



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2023 – 04:04 PM JST

PDB ID : 5ZJU  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

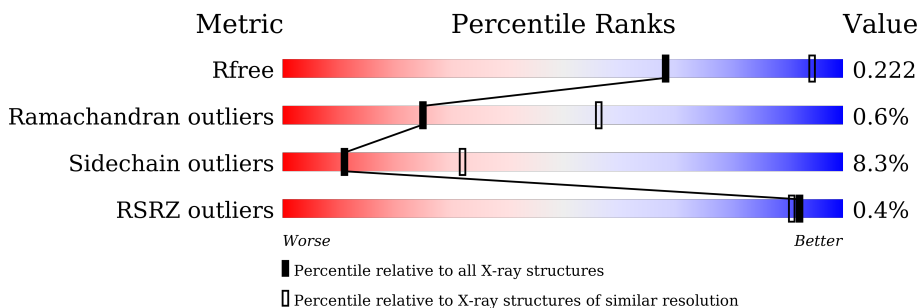
# 1 Overall quality at a glance

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.














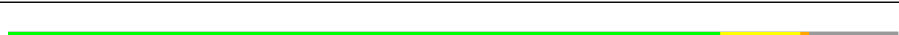

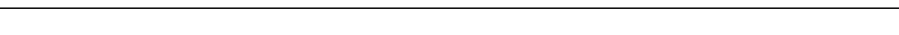
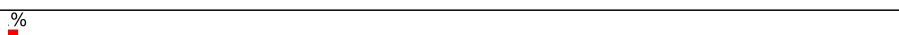
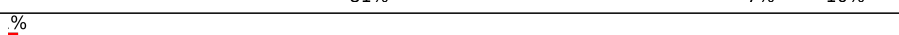

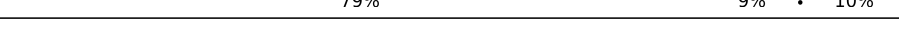







Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	 81% 8% • 10%
1	2	209	 81% 9% 10%
1	3	209	 80% 10% 10%
1	4	209	 81% 9% 10%
1	5	209	 80% 8% • 10%
1	6	209	 82% 8% 10%
1	7	209	 80% 9% • 10%



















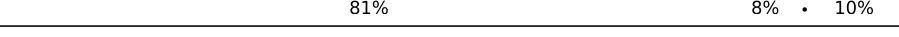






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Mol	Chain	Length	Quality of chain
1	8	209	 80% 8% • 10%
1	9	209	 80% 9% • 10%
1	A	209	 79% 10% • 10%
1	B	209	 81% 8% • 10%
1	C	209	 80% 9% • 10%
1	D	209	 79% 10% • 10%
1	E	209	 80% 8% • 10%
1	F	209	 80% 9% • 10%
1	G	209	 79% 10% • 10%
1	H	209	 81% 8% • 10%
1	I	209	 80% 9% • 10%
1	J	209	 80% 9% • 10%
1	K	209	 82% 6% • 10%
1	L	209	 79% 11% • 10%
1	M	209	 81% 7% • 10%
1	N	209	 79% 10% • 10%
1	O	209	 79% 9% • 10%
1	P	209	 80% 8% • 10%
1	Q	209	 81% 7% • 10%
1	R	209	 78% 11% • 10%
1	S	209	 82% 7% • 10%
1	T	209	 80% 9% • 10%
1	U	209	 82% 8% • 10%
1	V	209	 83% 6% • 10%
1	W	209	 80% 10% • 10%




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Mol	Chain	Length	Quality of chain
1	X	209	 % 80% 9% 10%
1	Y	209	 % 78% 11% 10%
1	Z	209	 % 82% 6% 10%
1	a	209	 % 79% 10% 10%
1	b	209	 % 81% 7% 10%
1	c	209	 % 78% 11% 10%
1	d	209	 % 78% 11% 10%
1	e	209	 % 81% 9% 10%
1	f	209	 % 82% 7% 10%
1	g	209	 % 79% 10% 10%
1	h	209	 % 82% 8% 10%
1	i	209	 % 80% 9% 10%
1	j	209	 % 81% 9% 10%
1	k	209	 % 82% 8% 10%
1	l	209	 % 81% 8% 10%
1	m	209	 % 79% 10% 10%
1	n	209	 % 80% 9% 10%
1	o	209	 % 79% 8% 10%
1	p	209	 % 81% 8% 10%
1	q	209	 % 79% 9% 10%
1	r	209	 % 81% 9% 10%
1	s	209	 % 80% 9% 10%
1	t	209	 % 81% 9% 10%
1	u	209	 % 78% 11% 10%
1	v	209	 % 80% 9% 10%

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Mol	Chain	Length	Quality of chain
1	w	209	 81% 7% • 10%
1	x	209	 80% 9% • 10%
1	y	209	 80% 9% • 10%

## 2 Entry composition [i](#)

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	189	Total	C	N	O	S	0	0	0
			1554	996	270	284	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	189	Total	C	N	O	S	0	0	0
			1554	996	270	284	4			
1	l	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	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	189	Total	C	N	O	S	0	0	0
			1554	996	270	284	4			
1	q	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	r	189	Total	C	N	O	S	0	0	0
			1554	996	270	284	4			
1	s	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	t	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	u	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	v	188	Total	C	N	O	S	0	0	0
			1546	990	269	283	4			
1	w	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
			Total	C	N	O	S			
1	x	189	1554	996	270	284	4	0	0	0
1	y	189	1554	996	270	284	4	0	0	0

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

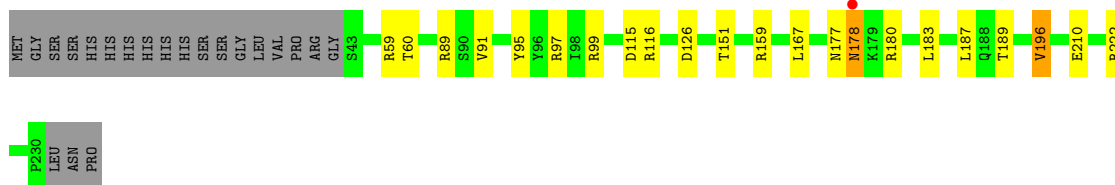


### 3 Residue-property plots [i](#)


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

Chain A: 




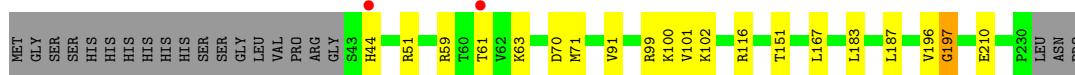
- Molecule 1: Capsid protein

Chain B: 




