



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 01:18 PM BST

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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	:	2.13
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)	:	2.13

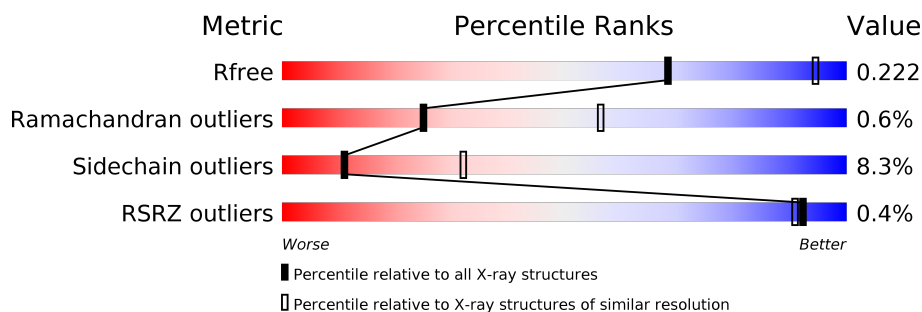
1 Overall quality at a glance ⓘ

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.

















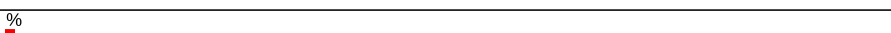




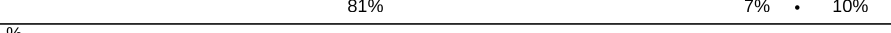





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	209	<div> <div>81%</div> <div>8%</div> <div>10%</div> </div>
1	2	209	<div> <div>81%</div> <div>9%</div> <div>10%</div> </div>
1	3	209	<div> <div>80%</div> <div>10%</div> <div>10%</div> </div>
1	4	209	<div> <div>81%</div> <div>9%</div> <div>10%</div> </div>
1	5	209	<div> <div>80%</div> <div>8%</div> <div>10%</div> </div>
1	6	209	<div> <div>82%</div> <div>8%</div> <div>10%</div> </div>
1	7	209	<div> <div>80%</div> <div>9%</div> <div>10%</div> </div>



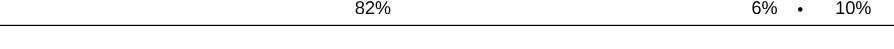
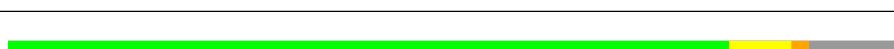



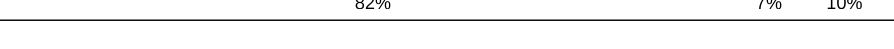


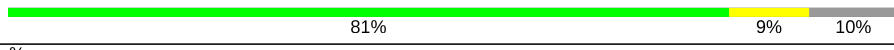





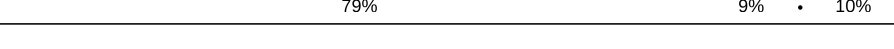
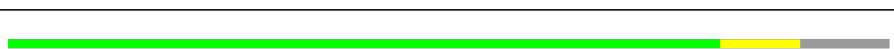






Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 97686 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Capsid protein.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

There are 1200 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...


Continued from previous page...

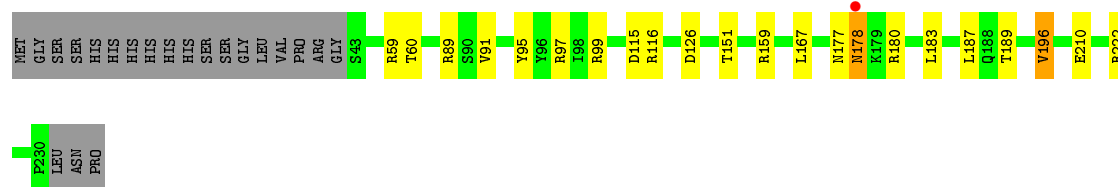
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	k	78	Total 78	O 78	0	0
2	l	81	Total 81	O 81	0	0
2	m	78	Total 78	O 78	0	0
2	n	94	Total 94	O 94	0	0
2	o	79	Total 79	O 79	0	0
2	p	78	Total 78	O 78	0	0
2	q	102	Total 102	O 102	0	0
2	r	74	Total 74	O 74	0	0
2	s	113	Total 113	O 113	0	0
2	t	76	Total 76	O 76	0	0
2	u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

