	33	HIS	-	expression tag	UNP G0Y2B2
q	34	HIS	-	expression tag	UNP G0Y2B2
q	35	SER	-	expression tag	UNP G0Y2B2
q	36	SER	-	expression tag	UNP G0Y2B2
q	37	GLY	-	expression tag	UNP G0Y2B2
q	38	LEU	-	expression tag	UNP G0Y2B2
q	39	VAL	-	expression tag	UNP G0Y2B2
q	40	PRO	-	expression tag	UNP G0Y2B2
q	41	ARG	-	expression tag	UNP G0Y2B2
q	42	GLY	-	expression tag	UNP G0Y2B2
q	43	SER	-	expression tag	UNP G0Y2B2
q	44	HIS	-	expression tag	UNP G0Y2B2
r	25	MET	-	expression tag	UNP G0Y2B2
r	26	GLY	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
r	27	SER	-	expression tag	UNP G0Y2B2
r	28	SER	-	expression tag	UNP G0Y2B2
r	29	HIS	-	expression tag	UNP G0Y2B2
r	30	HIS	-	expression tag	UNP G0Y2B2
r	31	HIS	-	expression tag	UNP G0Y2B2
r	32	HIS	-	expression tag	UNP G0Y2B2
r	33	HIS	-	expression tag	UNP G0Y2B2
r	34	HIS	-	expression tag	UNP G0Y2B2
r	35	SER	-	expression tag	UNP G0Y2B2
r	36	SER	-	expression tag	UNP G0Y2B2
r	37	GLY	-	expression tag	UNP G0Y2B2
r	38	LEU	-	expression tag	UNP G0Y2B2
r	39	VAL	-	expression tag	UNP G0Y2B2
r	40	PRO	-	expression tag	UNP G0Y2B2
r	41	ARG	-	expression tag	UNP G0Y2B2
r	42	GLY	-	expression tag	UNP G0Y2B2
r	43	SER	-	expression tag	UNP G0Y2B2
r	44	HIS	-	expression tag	UNP G0Y2B2
s	25	MET	-	expression tag	UNP G0Y2B2
s	26	GLY	-	expression tag	UNP G0Y2B2
s	27	SER	-	expression tag	UNP G0Y2B2
s	28	SER	-	expression tag	UNP G0Y2B2
s	29	HIS	-	expression tag	UNP G0Y2B2
s	30	HIS	-	expression tag	UNP G0Y2B2
s	31	HIS	-	expression tag	UNP G0Y2B2
s	32	HIS	-	expression tag	UNP G0Y2B2
s	33	HIS	-	expression tag	UNP G0Y2B2
s	34	HIS	-	expression tag	UNP G0Y2B2
s	35	SER	-	expression tag	UNP G0Y2B2
s	36	SER	-	expression tag	UNP G0Y2B2
s	37	GLY	-	expression tag	UNP G0Y2B2
s	38	LEU	-	expression tag	UNP G0Y2B2
s	39	VAL	-	expression tag	UNP G0Y2B2
s	40	PRO	-	expression tag	UNP G0Y2B2
s	41	ARG	-	expression tag	UNP G0Y2B2
s	42	GLY	-	expression tag	UNP G0Y2B2
s	43	SER	-	expression tag	UNP G0Y2B2
s	44	HIS	-	expression tag	UNP G0Y2B2
t	25	MET	-	expression tag	UNP G0Y2B2
t	26	GLY	-	expression tag	UNP G0Y2B2
t	27	SER	-	expression tag	UNP G0Y2B2
t	28	SER	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
t	29	HIS	-	expression tag	UNP G0Y2B2
t	30	HIS	-	expression tag	UNP G0Y2B2
t	31	HIS	-	expression tag	UNP G0Y2B2
t	32	HIS	-	expression tag	UNP G0Y2B2
t	33	HIS	-	expression tag	UNP G0Y2B2
t	34	HIS	-	expression tag	UNP G0Y2B2
t	35	SER	-	expression tag	UNP G0Y2B2
t	36	SER	-	expression tag	UNP G0Y2B2
t	37	GLY	-	expression tag	UNP G0Y2B2
t	38	LEU	-	expression tag	UNP G0Y2B2
t	39	VAL	-	expression tag	UNP G0Y2B2
t	40	PRO	-	expression tag	UNP G0Y2B2
t	41	ARG	-	expression tag	UNP G0Y2B2
t	42	GLY	-	expression tag	UNP G0Y2B2
t	43	SER	-	expression tag	UNP G0Y2B2
t	44	HIS	-	expression tag	UNP G0Y2B2
u	25	MET	-	expression tag	UNP G0Y2B2
u	26	GLY	-	expression tag	UNP G0Y2B2
u	27	SER	-	expression tag	UNP G0Y2B2
u	28	SER	-	expression tag	UNP G0Y2B2
u	29	HIS	-	expression tag	UNP G0Y2B2
u	30	HIS	-	expression tag	UNP G0Y2B2
u	31	HIS	-	expression tag	UNP G0Y2B2
u	32	HIS	-	expression tag	UNP G0Y2B2
u	33	HIS	-	expression tag	UNP G0Y2B2
u	34	HIS	-	expression tag	UNP G0Y2B2
u	35	SER	-	expression tag	UNP G0Y2B2
u	36	SER	-	expression tag	UNP G0Y2B2
u	37	GLY	-	expression tag	UNP G0Y2B2
u	38	LEU	-	expression tag	UNP G0Y2B2
u	39	VAL	-	expression tag	UNP G0Y2B2
u	40	PRO	-	expression tag	UNP G0Y2B2
u	41	ARG	-	expression tag	UNP G0Y2B2
u	42	GLY	-	expression tag	UNP G0Y2B2
u	43	SER	-	expression tag	UNP G0Y2B2
u	44	HIS	-	expression tag	UNP G0Y2B2
v	25	MET	-	expression tag	UNP G0Y2B2
v	26	GLY	-	expression tag	UNP G0Y2B2
v	27	SER	-	expression tag	UNP G0Y2B2
v	28	SER	-	expression tag	UNP G0Y2B2
v	29	HIS	-	expression tag	UNP G0Y2B2
v	30	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
v	31	HIS	-	expression tag	UNP G0Y2B2
v	32	HIS	-	expression tag	UNP G0Y2B2
v	33	HIS	-	expression tag	UNP G0Y2B2
v	34	HIS	-	expression tag	UNP G0Y2B2
v	35	SER	-	expression tag	UNP G0Y2B2
v	36	SER	-	expression tag	UNP G0Y2B2
v	37	GLY	-	expression tag	UNP G0Y2B2
v	38	LEU	-	expression tag	UNP G0Y2B2
v	39	VAL	-	expression tag	UNP G0Y2B2
v	40	PRO	-	expression tag	UNP G0Y2B2
v	41	ARG	-	expression tag	UNP G0Y2B2
v	42	GLY	-	expression tag	UNP G0Y2B2
v	43	SER	-	expression tag	UNP G0Y2B2
v	44	HIS	-	expression tag	UNP G0Y2B2
w	25	MET	-	expression tag	UNP G0Y2B2
w	26	GLY	-	expression tag	UNP G0Y2B2
w	27	SER	-	expression tag	UNP G0Y2B2
w	28	SER	-	expression tag	UNP G0Y2B2
w	29	HIS	-	expression tag	UNP G0Y2B2
w	30	HIS	-	expression tag	UNP G0Y2B2
w	31	HIS	-	expression tag	UNP G0Y2B2
w	32	HIS	-	expression tag	UNP G0Y2B2
w	33	HIS	-	expression tag	UNP G0Y2B2
w	34	HIS	-	expression tag	UNP G0Y2B2
w	35	SER	-	expression tag	UNP G0Y2B2
w	36	SER	-	expression tag	UNP G0Y2B2
w	37	GLY	-	expression tag	UNP G0Y2B2
w	38	LEU	-	expression tag	UNP G0Y2B2
w	39	VAL	-	expression tag	UNP G0Y2B2
w	40	PRO	-	expression tag	UNP G0Y2B2
w	41	ARG	-	expression tag	UNP G0Y2B2
w	42	GLY	-	expression tag	UNP G0Y2B2
w	43	SER	-	expression tag	UNP G0Y2B2
w	44	HIS	-	expression tag	UNP G0Y2B2
x	25	MET	-	expression tag	UNP G0Y2B2
x	26	GLY	-	expression tag	UNP G0Y2B2
x	27	SER	-	expression tag	UNP G0Y2B2
x	28	SER	-	expression tag	UNP G0Y2B2
x	29	HIS	-	expression tag	UNP G0Y2B2
x	30	HIS	-	expression tag	UNP G0Y2B2
x	31	HIS	-	expression tag	UNP G0Y2B2
x	32	HIS	-	expression tag	UNP G0Y2B2