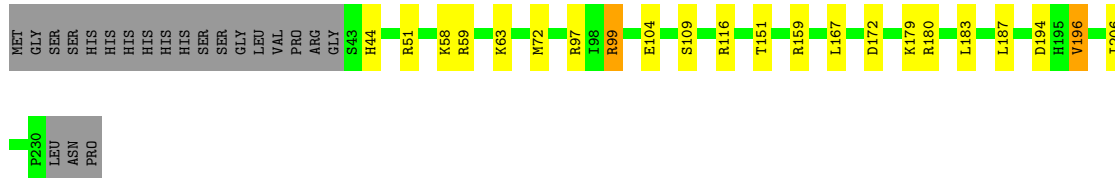
- Molecule 1: Capsid protein

Chain C: 




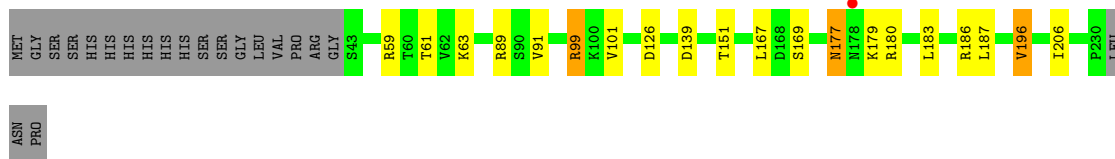
- Molecule 1: Capsid protein

Chain D: 

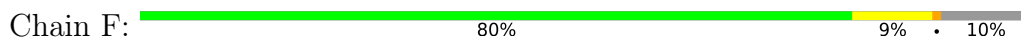


- Molecule 1: Capsid protein

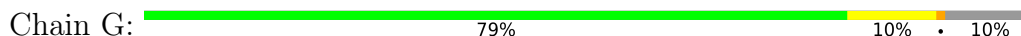
Chain E: 



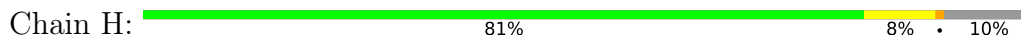
• Molecule 1: Capsid protein



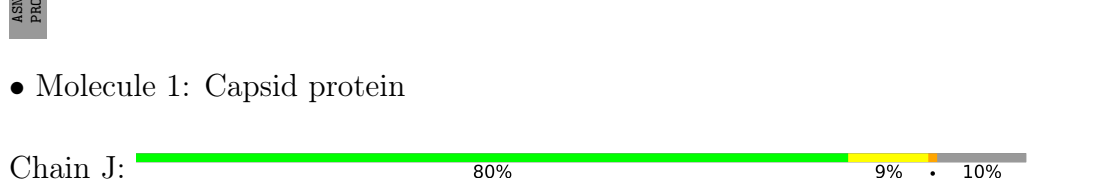
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein

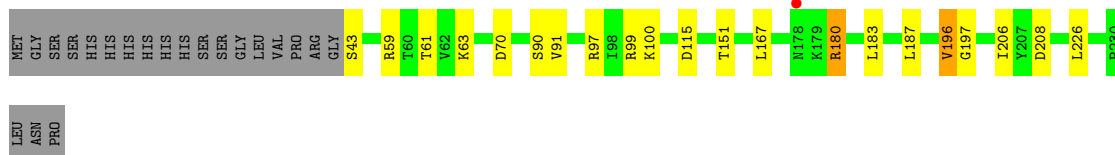


• Molecule 1: Capsid protein

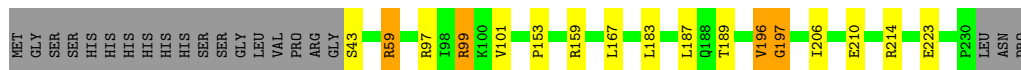
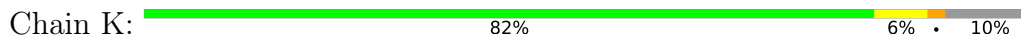


• Molecule 1: Capsid protein

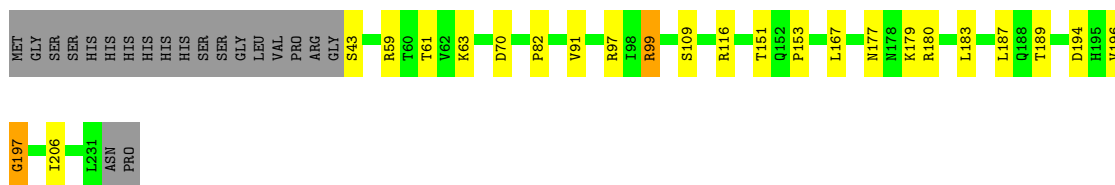
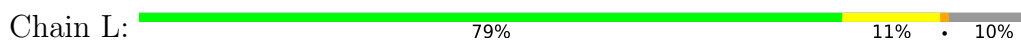




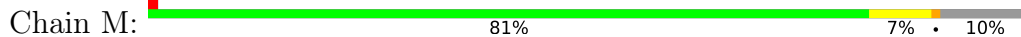
• Molecule 1: Capsid protein



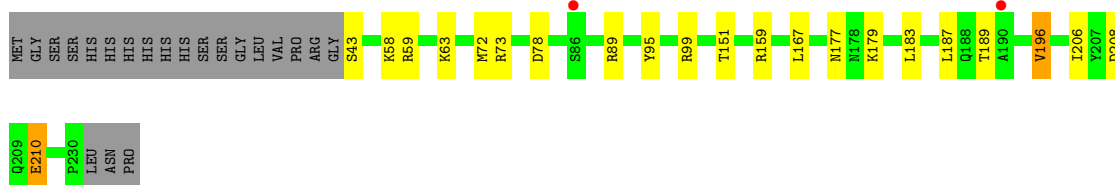
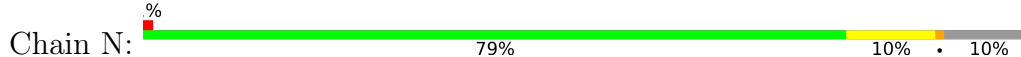
• Molecule 1: Capsid protein



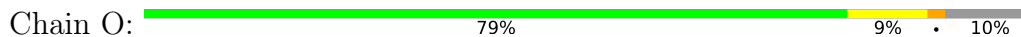
• Molecule 1: Capsid protein

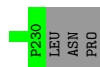


• Molecule 1: Capsid protein

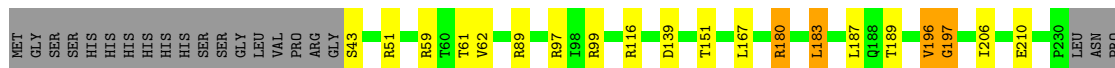
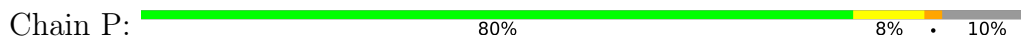