3 Residue-property plots


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: 



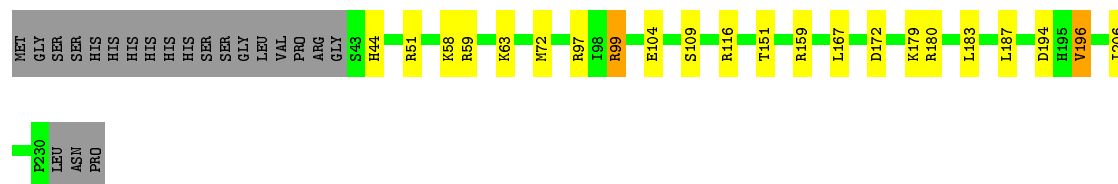
- Molecule 1: Capsid protein

Chain C: 




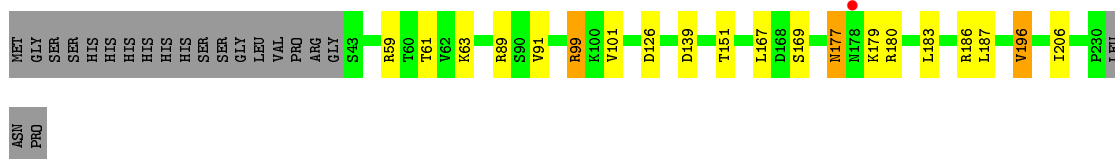
- Molecule 1: Capsid protein

Chain D: 



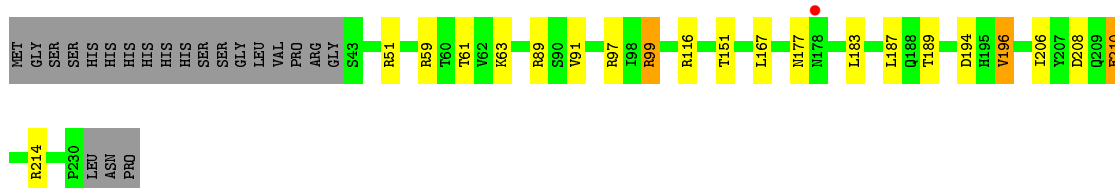
- Molecule 1: Capsid protein

Chain E: 