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Chain	Residue	Modelled	Actual	Comment	Reference
x	33	HIS	-	expression tag	UNP G0Y2B2
x	34	HIS	-	expression tag	UNP G0Y2B2
x	35	SER	-	expression tag	UNP G0Y2B2
x	36	SER	-	expression tag	UNP G0Y2B2
x	37	GLY	-	expression tag	UNP G0Y2B2
x	38	LEU	-	expression tag	UNP G0Y2B2
x	39	VAL	-	expression tag	UNP G0Y2B2
x	40	PRO	-	expression tag	UNP G0Y2B2
x	41	ARG	-	expression tag	UNP G0Y2B2
x	42	GLY	-	expression tag	UNP G0Y2B2
x	43	SER	-	expression tag	UNP G0Y2B2
x	44	HIS	-	expression tag	UNP G0Y2B2
y	25	MET	-	expression tag	UNP G0Y2B2
y	26	GLY	-	expression tag	UNP G0Y2B2
y	27	SER	-	expression tag	UNP G0Y2B2
y	28	SER	-	expression tag	UNP G0Y2B2
y	29	HIS	-	expression tag	UNP G0Y2B2
y	30	HIS	-	expression tag	UNP G0Y2B2
y	31	HIS	-	expression tag	UNP G0Y2B2
y	32	HIS	-	expression tag	UNP G0Y2B2
y	33	HIS	-	expression tag	UNP G0Y2B2
y	34	HIS	-	expression tag	UNP G0Y2B2
y	35	SER	-	expression tag	UNP G0Y2B2
y	36	SER	-	expression tag	UNP G0Y2B2
y	37	GLY	-	expression tag	UNP G0Y2B2
y	38	LEU	-	expression tag	UNP G0Y2B2
y	39	VAL	-	expression tag	UNP G0Y2B2
y	40	PRO	-	expression tag	UNP G0Y2B2
y	41	ARG	-	expression tag	UNP G0Y2B2
y	42	GLY	-	expression tag	UNP G0Y2B2
y	43	SER	-	expression tag	UNP G0Y2B2
y	44	HIS	-	expression tag	UNP G0Y2B2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	94	Total O 94 94	0	0
2	B	78	Total O 78 78	0	0
2	C	98	Total O 98 98	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	91	Total O 91 91	0	0
2	E	107	Total O 107 107	0	0
2	F	95	Total O 95 95	0	0
2	G	90	Total O 90 90	0	0
2	H	52	Total O 52 52	0	0
2	I	63	Total O 63 63	0	0
2	J	65	Total O 65 65	0	0
2	K	75	Total O 75 75	0	0
2	L	81	Total O 81 81	0	0
2	M	96	Total O 96 96	0	0
2	N	83	Total O 83 83	0	0
2	O	74	Total O 74 74	0	0
2	P	94	Total O 94 94	0	0
2	Q	83	Total O 83 83	0	0
2	R	86	Total O 86 86	0	0
2	S	87	Total O 87 87	0	0
2	T	74	Total O 74 74	0	0
2	U	68	Total O 68 68	0	0
2	V	53	Total O 53 53	0	0
2	W	55	Total O 55 55	0	0
2	X	72	Total O 72 72	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Y	57	Total O 57 57	0	0
2	Z	63	Total O 63 63	0	0
2	1	66	Total O 66 66	0	0
2	2	79	Total O 79 79	0	0
2	3	98	Total O 98 98	0	0
2	4	96	Total O 96 96	0	0
2	5	92	Total O 92 92	0	0
2	6	104	Total O 104 104	0	0
2	7	88	Total O 88 88	0	0
2	8	91	Total O 91 91	0	0
2	9	91	Total O 91 91	0	0
2	a	90	Total O 90 90	0	0
2	b	63	Total O 63 63	0	0
2	c	50	Total O 50 50	0	0
2	d	69	Total O 69 69	0	0
2	e	76	Total O 76 76	0	0
2	f	78	Total O 78 78	0	0
2	g	70	Total O 70 70	0	0
2	h	80	Total O 80 80	0	0
2	i	81	Total O 81 81	0	0
2	j	69	Total O 69 69	0	0

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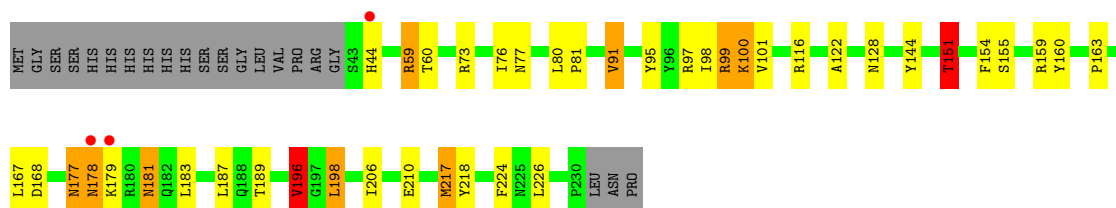
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	k	78	Total 78	O 78	0	0
2	l	81	Total 81	O 81	0	0
2	m	78	Total 78	O 78	0	0
2	n	94	Total 94	O 94	0	0
2	o	79	Total 79	O 79	0	0
2	p	78	Total 78	O 78	0	0
2	q	102	Total 102	O 102	0	0
2	r	74	Total 74	O 74	0	0
2	s	113	Total 113	O 113	0	0
2	t	76	Total 76	O 76	0	0
2	u	93	Total 93	O 93	0	0
2	v	82	Total 82	O 82	0	0
2	w	94	Total 94	O 94	0	0
2	x	81	Total 81	O 81	0	0
2	y	78	Total 78	O 78	0	0

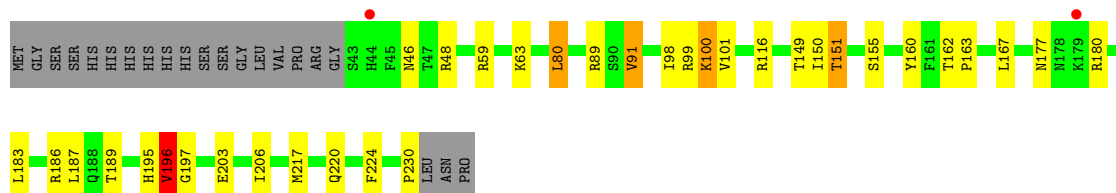
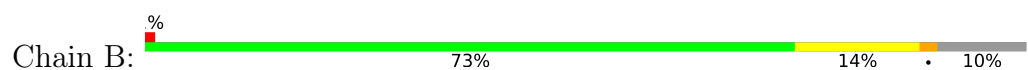
3 Residue-property plots [i](#)

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.

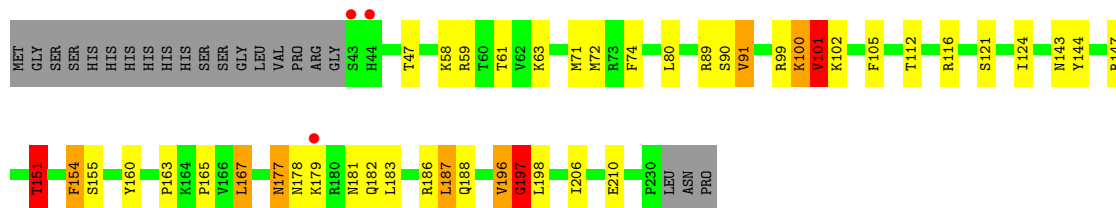
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

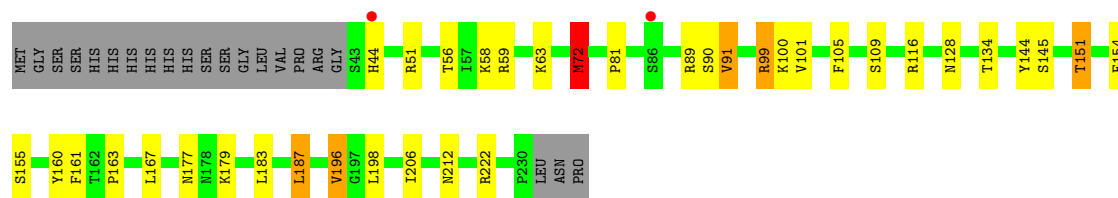


- Molecule 1: Capsid protein

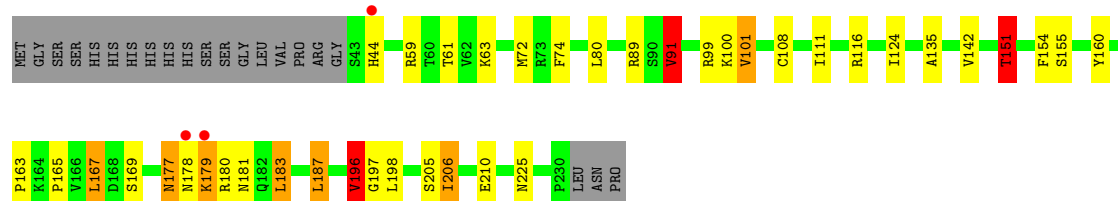


- Molecule 1: Capsid protein

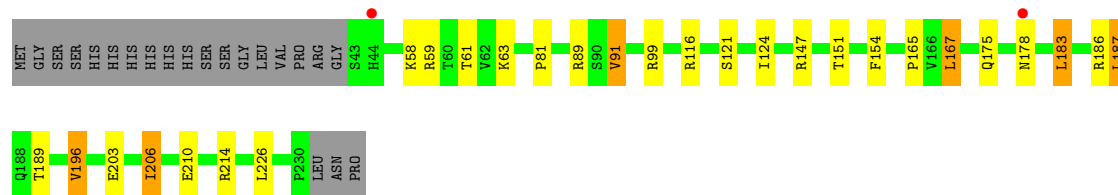
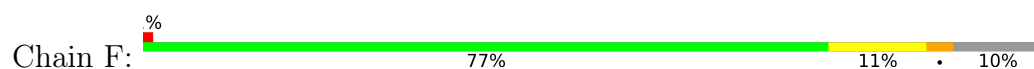