• Molecule 1: Capsid protein

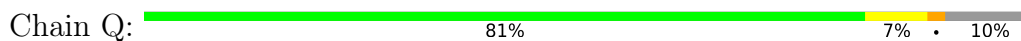




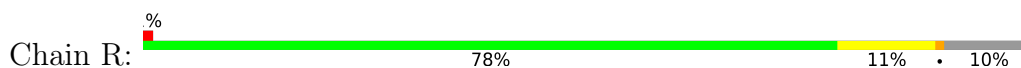
• Molecule 1: Capsid protein



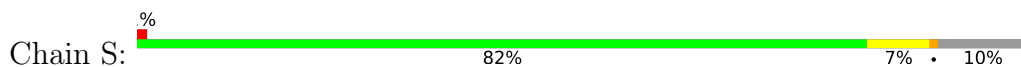
• Molecule 1: Capsid protein



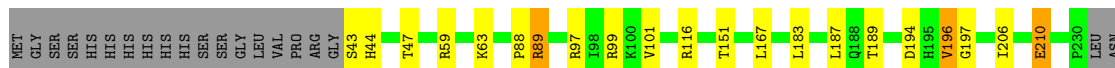
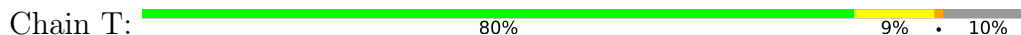
• Molecule 1: Capsid protein



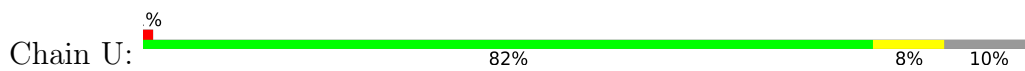
• Molecule 1: Capsid protein



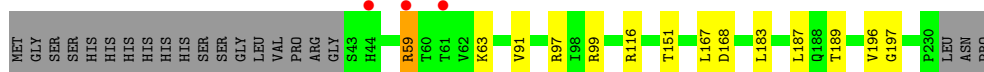
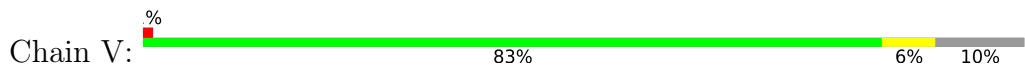
• Molecule 1: Capsid protein



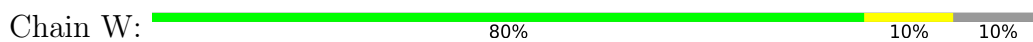
• Molecule 1: Capsid protein



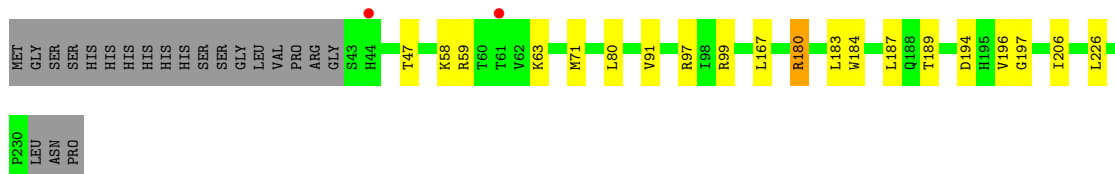
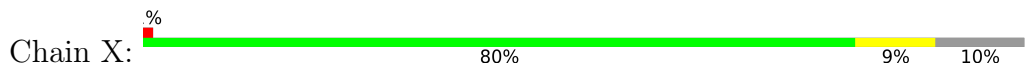
• Molecule 1: Capsid protein



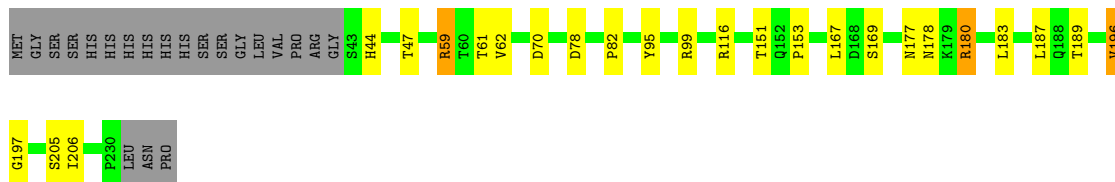
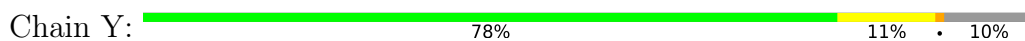
• Molecule 1: Capsid protein



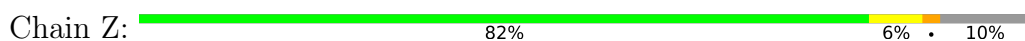
• Molecule 1: Capsid protein




• Molecule 1: Capsid protein



• Molecule 1: Capsid protein




• Molecule 1: Capsid protein

Chain 1:  81% 8% 10%




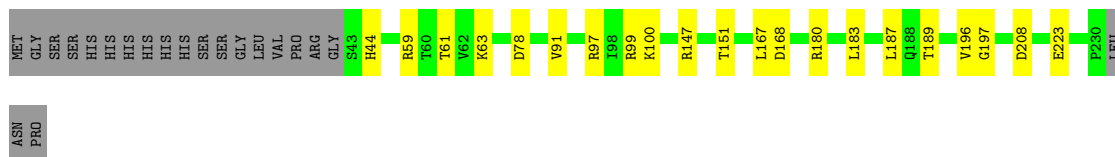
• Molecule 1: Capsid protein

Chain 2:  81% 9% 10%




• Molecule 1: Capsid protein

Chain 3:  80% 10% 10%




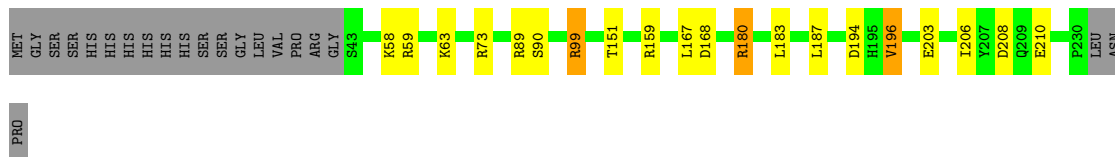
• Molecule 1: Capsid protein

Chain 4:  81% 9% 10%




• Molecule 1: Capsid protein

Chain 5:  80% 8% 10%

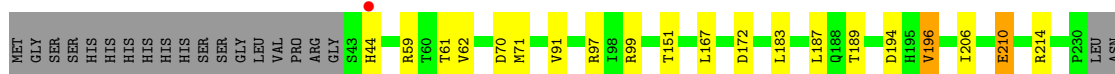
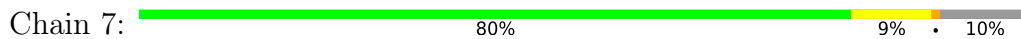


• Molecule 1: Capsid protein

Chain 6:  82% 8% 10%

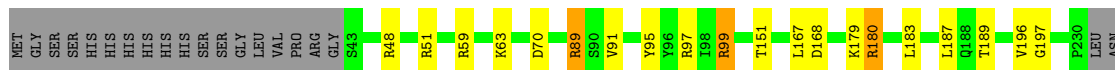
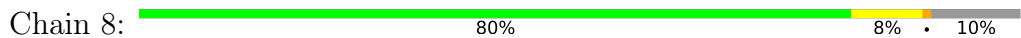