- Molecule 1: Capsid protein

Chain F: 80% 9% 10%



- Molecule 1: Capsid protein

Chain G: 79% 10% 10%



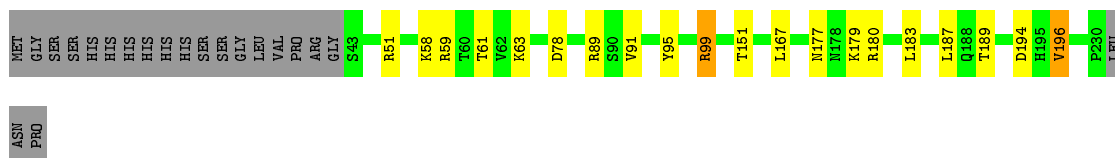
- Molecule 1: Capsid protein

Chain H: 81% 8% 10%



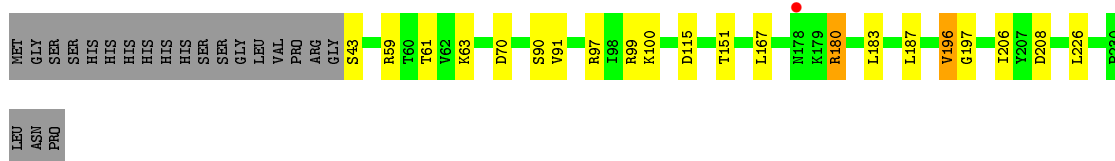
- Molecule 1: Capsid protein

Chain I: 80% 9% 10%



- Molecule 1: Capsid protein

Chain J: 80% 9% 10%



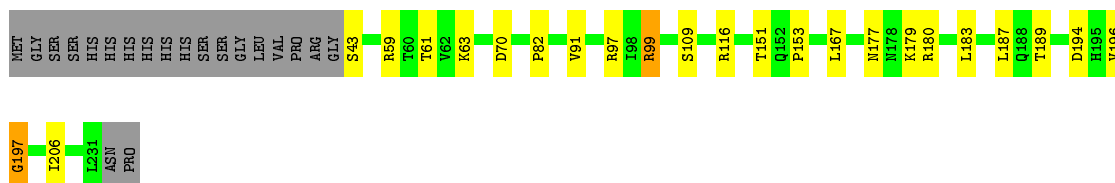
- Molecule 1: Capsid protein

Chain K: 82% 6% 10%



- Molecule 1: Capsid protein

Chain L: 79% 11% 10%



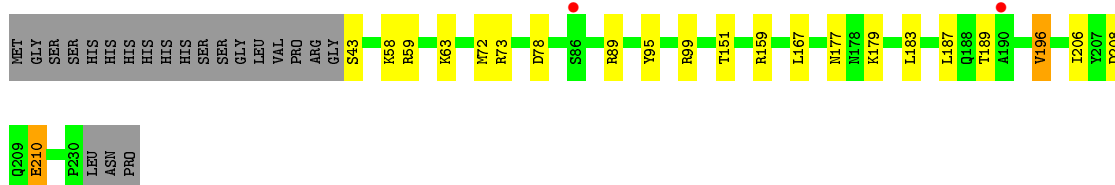
- Molecule 1: Capsid protein

Chain M: 81% 7% 10%



- Molecule 1: Capsid protein

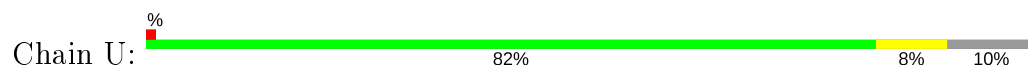
Chain N: 79% 10% 10%



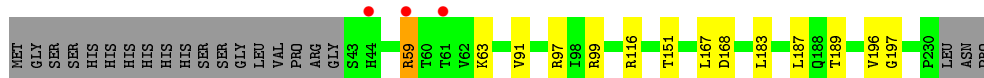
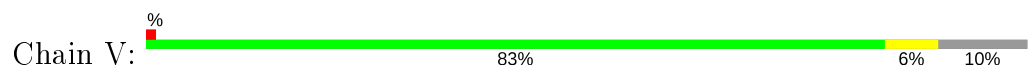
- Molecule 1: Capsid protein

Chain O: 79% 9% 10%

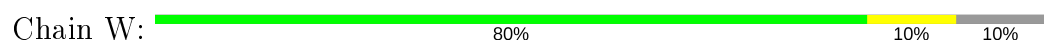




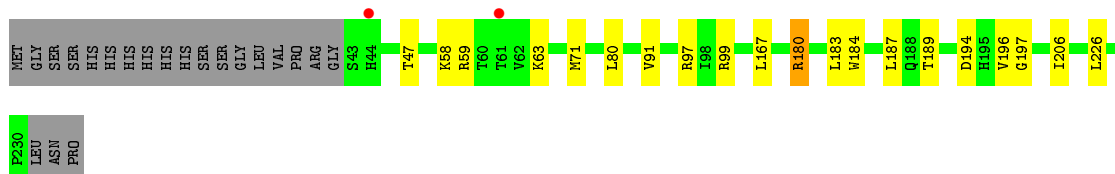
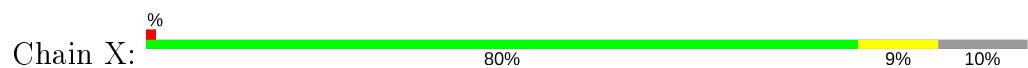
- Molecule 1: Capsid protein