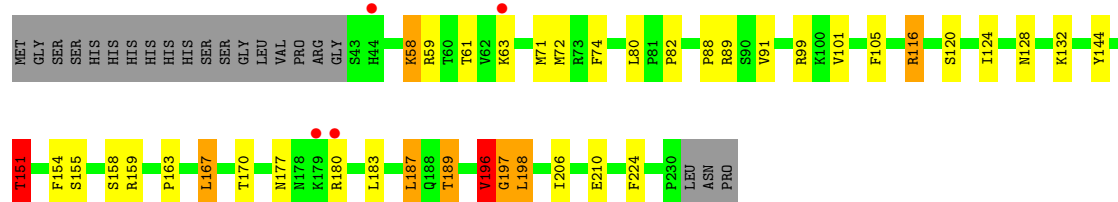
• Molecule 1: Capsid protein



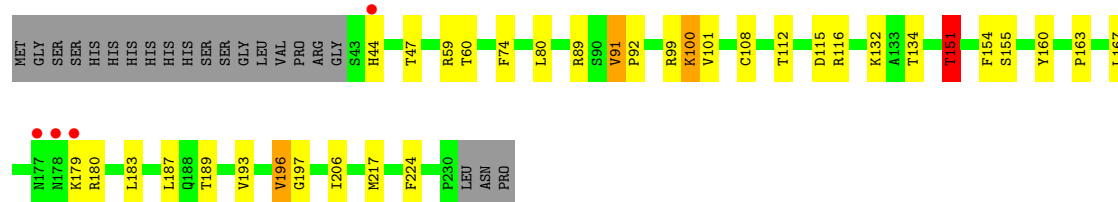
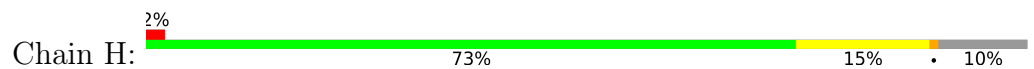
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein

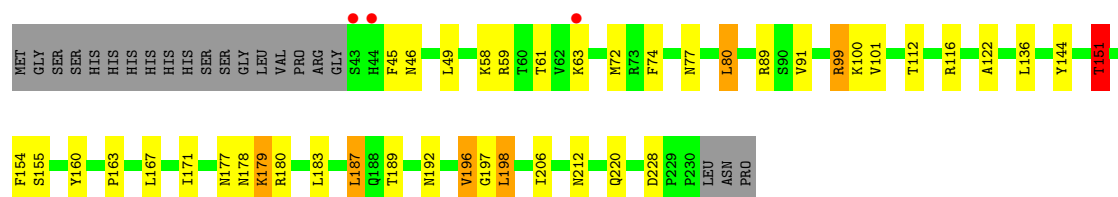


• Molecule 1: Capsid protein



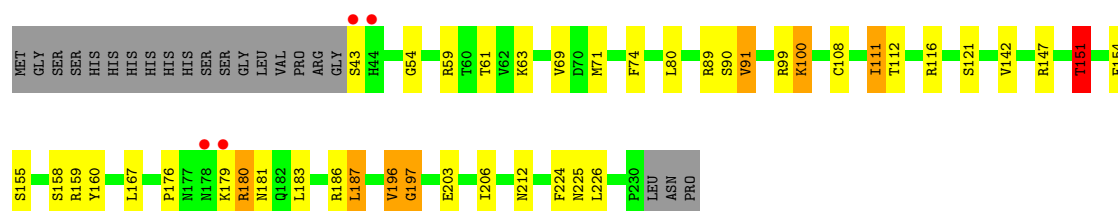
- Molecule 1: Capsid protein

Chain I: 



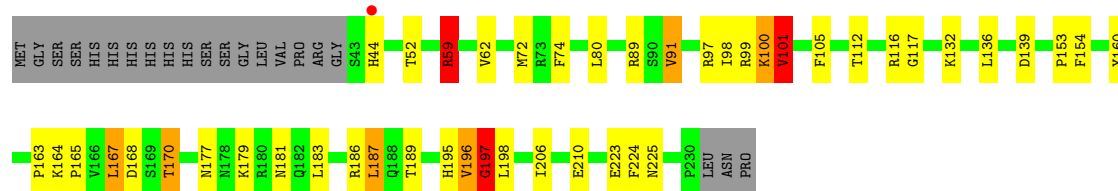
- Molecule 1: Capsid protein

Chain J: 



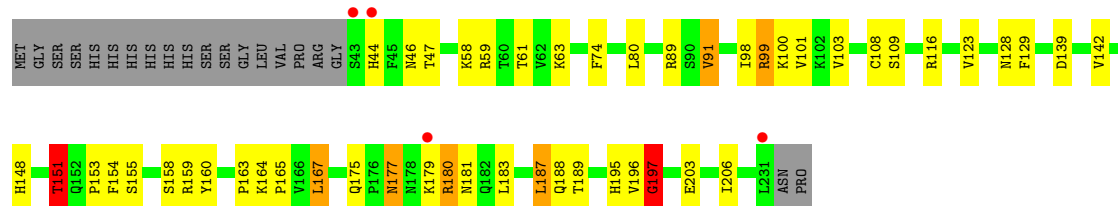
- Molecule 1: Capsid protein

Chain K: 



- Molecule 1: Capsid protein

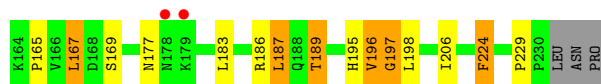
Chain L: 



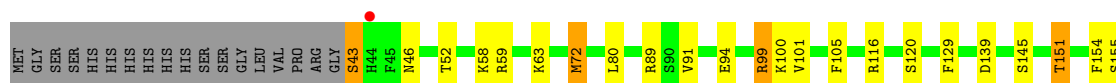
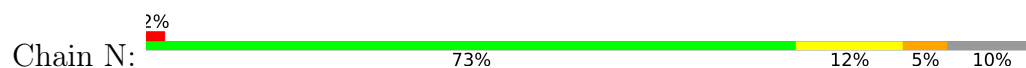
- Molecule 1: Capsid protein

Chain M: 

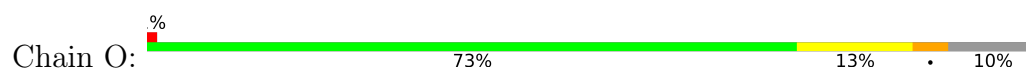




• Molecule 1: Capsid protein



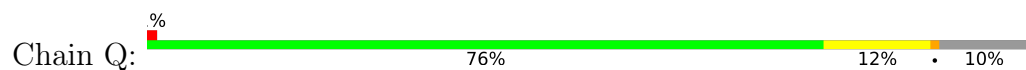
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein

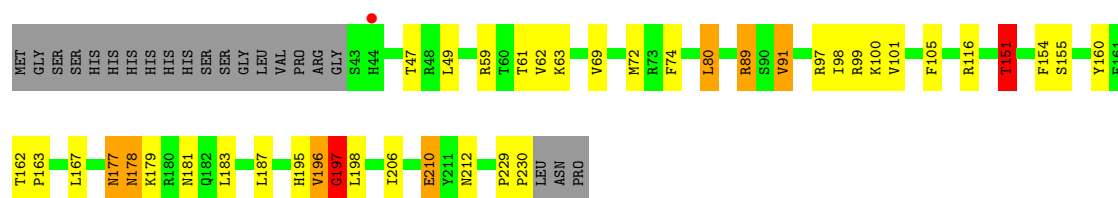


• Molecule 1: Capsid protein

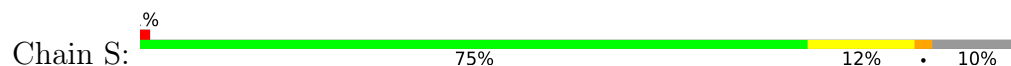


• Molecule 1: Capsid protein

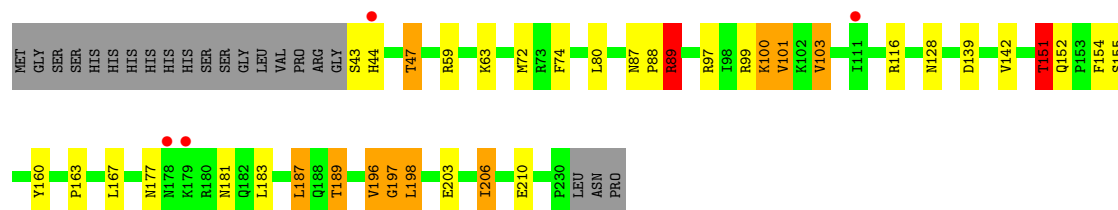
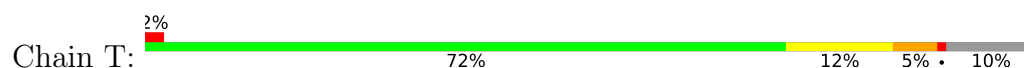




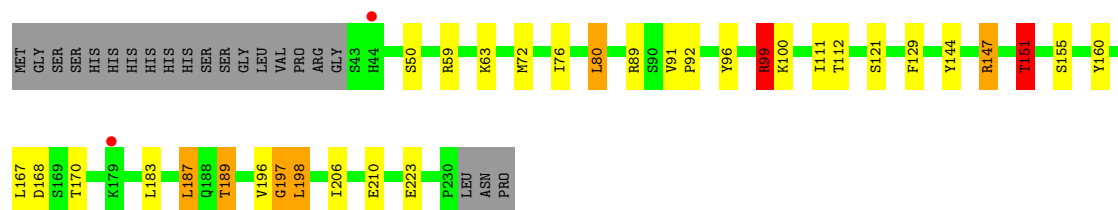
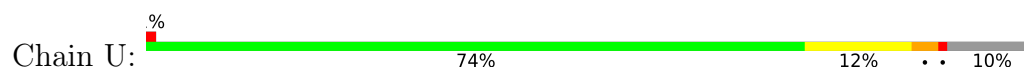
• Molecule 1: Capsid protein