• Molecule 1: Capsid protein



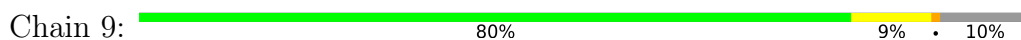
PRO

• Molecule 1: Capsid protein



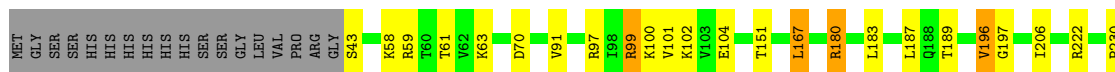
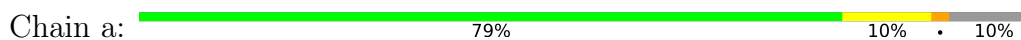
PRO

• Molecule 1: Capsid protein



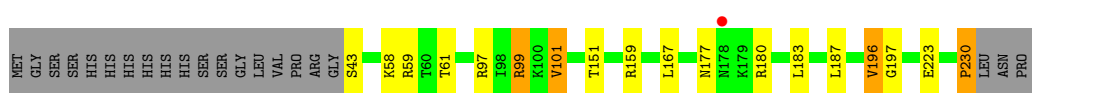
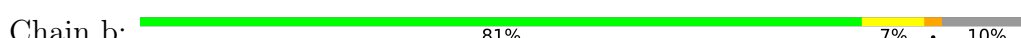
ASN  
PRO

• Molecule 1: Capsid protein

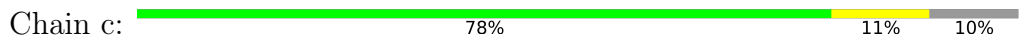


L231  
ASN  
PRO

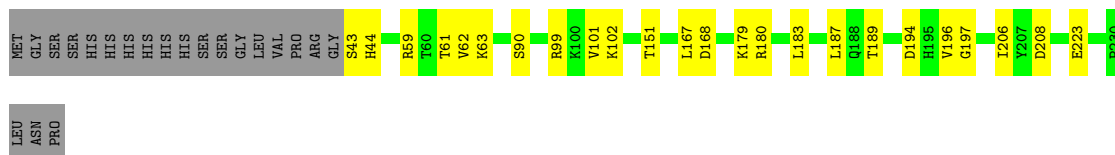
• Molecule 1: Capsid protein



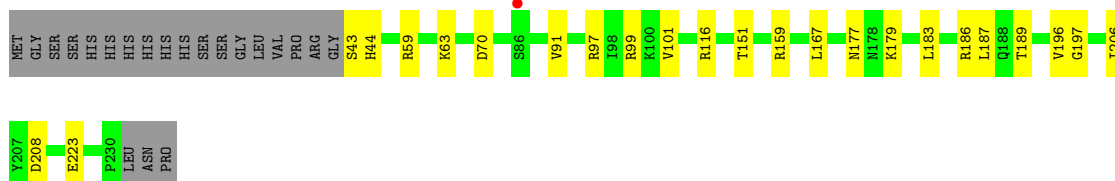
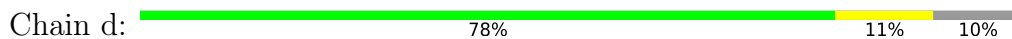
• Molecule 1: Capsid protein



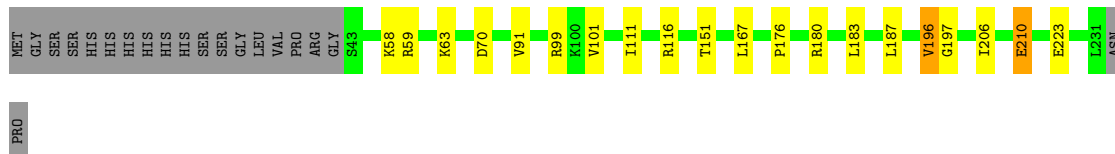
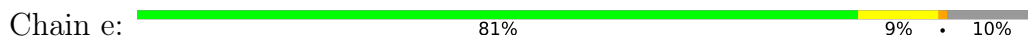




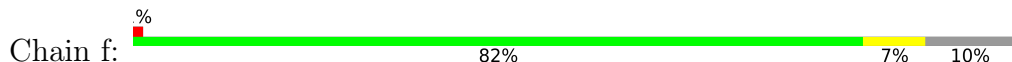
• Molecule 1: Capsid protein



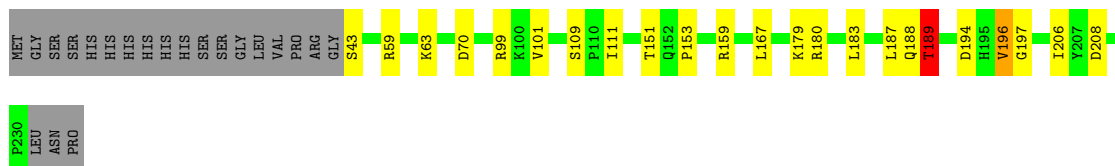
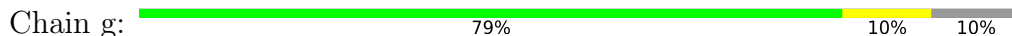
• Molecule 1: Capsid protein



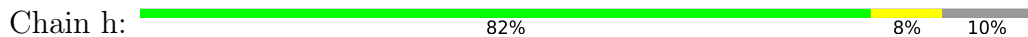
• Molecule 1: Capsid protein



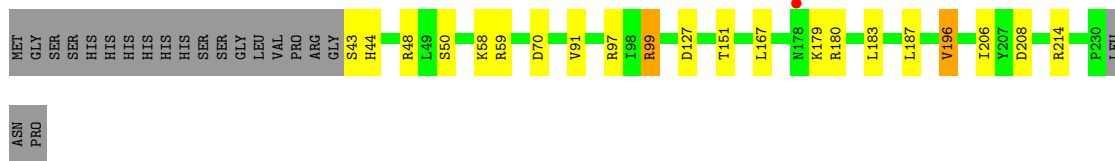
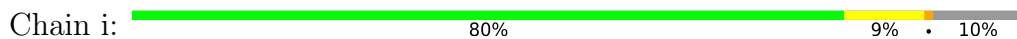
• Molecule 1: Capsid protein



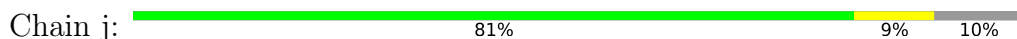
• Molecule 1: Capsid protein



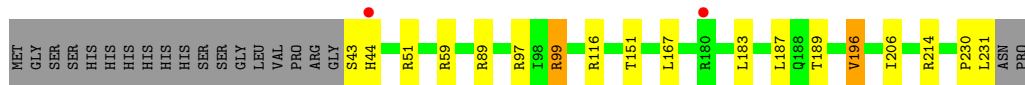
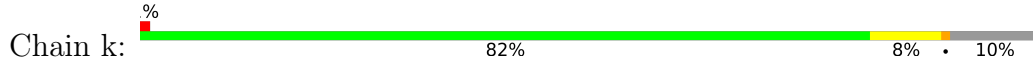
● Molecule 1: Capsid protein