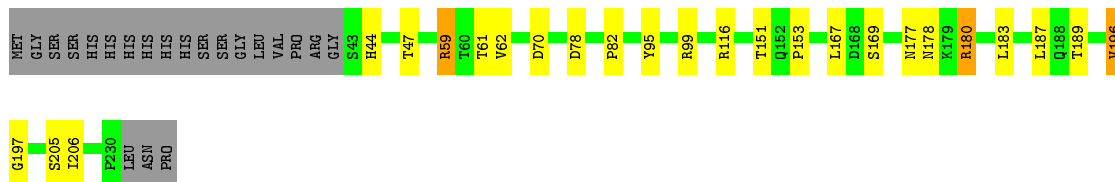
- Molecule 1: Capsid protein



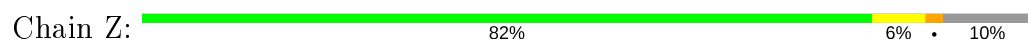
- Molecule 1: Capsid protein




- Molecule 1: Capsid protein

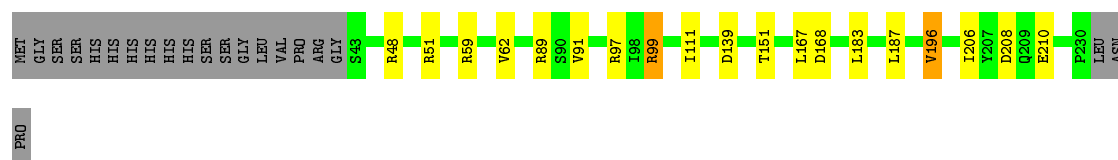


- Molecule 1: Capsid protein




- Molecule 1: Capsid protein

Chain 1:  81% 8% 10%



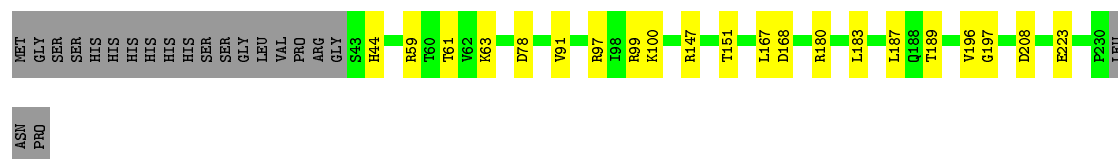
• Molecule 1: Capsid protein

Chain 2:  81% 9% 10%




• Molecule 1: Capsid protein

Chain 3:  80% 10% 10%




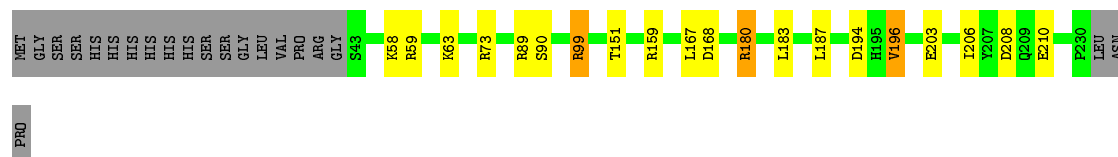
• Molecule 1: Capsid protein

Chain 4:  81% 9% 10%




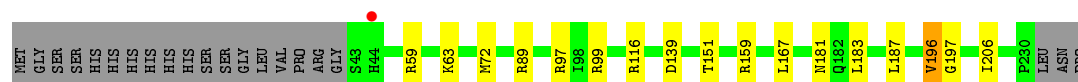
• Molecule 1: Capsid protein

Chain 5:  80% 8% 10%




• Molecule 1: Capsid protein

Chain 6:  82% 8% 10%