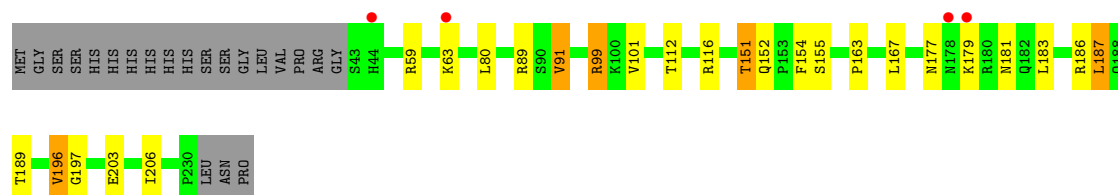
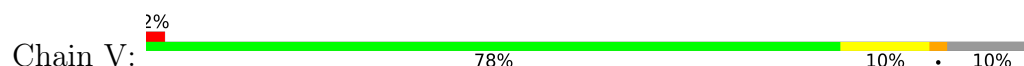
• Molecule 1: Capsid protein



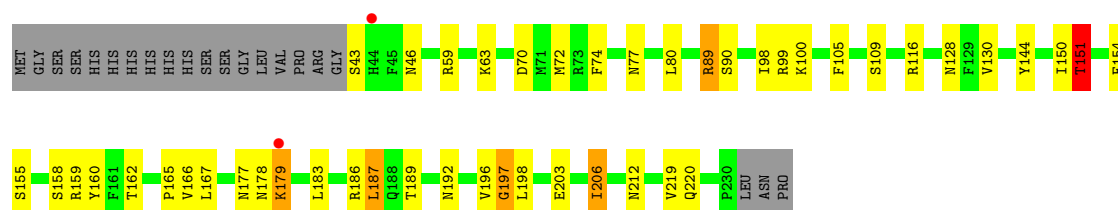
• Molecule 1: Capsid protein



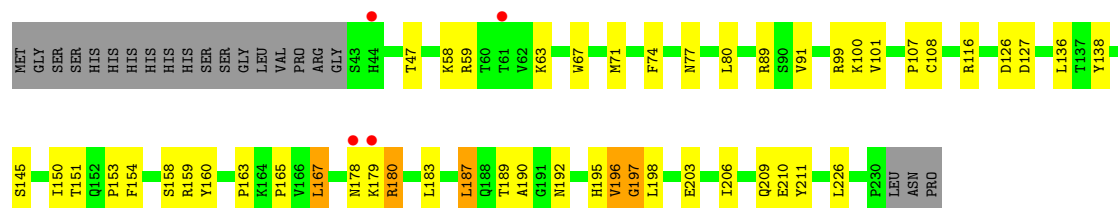
• Molecule 1: Capsid protein



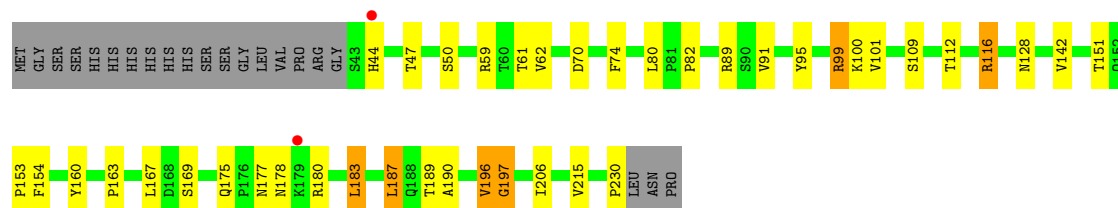
- Molecule 1: Capsid protein



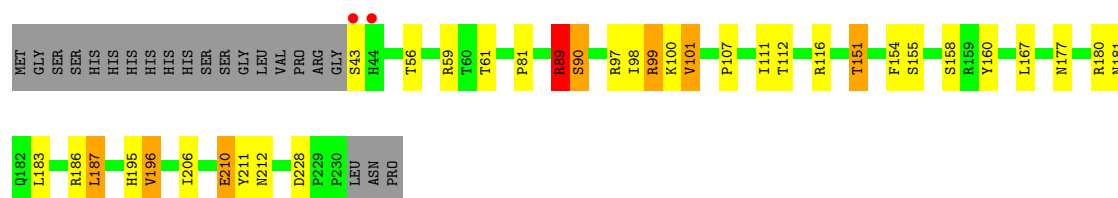
- Molecule 1: Capsid protein



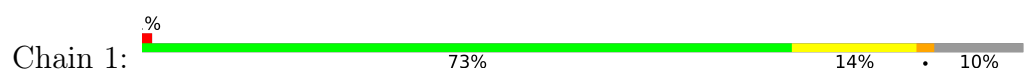
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

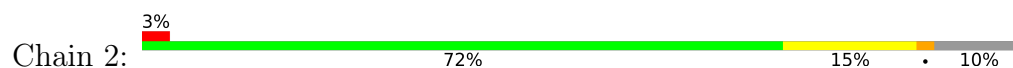


- Molecule 1: Capsid protein





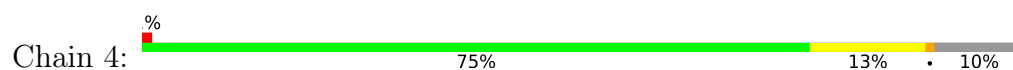
- Molecule 1: Capsid protein



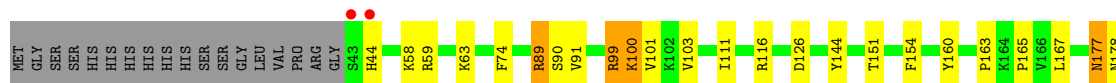
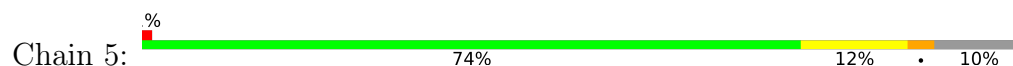
- Molecule 1: Capsid protein



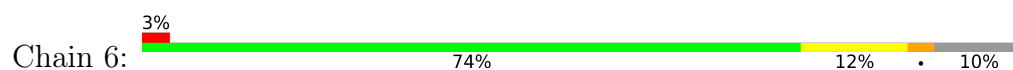
- Molecule 1: Capsid protein

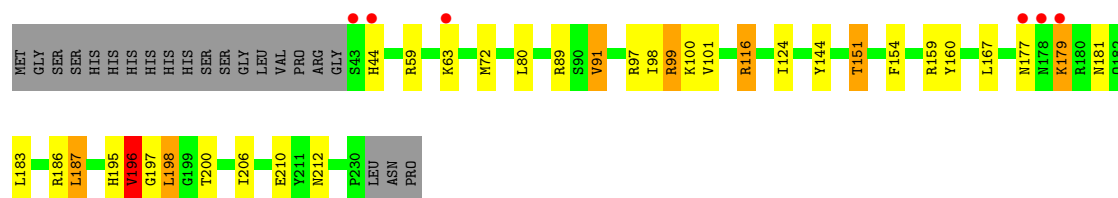


- Molecule 1: Capsid protein

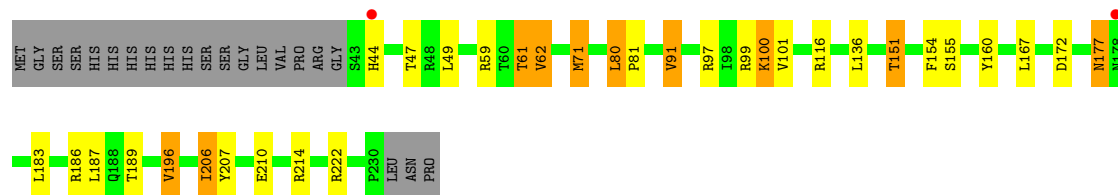
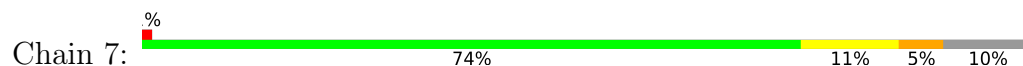