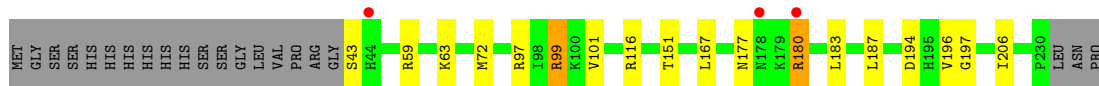
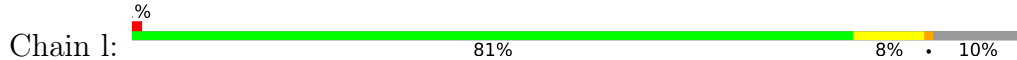
● Molecule 1: Capsid protein



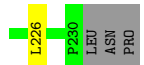
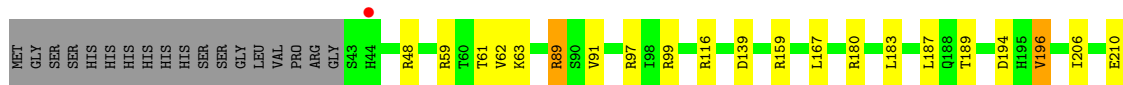
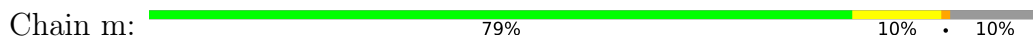
● Molecule 1: Capsid protein



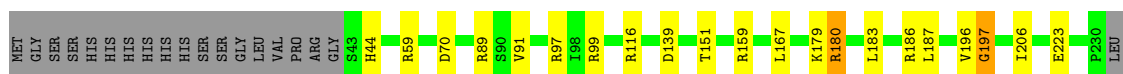
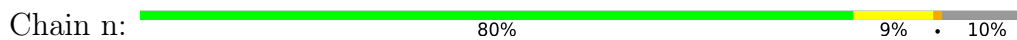
● Molecule 1: Capsid protein