- Molecule 1: Capsid protein

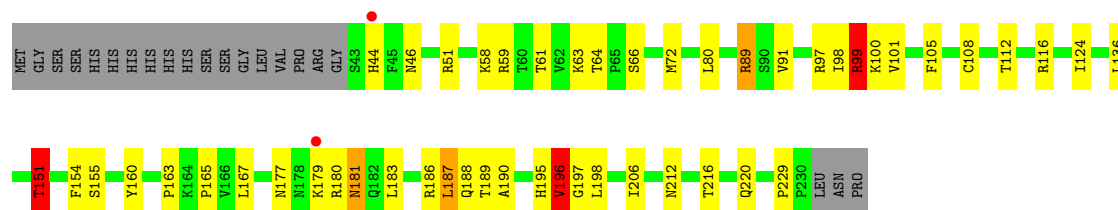




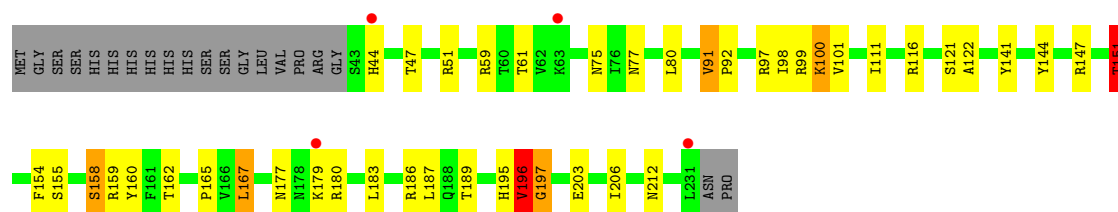
• Molecule 1: Capsid protein



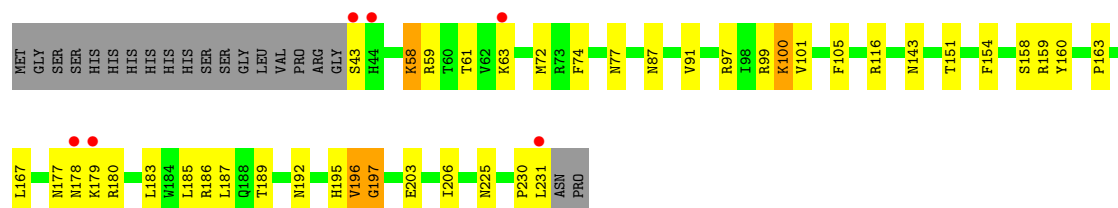
• Molecule 1: Capsid protein



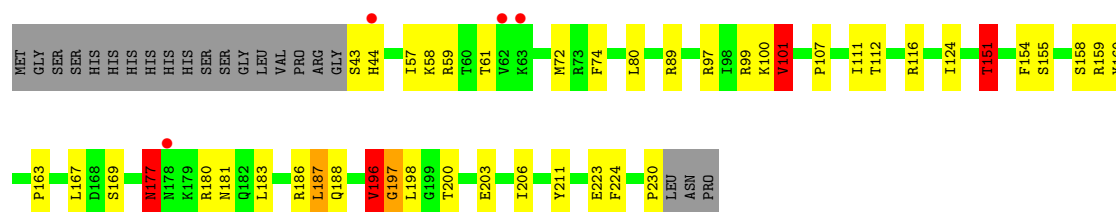
• Molecule 1: Capsid protein



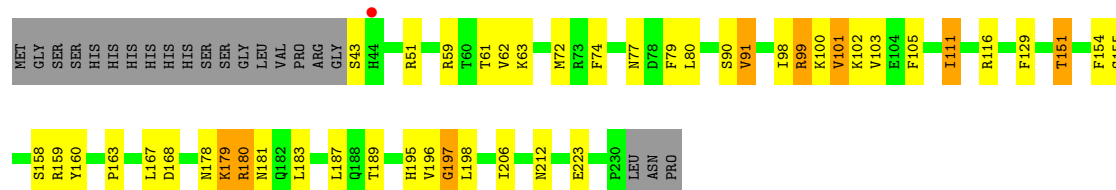
• Molecule 1: Capsid protein



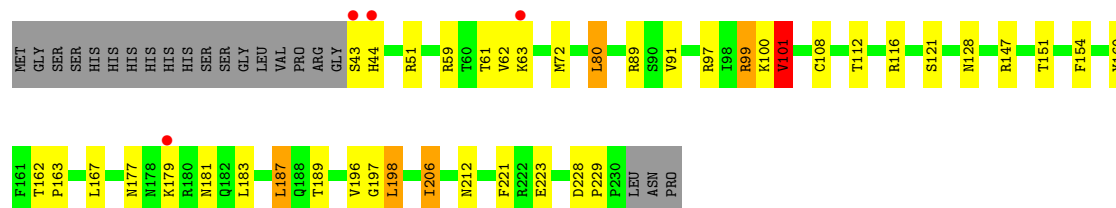
- Molecule 1: Capsid protein



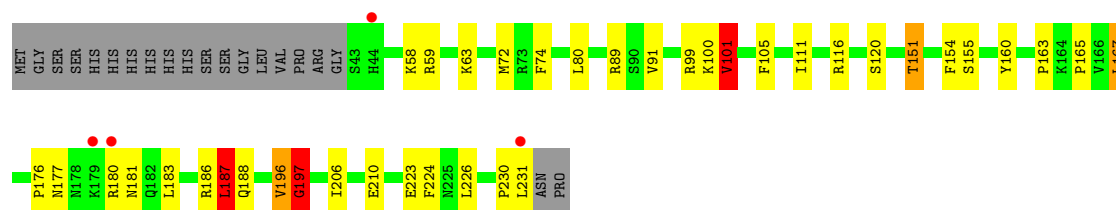
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

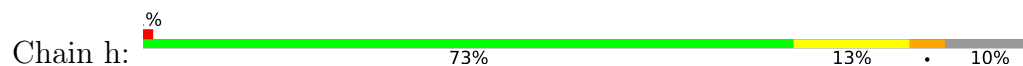




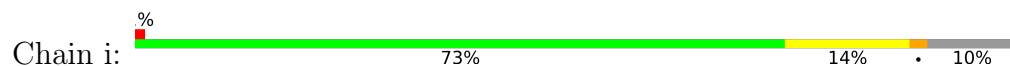
• Molecule 1: Capsid protein



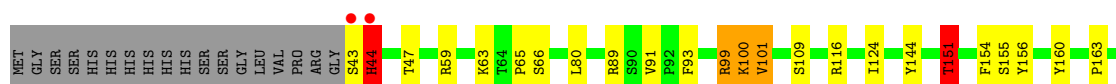
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein

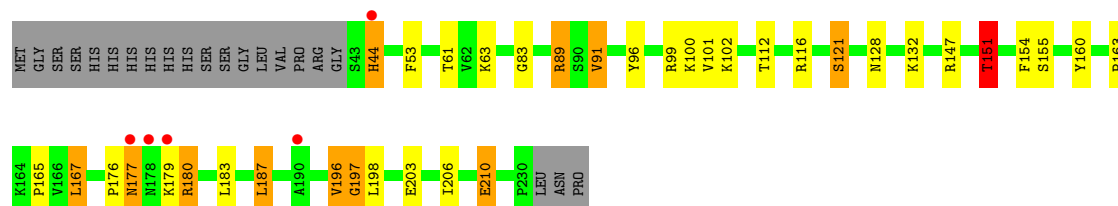


• Molecule 1: Capsid protein

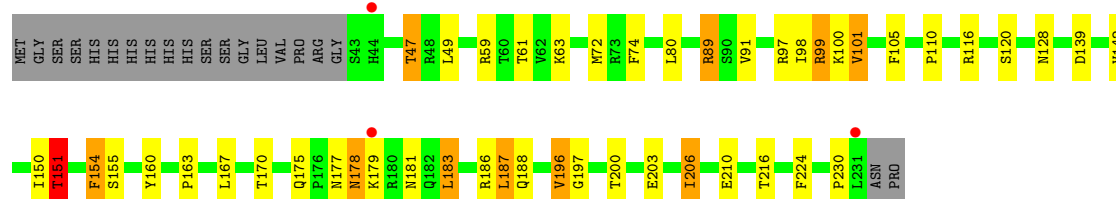


• Molecule 1: Capsid protein

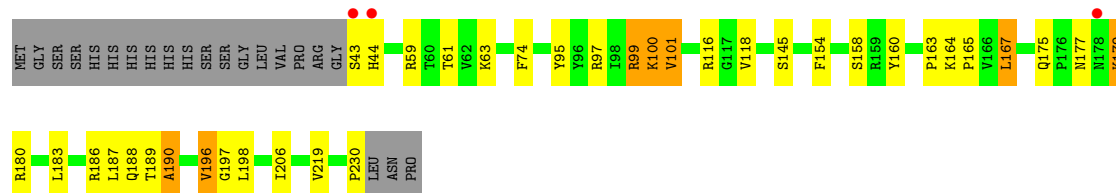
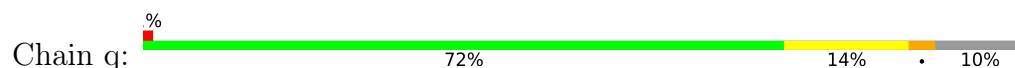




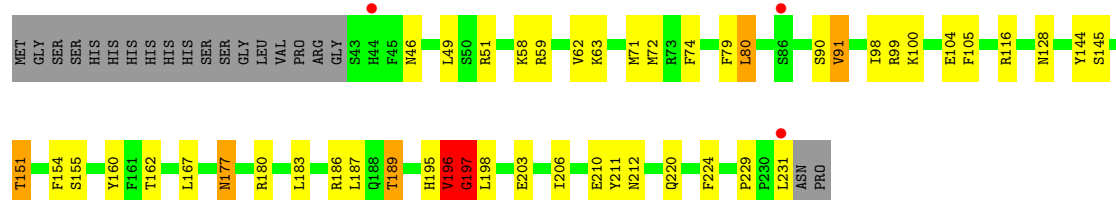
- Molecule 1: Capsid protein



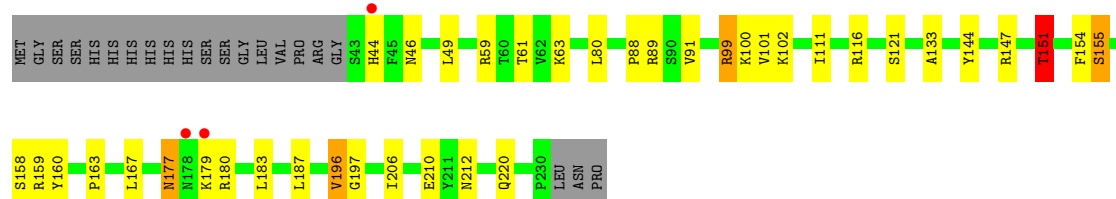
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

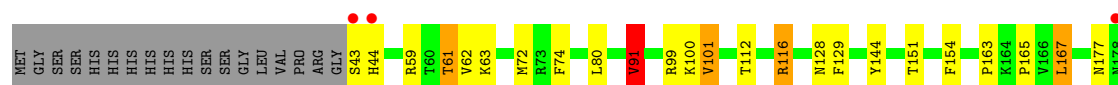
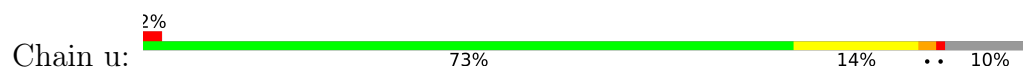


- Molecule 1: Capsid protein





• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



• Molecule 1: Capsid protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	194.12Å 201.88Å 231.28Å 90.00° 90.72° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.80) 99.0 (50.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.163 , 0.224 0.167 , 0.222	Depositor DCC
R_{free} test set	21255 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l 0.000 for k,h,-l 0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	97686	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.36% 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	1	1.21	4/1594 (0.3%)	1.23	4/2171 (0.2%)
1	2	1.21	2/1602 (0.1%)	1.25	11/2182 (0.5%)
1	3	1.30	4/1594 (0.3%)	1.21	7/2171 (0.3%)
1	4	1.26	3/1594 (0.2%)	1.29	9/2171 (0.4%)
1	5	1.26	6/1594 (0.4%)	1.24	3/2171 (0.1%)
1	6	1.35	6/1594 (0.4%)	1.31	10/2171 (0.5%)
1	7	1.32	4/1594 (0.3%)	1.26	8/2171 (0.4%)
1	8	1.31	8/1594 (0.5%)	1.29	13/2171 (0.6%)
1	9	1.30	3/1602 (0.2%)	1.25	7/2182 (0.3%)
1	A	1.36	8/1594 (0.5%)	1.33	10/2171 (0.5%)
1	B	1.30	6/1594 (0.4%)	1.25	5/2171 (0.2%)
1	C	1.31	4/1594 (0.3%)	1.25	8/2171 (0.4%)
1	D	1.34	3/1594 (0.2%)	1.27	8/2171 (0.4%)
1	E	1.32	7/1594 (0.4%)	1.27	11/2171 (0.5%)
1	F	1.33	1/1594 (0.1%)	1.24	6/2171 (0.3%)
1	G	1.26	4/1594 (0.3%)	1.27	5/2171 (0.2%)
1	H	1.22	2/1594 (0.1%)	1.17	2/2171 (0.1%)
1	I	1.20	1/1594 (0.1%)	1.22	8/2171 (0.4%)
1	J	1.23	2/1594 (0.1%)	1.25	5/2171 (0.2%)
1	K	1.33	10/1594 (0.6%)	1.30	9/2171 (0.4%)
1	L	1.21	7/1602 (0.4%)	1.25	9/2182 (0.4%)
1	M	1.28	2/1594 (0.1%)	1.25	11/2171 (0.5%)
1	N	1.28	2/1594 (0.1%)	1.22	3/2171 (0.1%)
1	O	1.36	7/1594 (0.4%)	1.26	5/2171 (0.2%)
1	P	1.35	7/1594 (0.4%)	1.32	14/2171 (0.6%)
1	Q	1.27	2/1594 (0.1%)	1.24	3/2171 (0.1%)
1	R	1.34	7/1594 (0.4%)	1.32	9/2171 (0.4%)
1	S	1.32	3/1594 (0.2%)	1.19	3/2171 (0.1%)
1	T	1.26	2/1594 (0.1%)	1.30	11/2171 (0.5%)
1	U	1.22	3/1594 (0.2%)	1.23	7/2171 (0.3%)
1	V	1.19	2/1594 (0.1%)	1.19	1/2171 (0.0%)
1	W	1.25	1/1594 (0.1%)	1.22	9/2171 (0.4%)
1	X	1.17	2/1594 (0.1%)	1.17	4/2171 (0.2%)
1	Y	1.21	1/1594 (0.1%)	1.19	4/2171 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Z	1.21	4/1594 (0.3%)	1.20	5/2171 (0.2%)
1	a	1.23	3/1602 (0.2%)	1.21	6/2182 (0.3%)
1	b	1.23	3/1594 (0.2%)	1.25	12/2171 (0.6%)
1	c	1.24	2/1594 (0.1%)	1.19	3/2171 (0.1%)
1	d	1.21	2/1594 (0.1%)	1.22	14/2171 (0.6%)
1	e	1.29	5/1602 (0.3%)	1.24	3/2182 (0.1%)
1	f	1.17	2/1594 (0.1%)	1.18	4/2171 (0.2%)
1	g	1.29	7/1594 (0.4%)	1.21	7/2171 (0.3%)
1	h	1.27	4/1594 (0.3%)	1.25	5/2171 (0.2%)
1	i	1.29	5/1594 (0.3%)	1.23	6/2171 (0.3%)
1	j	1.23	4/1594 (0.3%)	1.19	6/2171 (0.3%)
1	k	1.28	1/1602 (0.1%)	1.25	4/2182 (0.2%)
1	l	1.30	2/1594 (0.1%)	1.23	13/2171 (0.6%)
1	m	1.30	6/1594 (0.4%)	1.19	3/2171 (0.1%)
1	n	1.30	7/1594 (0.4%)	1.27	16/2171 (0.7%)
1	o	1.30	3/1594 (0.2%)	1.30	8/2171 (0.4%)
1	p	1.31	6/1602 (0.4%)	1.27	10/2182 (0.5%)
1	q	1.31	2/1594 (0.1%)	1.26	7/2171 (0.3%)
1	r	1.26	5/1602 (0.3%)	1.24	9/2182 (0.4%)
1	s	1.30	4/1594 (0.3%)	1.22	2/2171 (0.1%)
1	t	1.29	6/1594 (0.4%)	1.26	4/2171 (0.2%)
1	u	1.28	3/1594 (0.2%)	1.25	8/2171 (0.4%)
1	v	1.28	5/1594 (0.3%)	1.23	8/2171 (0.4%)
1	w	1.32	6/1594 (0.4%)	1.24	5/2171 (0.2%)
1	x	1.30	3/1602 (0.2%)	1.27	11/2182 (0.5%)
1	y	1.28	4/1602 (0.2%)	1.26	6/2182 (0.3%)
All	All	1.28	240/95720 (0.3%)	1.24	427/130370 (0.3%)

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	1	0	1
1	4	0	1
1	5	0	1
1	6	0	1
1	7	0	1
1	9	0	1
1	A	0	2
1	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
1	F	0	2
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	M	0	1
1	N	0	2
1	O	0	1
1	P	0	1
1	Q	0	1
1	S	0	1
1	T	0	1
1	U	0	1
1	Y	0	1
1	Z	0	1
1	a	0	1
1	b	0	1
1	e	0	1
1	f	0	1
1	g	0	2
1	h	0	1
1	i	0	1
1	k	0	1
1	m	0	1
1	o	0	2
1	p	0	2
1	q	0	3
1	r	0	2
1	s	0	1
1	t	0	1
1	u	0	1
1	v	0	1
1	w	0	1
1	x	0	1
All	All	0	54

The worst 5 of 240 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	189	THR	CA-C	9.40	1.65	1.52
1	g	189	THR	CA-CB	9.32	1.69	1.53
1	E	177	ASN	CA-CB	8.42	1.63	1.53
1	7	81	PRO	CA-C	7.59	1.59	1.52
1	R	196	VAL	C-O	7.53	1.31	1.24

The worst 5 of 427 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ASN	N-CA-C	8.70	123.73	113.20
1	4	80	LEU	CA-C-N	-8.41	111.72	120.38
1	4	80	LEU	C-N-CA	-8.41	111.72	120.38
1	K	101	VAL	CB-CA-C	-8.33	98.20	110.62
1	T	89	ARG	NE-CZ-NH2	8.23	126.61	119.20

There are no chirality outliers.