● Molecule 1: Capsid protein



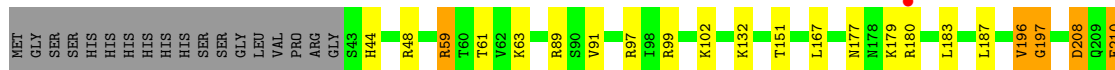
● Molecule 1: Capsid protein



ASN  
PRO

• Molecule 1: Capsid protein

Chain o: 79% 8% 10%



P230  
LEU  
ASN  
PRO

• Molecule 1: Capsid protein

Chain p: 81% 8% 10%



• Molecule 1: Capsid protein

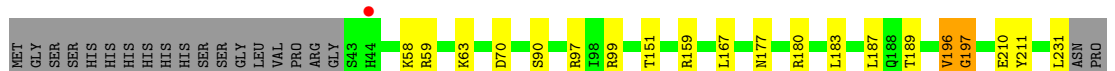
Chain q: 79% 9% 10%



P230  
LEU  
ASN  
PRO

• Molecule 1: Capsid protein

Chain r: 81% 9% 10%



• Molecule 1: Capsid protein

Chain s: 80% 9% 10%



ASN  
PRO

• Molecule 1: Capsid protein

Chain t: 81% 9% 10%



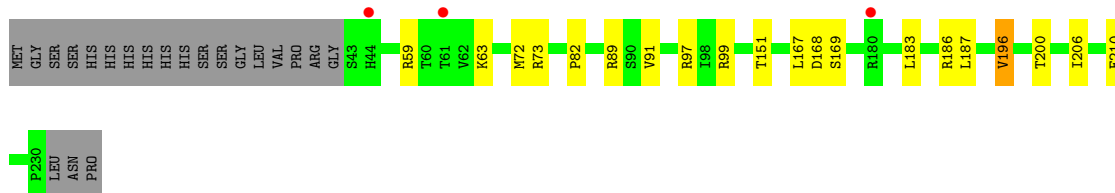
• Molecule 1: Capsid protein

Chain u: 78% 11% 10%



• Molecule 1: Capsid protein

Chain v: 80% 9% 10%



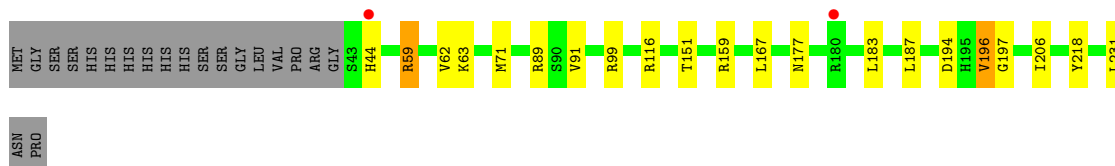
• Molecule 1: Capsid protein

Chain w: 81% 7% 10%



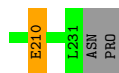
• Molecule 1: Capsid protein

Chain x: 80% 9% 10%



• Molecule 1: Capsid protein

Chain y: 80% 9% 10%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	194.12Å 201.88Å 231.28Å 90.00° 90.72° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.75 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.80) 99.1 (49.75-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 2.81Å)	Xtrriage
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 (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.7	Xtrriage
Anisotropy	0.025	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.000 for -k,-h,-l 0.000 for k,h,-l 0.000 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	97686	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.93	0/1594	1.07	11/2171 (0.5%)
1	2	0.93	0/1602	1.03	5/2182 (0.2%)
1	3	1.01	0/1594	1.08	5/2171 (0.2%)
1	4	0.96	0/1594	1.09	6/2171 (0.3%)
1	5	1.00	0/1594	1.10	11/2171 (0.5%)
1	6	1.03	0/1594	1.10	11/2171 (0.5%)
1	7	1.02	3/1594 (0.2%)	1.11	5/2171 (0.2%)
1	8	0.99	0/1594	1.11	8/2171 (0.4%)
1	9	1.00	0/1602	1.11	8/2182 (0.4%)
1	A	1.04	0/1594	1.15	10/2171 (0.5%)
1	B	1.03	1/1594 (0.1%)	1.07	7/2171 (0.3%)
1	C	1.03	0/1594	1.06	6/2171 (0.3%)
1	D	1.04	1/1594 (0.1%)	1.11	10/2171 (0.5%)
1	E	1.02	1/1594 (0.1%)	1.07	7/2171 (0.3%)
1	F	1.05	1/1594 (0.1%)	1.09	9/2171 (0.4%)
1	G	0.99	0/1594	1.09	8/2171 (0.4%)
1	H	0.93	1/1594 (0.1%)	0.99	2/2171 (0.1%)
1	I	0.94	0/1594	1.07	8/2171 (0.4%)
1	J	0.95	0/1594	1.04	4/2171 (0.2%)
1	K	1.04	3/1594 (0.2%)	1.08	7/2171 (0.3%)
1	L	0.96	0/1602	1.06	5/2182 (0.2%)
1	M	1.01	1/1594 (0.1%)	1.07	6/2171 (0.3%)
1	N	1.01	2/1594 (0.1%)	1.08	6/2171 (0.3%)
1	O	1.03	0/1594	1.11	10/2171 (0.5%)
1	P	1.07	2/1594 (0.1%)	1.17	12/2171 (0.6%)
1	Q	1.00	2/1594 (0.1%)	1.05	8/2171 (0.4%)
1	R	1.03	3/1594 (0.2%)	1.12	10/2171 (0.5%)
1	S	1.01	2/1594 (0.1%)	1.04	4/2171 (0.2%)
1	T	0.97	2/1594 (0.1%)	1.13	9/2171 (0.4%)
1	U	0.92	0/1594	1.00	1/2171 (0.0%)
1	V	0.91	0/1594	1.04	5/2171 (0.2%)
1	W	0.95	0/1594	1.02	2/2171 (0.1%)
1	X	0.91	1/1594 (0.1%)	1.00	3/2171 (0.1%)
1	Y	0.94	0/1594	1.02	5/2171 (0.2%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	Z	0.93	0/1594	1.02	8/2171 (0.4%)
1	a	0.95	0/1602	1.11	11/2182 (0.5%)
1	b	0.95	0/1594	1.07	6/2171 (0.3%)
1	c	0.96	0/1594	1.05	5/2171 (0.2%)
1	d	0.94	0/1594	1.06	7/2171 (0.3%)
1	e	0.99	2/1602 (0.1%)	1.04	2/2182 (0.1%)
1	f	0.91	0/1594	1.02	5/2171 (0.2%)
1	g	0.96	2/1594 (0.1%)	1.04	6/2171 (0.3%)
1	h	0.98	0/1594	1.08	6/2171 (0.3%)
1	i	1.02	1/1594 (0.1%)	1.08	8/2171 (0.4%)
1	j	0.95	2/1594 (0.1%)	1.02	0/2171
1	k	0.99	0/1602	1.08	8/2182 (0.4%)
1	l	0.98	1/1594 (0.1%)	1.05	9/2171 (0.4%)
1	m	1.02	0/1594	1.06	8/2171 (0.4%)
1	n	1.01	1/1594 (0.1%)	1.10	8/2171 (0.4%)
1	o	1.02	3/1594 (0.2%)	1.09	5/2171 (0.2%)
1	p	1.03	2/1602 (0.1%)	1.07	4/2182 (0.2%)
1	q	1.03	0/1594	1.11	11/2171 (0.5%)
1	r	0.97	2/1602 (0.1%)	1.05	3/2182 (0.1%)
1	s	1.00	0/1594	1.05	6/2171 (0.3%)
1	t	1.02	0/1594	1.07	7/2171 (0.3%)
1	u	1.01	2/1594 (0.1%)	1.09	7/2171 (0.3%)
1	v	0.96	0/1594	1.07	8/2171 (0.4%)
1	w	1.02	1/1594 (0.1%)	1.08	3/2171 (0.1%)
1	x	1.00	1/1602 (0.1%)	1.15	10/2182 (0.5%)
1	y	1.01	1/1602 (0.1%)	1.13	12/2182 (0.5%)
All	All	0.99	47/95720 (0.0%)	1.07	407/130370 (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 47 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	w	210	GLU	CG-CD	7.82	1.63	1.51
1	P	197	GLY	N-CA	-7.66	1.34	1.46
1	o	210	GLU	CG-CD	7.29	1.62	1.51
1	r	197	GLY	N-CA	-6.67	1.36	1.46
1	R	210	GLU	CG-CD	6.65	1.61	1.51

The worst 5 of 407 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	89	ARG	NE-CZ-NH2	12.61	126.61	120.30
1	3	97	ARG	NE-CZ-NH1	-10.43	115.09	120.30
1	3	97	ARG	NE-CZ-NH2	10.07	125.33	120.30
1	9	97	ARG	NE-CZ-NH2	9.90	125.25	120.30
1	P	89	ARG	NE-CZ-NH2	9.64	125.12	120.30