5 of 54 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	ASN	Peptide
1	A	196	VAL	Peptide
1	B	196	VAL	Peptide
1	D	196	VAL	Peptide
1	E	196	VAL	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	1	1546	0	1490	14	0
1	2	1554	0	1501	16	0
1	3	1546	0	1490	14	0
1	4	1546	0	1490	8	0
1	5	1546	0	1490	12	0
1	6	1546	0	1490	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	7	1546	0	1490	16	0
1	8	1546	0	1490	19	0
1	9	1554	0	1501	18	0
1	A	1546	0	1490	17	0
1	B	1546	0	1490	15	0
1	C	1546	0	1490	20	0
1	D	1546	0	1490	14	0
1	E	1546	0	1490	18	0
1	F	1546	0	1490	10	0
1	G	1546	0	1490	19	0
1	H	1546	0	1490	14	0
1	I	1546	0	1490	20	0
1	J	1546	0	1490	18	0
1	K	1546	0	1490	22	0
1	L	1554	0	1501	20	0
1	M	1546	0	1490	20	0
1	N	1546	0	1490	19	0
1	O	1546	0	1490	10	0
1	P	1546	0	1490	19	0
1	Q	1546	0	1490	11	0
1	R	1546	0	1490	15	0
1	S	1546	0	1490	17	0
1	T	1546	0	1490	19	0
1	U	1546	0	1490	12	0
1	V	1546	0	1490	13	0
1	W	1546	0	1490	21	0
1	X	1546	0	1490	19	0
1	Y	1546	0	1490	13	0
1	Z	1546	0	1490	16	0
1	a	1554	0	1501	15	0
1	b	1546	0	1490	18	0
1	c	1546	0	1490	20	0
1	d	1546	0	1490	16	0
1	e	1554	0	1501	14	0
1	f	1546	0	1490	16	0
1	g	1546	0	1490	16	0
1	h	1546	0	1490	14	0
1	i	1546	0	1490	13	0
1	j	1546	0	1490	14	0
1	k	1554	0	1501	17	0
1	l	1546	0	1490	13	0
1	m	1546	0	1490	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	n	1546	0	1490	14	0
1	o	1546	0	1490	18	0
1	p	1554	0	1501	22	0
1	q	1546	0	1490	12	0
1	r	1554	0	1501	23	0
1	s	1546	0	1490	15	0
1	t	1546	0	1490	18	0
1	u	1546	0	1490	14	0
1	v	1546	0	1490	20	0
1	w	1546	0	1490	20	0
1	x	1554	0	1501	23	0
1	y	1554	0	1501	19	0
2	1	66	0	0	0	0
2	2	79	0	0	3	0
2	3	98	0	0	1	0
2	4	96	0	0	0	0
2	5	92	0	0	1	0
2	6	104	0	0	4	1
2	7	88	0	0	4	0
2	8	91	0	0	2	0
2	9	91	0	0	2	0
2	A	94	0	0	2	0
2	B	78	0	0	1	0
2	C	98	0	0	2	0
2	D	91	0	0	3	0
2	E	107	0	0	2	0
2	F	95	0	0	1	0
2	G	90	0	0	1	0
2	H	52	0	0	0	0
2	I	63	0	0	0	0
2	J	65	0	0	0	0
2	K	75	0	0	4	0
2	L	81	0	0	2	0
2	M	96	0	0	3	0
2	N	83	0	0	2	0
2	O	74	0	0	1	0
2	P	94	0	0	3	0
2	Q	83	0	0	4	0
2	R	86	0	0	1	0
2	S	87	0	0	2	0
2	T	74	0	0	4	0
2	U	68	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	53	0	0	2	0
2	W	55	0	0	2	0
2	X	72	0	0	2	0
2	Y	57	0	0	1	0
2	Z	63	0	0	0	0
2	a	90	0	0	2	0
2	b	63	0	0	1	0
2	c	50	0	0	1	0
2	d	69	0	0	2	0
2	e	76	0	0	1	0
2	f	78	0	0	1	0
2	g	70	0	0	5	0
2	h	80	0	0	1	0
2	i	81	0	0	3	0
2	j	69	0	0	4	0
2	k	78	0	0	2	0
2	l	81	0	0	0	0
2	m	78	0	0	1	0
2	n	94	0	0	2	0
2	o	79	0	0	4	0
2	p	78	0	0	0	0
2	q	102	0	0	2	1
2	r	74	0	0	3	0
2	s	113	0	0	1	0
2	t	76	0	0	1	0
2	u	93	0	0	3	0
2	v	82	0	0	2	0
2	w	94	0	0	5	0
2	x	81	0	0	6	0
2	y	78	0	0	2	0
All	All	97686	0	89510	872	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 5.

The worst 5 of 872 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:g:44:HIS:HB3	2:g:358:HOH:O	1.46	1.12
1:6:101:VAL:HB	2:6:371:HOH:O	1.47	1.11
1:x:44:HIS:HB2	2:x:371:HOH:O	1.49	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:101:VAL:HB	2:i:343:HOH:O	1.55	1.06
1:M:101:VAL:HB	2:M:367:HOH:O	1.56	1.05

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)
2:6:385:HOH:O	2:q:376:HOH:O[2_555]	2.13	0.07

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	1	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	24	55
1	2	187/209 (90%)	174 (93%)	12 (6%)	1 (0%)	24	55
1	3	186/209 (89%)	175 (94%)	9 (5%)	2 (1%)	11	36
1	4	186/209 (89%)	172 (92%)	13 (7%)	1 (0%)	24	55
1	5	186/209 (89%)	179 (96%)	7 (4%)	0	100	100
1	6	186/209 (89%)	178 (96%)	7 (4%)	1 (0%)	24	55
1	7	186/209 (89%)	178 (96%)	6 (3%)	2 (1%)	11	36
1	8	186/209 (89%)	172 (92%)	13 (7%)	1 (0%)	24	55
1	9	187/209 (90%)	177 (95%)	8 (4%)	2 (1%)	11	36
1	A	186/209 (89%)	178 (96%)	7 (4%)	1 (0%)	24	55
1	B	186/209 (89%)	176 (95%)	9 (5%)	1 (0%)	24	55
1	C	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	24	55
1	D	186/209 (89%)	176 (95%)	10 (5%)	0	100	100
1	E	186/209 (89%)	176 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	186/209 (89%)	173 (93%)	13 (7%)	0	100	100
1	G	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	24	55
1	H	186/209 (89%)	173 (93%)	12 (6%)	1 (0%)	24	55
1	I	186/209 (89%)	176 (95%)	10 (5%)	0	100	100
1	J	186/209 (89%)	173 (93%)	12 (6%)	1 (0%)	24	55
1	K	186/209 (89%)	172 (92%)	12 (6%)	2 (1%)	11	36
1	L	187/209 (90%)	179 (96%)	7 (4%)	1 (0%)	24	55
1	M	186/209 (89%)	176 (95%)	8 (4%)	2 (1%)	11	36
1	N	186/209 (89%)	175 (94%)	11 (6%)	0	100	100
1	O	186/209 (89%)	173 (93%)	12 (6%)	1 (0%)	24	55
1	P	186/209 (89%)	174 (94%)	10 (5%)	2 (1%)	11	36
1	Q	186/209 (89%)	177 (95%)	8 (4%)	1 (0%)	24	55
1	R	186/209 (89%)	173 (93%)	11 (6%)	2 (1%)	11	36
1	S	186/209 (89%)	179 (96%)	6 (3%)	1 (0%)	24	55
1	T	186/209 (89%)	177 (95%)	8 (4%)	1 (0%)	24	55
1	U	186/209 (89%)	173 (93%)	10 (5%)	3 (2%)	7	27
1	V	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	24	55
1	W	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	24	55
1	X	186/209 (89%)	170 (91%)	15 (8%)	1 (0%)	24	55
1	Y	186/209 (89%)	171 (92%)	12 (6%)	3 (2%)	7	27
1	Z	186/209 (89%)	173 (93%)	13 (7%)	0	100	100
1	a	187/209 (90%)	176 (94%)	9 (5%)	2 (1%)	11	36
1	b	186/209 (89%)	176 (95%)	8 (4%)	2 (1%)	11	36
1	c	186/209 (89%)	175 (94%)	8 (4%)	3 (2%)	7	27
1	d	186/209 (89%)	172 (92%)	12 (6%)	2 (1%)	11	36
1	e	187/209 (90%)	178 (95%)	7 (4%)	2 (1%)	11	36
1	f	186/209 (89%)	175 (94%)	11 (6%)	0	100	100
1	g	186/209 (89%)	174 (94%)	10 (5%)	2 (1%)	11	36
1	h	186/209 (89%)	169 (91%)	16 (9%)	1 (0%)	24	55
1	i	186/209 (89%)	175 (94%)	11 (6%)	0	100	100
1	j	186/209 (89%)	172 (92%)	12 (6%)	2 (1%)	11	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	k	187/209 (90%)	172 (92%)	13 (7%)	2 (1%)	11	36
1	l	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	24	55
1	m	186/209 (89%)	177 (95%)	8 (4%)	1 (0%)	24	55
1	n	186/209 (89%)	177 (95%)	7 (4%)	2 (1%)	11	36
1	o	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	24	55
1	p	187/209 (90%)	179 (96%)	8 (4%)	0	100	100
1	q	186/209 (89%)	176 (95%)	9 (5%)	1 (0%)	24	55
1	r	187/209 (90%)	179 (96%)	7 (4%)	1 (0%)	24	55
1	s	186/209 (89%)	177 (95%)	8 (4%)	1 (0%)	24	55
1	t	186/209 (89%)	177 (95%)	8 (4%)	1 (0%)	24	55
1	u	186/209 (89%)	173 (93%)	11 (6%)	2 (1%)	11	36
1	v	186/209 (89%)	177 (95%)	9 (5%)	0	100	100
1	w	186/209 (89%)	177 (95%)	8 (4%)	1 (0%)	24	55
1	x	187/209 (90%)	177 (95%)	8 (4%)	2 (1%)	11	36
1	y	187/209 (90%)	173 (92%)	13 (7%)	1 (0%)	24	55
All	All	11170/12540 (89%)	10499 (94%)	599 (5%)	72 (1%)	21	51

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	62	VAL
1	g	189	THR
1	Y	62	VAL
1	k	59	ARG
1	A	178	ASN