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 [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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%)	29	61
1	2	187/209 (90%)	174 (93%)	12 (6%)	1 (0%)	29	61
1	3	186/209 (89%)	175 (94%)	9 (5%)	2 (1%)	14	41
1	4	186/209 (89%)	172 (92%)	13 (7%)	1 (0%)	29	61
1	5	186/209 (89%)	179 (96%)	7 (4%)	0	100	100
1	6	186/209 (89%)	178 (96%)	7 (4%)	1 (0%)	29	61
1	7	186/209 (89%)	178 (96%)	6 (3%)	2 (1%)	14	41
1	8	186/209 (89%)	172 (92%)	13 (7%)	1 (0%)	29	61
1	9	187/209 (90%)	177 (95%)	8 (4%)	2 (1%)	14	41
1	A	186/209 (89%)	178 (96%)	7 (4%)	1 (0%)	29	61
1	B	186/209 (89%)	176 (95%)	9 (5%)	1 (0%)	29	61
1	C	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	29	61
1	D	186/209 (89%)	176 (95%)	10 (5%)	0	100	100
1	E	186/209 (89%)	176 (95%)	10 (5%)	0	100	100
1	F	186/209 (89%)	173 (93%)	13 (7%)	0	100	100
1	G	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	29	61
1	H	186/209 (89%)	173 (93%)	12 (6%)	1 (0%)	29	61
1	I	186/209 (89%)	176 (95%)	10 (5%)	0	100	100
1	J	186/209 (89%)	173 (93%)	12 (6%)	1 (0%)	29	61
1	K	186/209 (89%)	172 (92%)	12 (6%)	2 (1%)	14	41
1	L	187/209 (90%)	179 (96%)	7 (4%)	1 (0%)	29	61
1	M	186/209 (89%)	176 (95%)	8 (4%)	2 (1%)	14	41
1	N	186/209 (89%)	175 (94%)	11 (6%)	0	100	100
1	O	186/209 (89%)	173 (93%)	12 (6%)	1 (0%)	29	61
1	P	186/209 (89%)	174 (94%)	10 (5%)	2 (1%)	14	41
1	Q	186/209 (89%)	177 (95%)	8 (4%)	1 (0%)	29	61
1	R	186/209 (89%)	173 (93%)	11 (6%)	2 (1%)	14	41
1	S	186/209 (89%)	179 (96%)	6 (3%)	1 (0%)	29	61
1	T	186/209 (89%)	177 (95%)	8 (4%)	1 (0%)	29	61
1	U	186/209 (89%)	173 (93%)	10 (5%)	3 (2%)	9	31
1	V	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	29	61
1	W	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	186/209 (89%)	170 (91%)	15 (8%)	1 (0%)	29	61
1	Y	186/209 (89%)	171 (92%)	12 (6%)	3 (2%)	9	31
1	Z	186/209 (89%)	173 (93%)	13 (7%)	0	100	100
1	a	187/209 (90%)	176 (94%)	9 (5%)	2 (1%)	14	41
1	b	186/209 (89%)	176 (95%)	8 (4%)	2 (1%)	14	41
1	c	186/209 (89%)	175 (94%)	8 (4%)	3 (2%)	9	31
1	d	186/209 (89%)	172 (92%)	12 (6%)	2 (1%)	14	41
1	e	187/209 (90%)	178 (95%)	7 (4%)	2 (1%)	14	41
1	f	186/209 (89%)	175 (94%)	11 (6%)	0	100	100
1	g	186/209 (89%)	174 (94%)	10 (5%)	2 (1%)	14	41
1	h	186/209 (89%)	169 (91%)	16 (9%)	1 (0%)	29	61
1	i	186/209 (89%)	175 (94%)	11 (6%)	0	100	100
1	j	186/209 (89%)	172 (92%)	12 (6%)	2 (1%)	14	41
1	k	187/209 (90%)	172 (92%)	13 (7%)	2 (1%)	14	41
1	l	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	29	61
1	m	186/209 (89%)	177 (95%)	8 (4%)	1 (0%)	29	61
1	n	186/209 (89%)	177 (95%)	7 (4%)	2 (1%)	14	41
1	o	186/209 (89%)	174 (94%)	11 (6%)	1 (0%)	29	61
1	p	187/209 (90%)	179 (96%)	8 (4%)	0	100	100
1	q	186/209 (89%)	176 (95%)	9 (5%)	1 (0%)	29	61
1	r	187/209 (90%)	179 (96%)	7 (4%)	1 (0%)	29	61
1	s	186/209 (89%)	177 (95%)	8 (4%)	1 (0%)	29	61
1	t	186/209 (89%)	177 (95%)	8 (4%)	1 (0%)	29	61
1	u	186/209 (89%)	173 (93%)	11 (6%)	2 (1%)	14	41
1	v	186/209 (89%)	177 (95%)	9 (5%)	0	100	100
1	w	186/209 (89%)	177 (95%)	8 (4%)	1 (0%)	29	61
1	x	187/209 (90%)	177 (95%)	8 (4%)	2 (1%)	14	41
1	y	187/209 (90%)	173 (92%)	13 (7%)	1 (0%)	29	61
All	All	11170/12540 (89%)	10499 (94%)	599 (5%)	72 (1%)	25	56

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 [i](#)

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%)	161 (94%)	11 (6%)	17	45
1	2	173/190 (91%)	160 (92%)	13 (8%)	13	37
1	3	172/190 (90%)	157 (91%)	15 (9%)	10	30
1	4	172/190 (90%)	159 (92%)	13 (8%)	13	36
1	5	172/190 (90%)	159 (92%)	13 (8%)	13	36
1	6	172/190 (90%)	163 (95%)	9 (5%)	23	55
1	7	172/190 (90%)	158 (92%)	14 (8%)	11	33
1	8	172/190 (90%)	157 (91%)	15 (9%)	10	30
1	9	173/190 (91%)	160 (92%)	13 (8%)	13	37
1	A	172/190 (90%)	160 (93%)	12 (7%)	15	40
1	B	172/190 (90%)	158 (92%)	14 (8%)	11	33
1	C	172/190 (90%)	157 (91%)	15 (9%)	10	30
1	D	172/190 (90%)	158 (92%)	14 (8%)	11	33
1	E	172/190 (90%)	156 (91%)	16 (9%)	9	26
1	F	172/190 (90%)	159 (92%)	13 (8%)	13	36
1	G	172/190 (90%)	155 (90%)	17 (10%)	8	23
1	H	172/190 (90%)	157 (91%)	15 (9%)	10	30
1	I	172/190 (90%)	157 (91%)	15 (9%)	10	30
1	J	172/190 (90%)	155 (90%)	17 (10%)	8	23
1	K	172/190 (90%)	162 (94%)	10 (6%)	20	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	173/190 (91%)	153 (88%)	20 (12%)	5	17
1	M	172/190 (90%)	159 (92%)	13 (8%)	13	36
1	N	172/190 (90%)	157 (91%)	15 (9%)	10	30
1	O	172/190 (90%)	157 (91%)	15 (9%)	10	30
1	P	172/190 (90%)	160 (93%)	12 (7%)	15	40
1	Q	172/190 (90%)	159 (92%)	13 (8%)	13	36
1	R	172/190 (90%)	156 (91%)	16 (9%)	9	26
1	S	172/190 (90%)	161 (94%)	11 (6%)	17	45
1	T	172/190 (90%)	156 (91%)	16 (9%)	9	26
1	U	172/190 (90%)	159 (92%)	13 (8%)	13	36
1	V	172/190 (90%)	162 (94%)	10 (6%)	20	50
1	W	172/190 (90%)	155 (90%)	17 (10%)	8	23
1	X	172/190 (90%)	156 (91%)	16 (9%)	9	26
1	Y	172/190 (90%)	152 (88%)	20 (12%)	5	17
1	Z	172/190 (90%)	157 (91%)	15 (9%)	10	30
1	a	173/190 (91%)	156 (90%)	17 (10%)	8	24
1	b	172/190 (90%)	158 (92%)	14 (8%)	11	33
1	c	172/190 (90%)	155 (90%)	17 (10%)	8	23
1	d	172/190 (90%)	156 (91%)	16 (9%)	9	26
1	e	173/190 (91%)	157 (91%)	16 (9%)	9	27
1	f	172/190 (90%)	159 (92%)	13 (8%)	13	36
1	g	172/190 (90%)	157 (91%)	15 (9%)	10	30
1	h	172/190 (90%)	161 (94%)	11 (6%)	17	45
1	i	172/190 (90%)	156 (91%)	16 (9%)	9	26
1	j	172/190 (90%)	155 (90%)	17 (10%)	8	23
1	k	173/190 (91%)	161 (93%)	12 (7%)	15	41
1	l	172/190 (90%)	160 (93%)	12 (7%)	15	40
1	m	172/190 (90%)	157 (91%)	15 (9%)	10	30
1	n	172/190 (90%)	159 (92%)	13 (8%)	13	36
1	o	172/190 (90%)	155 (90%)	17 (10%)	8	23
1	p	173/190 (91%)	160 (92%)	13 (8%)	13	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	q	172/190 (90%)	159 (92%)	13 (8%)	13	36
1	r	173/190 (91%)	159 (92%)	14 (8%)	11	33
1	s	172/190 (90%)	158 (92%)	14 (8%)	11	33
1	t	172/190 (90%)	160 (93%)	12 (7%)	15	40
1	u	172/190 (90%)	157 (91%)	15 (9%)	10	30
1	v	172/190 (90%)	159 (92%)	13 (8%)	13	36
1	w	172/190 (90%)	157 (91%)	15 (9%)	10	30
1	x	173/190 (91%)	160 (92%)	13 (8%)	13	37
1	y	173/190 (91%)	159 (92%)	14 (8%)	11	33
All	All	10330/11400 (91%)	9477 (92%)	853 (8%)	11	32