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	1	172/190 (90%)	160 (93%)	12 (7%)	14	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	173/190 (91%)	160 (92%)	13 (8%)	12	37
1	3	172/190 (90%)	155 (90%)	17 (10%)	7	24
1	4	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	5	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	6	172/190 (90%)	161 (94%)	11 (6%)	16	44
1	7	172/190 (90%)	158 (92%)	14 (8%)	11	33
1	8	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	9	173/190 (91%)	158 (91%)	15 (9%)	9	30
1	A	172/190 (90%)	157 (91%)	15 (9%)	9	30
1	B	172/190 (90%)	157 (91%)	15 (9%)	9	30
1	C	172/190 (90%)	153 (89%)	19 (11%)	6	20
1	D	172/190 (90%)	157 (91%)	15 (9%)	9	30
1	E	172/190 (90%)	157 (91%)	15 (9%)	9	30
1	F	172/190 (90%)	159 (92%)	13 (8%)	12	36
1	G	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	H	172/190 (90%)	155 (90%)	17 (10%)	7	24
1	I	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	J	172/190 (90%)	153 (89%)	19 (11%)	6	20
1	K	172/190 (90%)	158 (92%)	14 (8%)	11	33
1	L	173/190 (91%)	155 (90%)	18 (10%)	7	22
1	M	172/190 (90%)	158 (92%)	14 (8%)	11	33
1	N	172/190 (90%)	159 (92%)	13 (8%)	12	36
1	O	172/190 (90%)	155 (90%)	17 (10%)	7	24
1	P	172/190 (90%)	159 (92%)	13 (8%)	12	36
1	Q	172/190 (90%)	159 (92%)	13 (8%)	12	36
1	R	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	S	172/190 (90%)	159 (92%)	13 (8%)	12	36
1	T	172/190 (90%)	155 (90%)	17 (10%)	7	24
1	U	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	V	172/190 (90%)	161 (94%)	11 (6%)	16	44
1	W	172/190 (90%)	156 (91%)	16 (9%)	8	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	172/190 (90%)	154 (90%)	18 (10%)	6	22
1	Y	172/190 (90%)	151 (88%)	21 (12%)	5	16
1	Z	172/190 (90%)	157 (91%)	15 (9%)	9	30
1	a	173/190 (91%)	155 (90%)	18 (10%)	7	22
1	b	172/190 (90%)	157 (91%)	15 (9%)	9	30
1	c	172/190 (90%)	153 (89%)	19 (11%)	6	20
1	d	172/190 (90%)	157 (91%)	15 (9%)	9	30
1	e	173/190 (91%)	156 (90%)	17 (10%)	7	25
1	f	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	g	172/190 (90%)	155 (90%)	17 (10%)	7	24
1	h	172/190 (90%)	157 (91%)	15 (9%)	9	30
1	i	172/190 (90%)	154 (90%)	18 (10%)	6	22
1	j	172/190 (90%)	153 (89%)	19 (11%)	6	20
1	k	173/190 (91%)	158 (91%)	15 (9%)	9	30
1	l	172/190 (90%)	160 (93%)	12 (7%)	14	40
1	m	172/190 (90%)	157 (91%)	15 (9%)	9	30
1	n	172/190 (90%)	160 (93%)	12 (7%)	14	40
1	o	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	p	173/190 (91%)	159 (92%)	14 (8%)	11	33
1	q	172/190 (90%)	159 (92%)	13 (8%)	12	36
1	r	173/190 (91%)	157 (91%)	16 (9%)	8	27
1	s	172/190 (90%)	158 (92%)	14 (8%)	11	33
1	t	172/190 (90%)	158 (92%)	14 (8%)	11	33
1	u	172/190 (90%)	156 (91%)	16 (9%)	8	27
1	v	172/190 (90%)	159 (92%)	13 (8%)	12	36
1	w	172/190 (90%)	158 (92%)	14 (8%)	11	33
1	x	173/190 (91%)	160 (92%)	13 (8%)	12	37
1	y	173/190 (91%)	157 (91%)	16 (9%)	8	27
All	All	10330/11400 (91%)	9413 (91%)	917 (9%)	9	29

5 of 917 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	5	58	LYS
1	w	206	ILE
1	c	91	VAL
1	w	71	MET
1	q	196	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 147 such sidechains are listed below:

Mol	Chain	Res	Type
1	j	212	ASN
1	x	181	ASN
1	k	212	ASN
1	q	188	GLN
1	S	204	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1	188/209 (89%)	-0.40	3 (1%) 70 61	32, 44, 71, 102	0
1	2	189/209 (90%)	-0.38	6 (3%) 50 40	32, 43, 69, 111	0
1	3	188/209 (89%)	-0.58	2 (1%) 78 70	26, 36, 60, 98	0
1	4	188/209 (89%)	-0.59	2 (1%) 78 70	27, 38, 65, 96	0
1	5	188/209 (89%)	-0.52	3 (1%) 70 61	29, 39, 66, 110	0
1	6	188/209 (89%)	-0.54	6 (3%) 50 40	26, 37, 59, 96	0
1	7	188/209 (89%)	-0.61	2 (1%) 78 70	27, 35, 61, 96	0
1	8	188/209 (89%)	-0.56	2 (1%) 78 70	24, 37, 63, 105	0
1	9	189/209 (90%)	-0.51	4 (2%) 63 54	29, 38, 63, 102	0
1	A	188/209 (89%)	-0.62	3 (1%) 70 61	26, 35, 57, 99	0
1	B	188/209 (89%)	-0.46	2 (1%) 78 70	32, 40, 63, 111	0
1	C	188/209 (89%)	-0.49	3 (1%) 70 61	27, 36, 64, 100	0
1	D	188/209 (89%)	-0.61	2 (1%) 78 70	26, 35, 59, 95	0
1	E	188/209 (89%)	-0.59	3 (1%) 70 61	25, 34, 58, 99	0
1	F	188/209 (89%)	-0.57	2 (1%) 78 70	25, 36, 61, 90	0
1	G	188/209 (89%)	-0.49	4 (2%) 63 54	28, 39, 69, 100	0
1	H	188/209 (89%)	-0.41	4 (2%) 63 54	34, 45, 70, 106	0
1	I	188/209 (89%)	-0.43	3 (1%) 70 61	33, 44, 70, 106	0
1	J	188/209 (89%)	-0.36	4 (2%) 63 54	32, 45, 73, 104	0
1	K	188/209 (89%)	-0.48	1 (0%) 87 82	24, 38, 64, 96	0
1	L	189/209 (90%)	-0.38	4 (2%) 63 54	33, 43, 69, 102	0
1	M	188/209 (89%)	-0.51	4 (2%) 63 54	30, 40, 66, 105	0
1	N	188/209 (89%)	-0.55	4 (2%) 63 54	27, 37, 66, 105	0
1	O	188/209 (89%)	-0.59	3 (1%) 70 61	25, 35, 61, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	P	188/209 (89%)	-0.59	3 (1%) 70 61	27, 35, 60, 95	0
1	Q	188/209 (89%)	-0.56	2 (1%) 78 70	28, 38, 62, 99	0
1	R	188/209 (89%)	-0.63	1 (0%) 87 82	27, 35, 63, 94	0
1	S	188/209 (89%)	-0.46	2 (1%) 78 70	29, 41, 69, 99	0
1	T	188/209 (89%)	-0.47	4 (2%) 63 54	30, 41, 69, 108	0
1	U	188/209 (89%)	-0.45	2 (1%) 78 70	29, 45, 69, 100	0
1	V	188/209 (89%)	-0.35	4 (2%) 63 54	35, 46, 73, 108	0
1	W	188/209 (89%)	-0.37	2 (1%) 78 70	35, 44, 73, 120	0
1	X	188/209 (89%)	-0.37	4 (2%) 63 54	35, 46, 71, 106	0
1	Y	188/209 (89%)	-0.36	2 (1%) 78 70	33, 46, 74, 106	0
1	Z	188/209 (89%)	-0.42	2 (1%) 78 70	32, 43, 73, 97	0
1	a	189/209 (90%)	-0.48	6 (3%) 50 40	30, 41, 66, 107	0
1	b	188/209 (89%)	-0.38	4 (2%) 63 54	32, 46, 73, 110	0
1	c	188/209 (89%)	-0.37	1 (0%) 87 82	33, 45, 68, 112	0
1	d	188/209 (89%)	-0.38	4 (2%) 63 54	35, 44, 69, 100	0
1	e	189/209 (90%)	-0.48	4 (2%) 63 54	29, 39, 64, 109	0
1	f	188/209 (89%)	-0.39	2 (1%) 78 70	32, 45, 72, 101	0
1	g	188/209 (89%)	-0.39	4 (2%) 63 54	32, 45, 71, 96	0
1	h	188/209 (89%)	-0.41	3 (1%) 70 61	32, 42, 65, 111	0
1	i	188/209 (89%)	-0.51	3 (1%) 70 61	30, 41, 64, 105	0
1	j	188/209 (89%)	-0.39	3 (1%) 70 61	35, 45, 70, 104	0
1	k	189/209 (90%)	-0.44	5 (2%) 57 47	29, 40, 72, 107	0
1	l	188/209 (89%)	-0.48	2 (1%) 78 70	28, 40, 68, 101	0
1	m	188/209 (89%)	-0.59	3 (1%) 70 61	27, 36, 64, 105	0
1	n	188/209 (89%)	-0.57	3 (1%) 70 61	26, 36, 65, 95	0
1	o	188/209 (89%)	-0.53	5 (2%) 56 46	27, 37, 64, 111	0
1	p	189/209 (90%)	-0.56	3 (1%) 70 61	26, 38, 62, 106	0
1	q	188/209 (89%)	-0.57	3 (1%) 70 61	28, 35, 64, 99	0
1	r	189/209 (90%)	-0.48	3 (1%) 70 61	30, 41, 64, 94	0
1	s	188/209 (89%)	-0.59	3 (1%) 70 61	28, 36, 63, 102	0
1	t	188/209 (89%)	-0.53	2 (1%) 78 70	27, 38, 64, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	u	188/209 (89%)	-0.57	5 (2%) 56 46	25, 36, 60, 98	0
1	v	188/209 (89%)	-0.53	4 (2%) 63 54	31, 40, 64, 102	0
1	w	188/209 (89%)	-0.57	0 100 100	29, 37, 65, 94	0
1	x	189/209 (90%)	-0.54	5 (2%) 57 47	27, 37, 63, 99	0
1	y	189/209 (90%)	-0.51	5 (2%) 57 47	27, 37, 62, 107	0
All	All	11290/12540 (90%)	-0.49	189 (1%) 69 60	24, 40, 67, 120	0

The worst 5 of 189 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	231	LEU	6.4
1	y	231	LEU	5.9
1	e	231	LEU	5.7
1	p	231	LEU	5.5
1	k	231	LEU	5.3

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.