5 of 853 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	7	187	LEU
1	e	196	VAL
1	v	63	LYS
1	8	167	LEU
1	7	183	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	o	212	ASN
1	r	177	ASN
1	v	148	HIS
1	W	177	ASN
1	W	44	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	1	188/209 (89%)	-0.44	0 100 100	32, 44, 71, 102	0
1	2	189/209 (90%)	-0.41	1 (0%) 91 88	32, 43, 69, 111	0
1	3	188/209 (89%)	-0.56	0 100 100	26, 36, 60, 98	0
1	4	188/209 (89%)	-0.59	0 100 100	27, 38, 65, 96	0
1	5	188/209 (89%)	-0.59	0 100 100	29, 39, 66, 110	0
1	6	188/209 (89%)	-0.72	1 (0%) 91 88	26, 37, 59, 96	0
1	7	188/209 (89%)	-0.65	1 (0%) 91 88	27, 35, 61, 96	0
1	8	188/209 (89%)	-0.54	0 100 100	24, 37, 63, 105	0
1	9	189/209 (90%)	-0.62	0 100 100	29, 38, 63, 102	0
1	A	188/209 (89%)	-0.75	1 (0%) 91 88	26, 35, 57, 99	0
1	B	188/209 (89%)	-0.57	1 (0%) 91 88	32, 40, 63, 111	0
1	C	188/209 (89%)	-0.63	2 (1%) 80 75	27, 36, 64, 100	0
1	D	188/209 (89%)	-0.61	0 100 100	26, 35, 59, 95	0
1	E	188/209 (89%)	-0.70	1 (0%) 91 88	25, 34, 58, 99	0
1	F	188/209 (89%)	-0.54	1 (0%) 91 88	25, 36, 61, 90	0
1	G	188/209 (89%)	-0.61	1 (0%) 91 88	28, 39, 69, 100	0
1	H	188/209 (89%)	-0.59	1 (0%) 91 88	34, 45, 70, 106	0
1	I	188/209 (89%)	-0.44	0 100 100	33, 44, 70, 106	0
1	J	188/209 (89%)	-0.34	1 (0%) 91 88	32, 45, 73, 104	0
1	K	188/209 (89%)	-0.64	0 100 100	24, 38, 64, 96	0
1	L	189/209 (90%)	-0.58	0 100 100	33, 43, 69, 102	0
1	M	188/209 (89%)	-0.61	2 (1%) 80 75	30, 40, 66, 105	0
1	N	188/209 (89%)	-0.60	2 (1%) 80 75	27, 37, 66, 105	0
1	O	188/209 (89%)	-0.68	0 100 100	25, 35, 61, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	P	188/209 (89%)	-0.66	0 100 100	27, 35, 60, 95	0
1	Q	188/209 (89%)	-0.59	1 (0%) 91 88	28, 38, 62, 99	0
1	R	188/209 (89%)	-0.64	2 (1%) 80 75	27, 35, 63, 94	0
1	S	188/209 (89%)	-0.42	3 (1%) 72 66	29, 41, 69, 99	0
1	T	188/209 (89%)	-0.55	0 100 100	30, 41, 69, 108	0
1	U	188/209 (89%)	-0.47	2 (1%) 80 75	29, 45, 69, 100	0
1	V	188/209 (89%)	-0.28	3 (1%) 72 66	35, 46, 73, 108	0
1	W	188/209 (89%)	-0.60	1 (0%) 91 88	35, 44, 73, 120	0
1	X	188/209 (89%)	-0.45	2 (1%) 80 75	35, 46, 71, 106	0
1	Y	188/209 (89%)	-0.59	0 100 100	33, 46, 74, 106	0
1	Z	188/209 (89%)	-0.62	1 (0%) 91 88	32, 43, 73, 97	0
1	a	189/209 (90%)	-0.55	0 100 100	30, 41, 66, 107	0
1	b	188/209 (89%)	-0.45	1 (0%) 91 88	32, 46, 73, 110	0
1	c	188/209 (89%)	-0.39	0 100 100	33, 45, 68, 112	0
1	d	188/209 (89%)	-0.53	1 (0%) 91 88	35, 44, 69, 100	0
1	e	189/209 (90%)	-0.58	0 100 100	29, 39, 64, 109	0
1	f	188/209 (89%)	-0.51	2 (1%) 80 75	32, 45, 72, 101	0
1	g	188/209 (89%)	-0.47	0 100 100	32, 45, 71, 96	0
1	h	188/209 (89%)	-0.63	0 100 100	32, 42, 65, 111	0
1	i	188/209 (89%)	-0.62	1 (0%) 91 88	30, 41, 64, 105	0
1	j	188/209 (89%)	-0.59	0 100 100	35, 45, 70, 104	0
1	k	189/209 (90%)	-0.60	2 (1%) 80 75	29, 40, 72, 107	0
1	l	188/209 (89%)	-0.47	3 (1%) 72 66	28, 40, 68, 101	0
1	m	188/209 (89%)	-0.58	1 (0%) 91 88	27, 36, 64, 105	0
1	n	188/209 (89%)	-0.69	0 100 100	26, 36, 65, 95	0
1	o	188/209 (89%)	-0.72	1 (0%) 91 88	27, 37, 64, 111	0
1	p	189/209 (90%)	-0.57	0 100 100	26, 38, 62, 106	0
1	q	188/209 (89%)	-0.57	0 100 100	28, 35, 64, 99	0
1	r	189/209 (90%)	-0.58	1 (0%) 91 88	30, 41, 64, 94	0
1	s	188/209 (89%)	-0.61	0 100 100	28, 36, 63, 102	0
1	t	188/209 (89%)	-0.56	0 100 100	27, 38, 64, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	u	188/209 (89%)	-0.68	0 100 100	25, 36, 60, 98	0
1	v	188/209 (89%)	-0.56	3 (1%) 72 66	31, 40, 64, 102	0
1	w	188/209 (89%)	-0.66	0 100 100	29, 37, 65, 94	0
1	x	189/209 (90%)	-0.71	2 (1%) 80 75	27, 37, 63, 99	0
1	y	189/209 (90%)	-0.58	0 100 100	27, 37, 62, 107	0
All	All	11290/12540 (90%)	-0.57	49 (0%) 92 91	24, 40, 67, 120	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	61	THR	3.8
1	U	180	ARG	3.4
1	d	86	SER	3.3
1	l	180	ARG	3.1
1	V	61	THR	3.0

## 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 monosaccharides 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.