• Molecule 1: Capsid protein

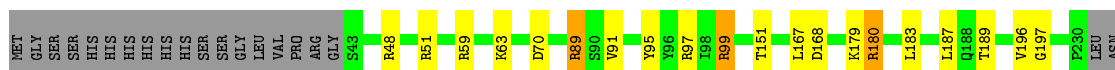
Chain 7:  80% 9% • 10%



PRO

- Molecule 1: Capsid protein

Chain 8:  80% 8% • 10%



PRO


- Molecule 1: Capsid protein

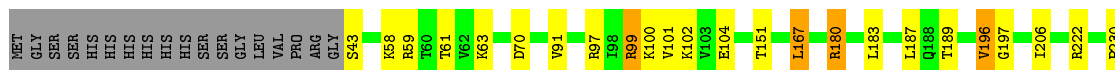
Chain 9:  80% 9% • 10%



ASN
PRO


- Molecule 1: Capsid protein

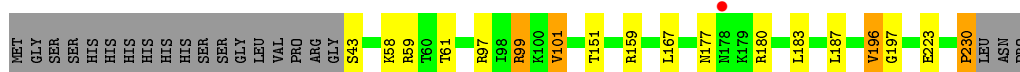
Chain a:  79% 10% • 10%



L231
ASN
PRO

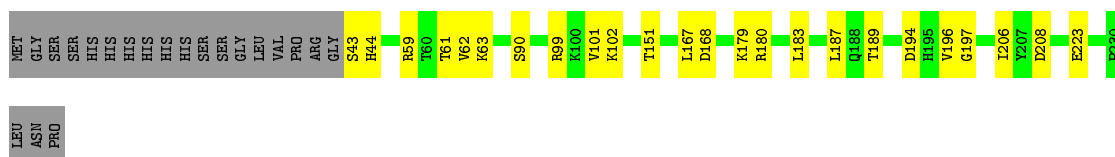
- Molecule 1: Capsid protein

Chain b:  81% 7% • 10%



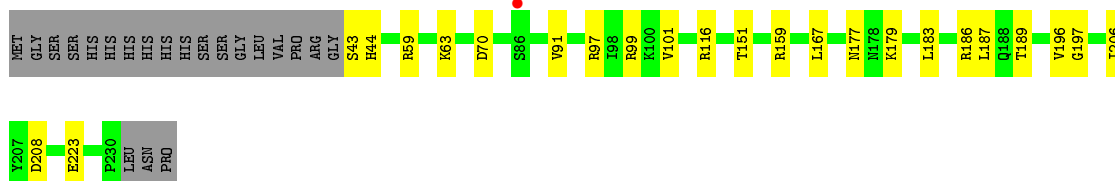
- Molecule 1: Capsid protein

Chain c:  78% 11% 10%



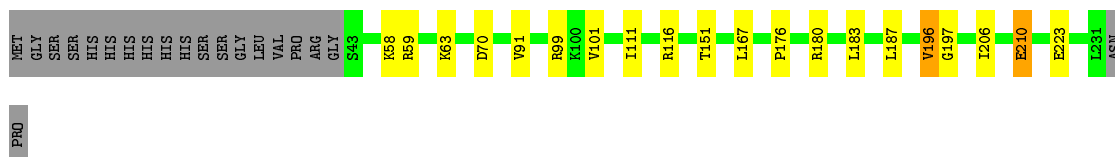
- Molecule 1: Capsid protein

Chain d: 78% 11% 10%



- Molecule 1: Capsid protein

Chain e: 81% 9% 10%



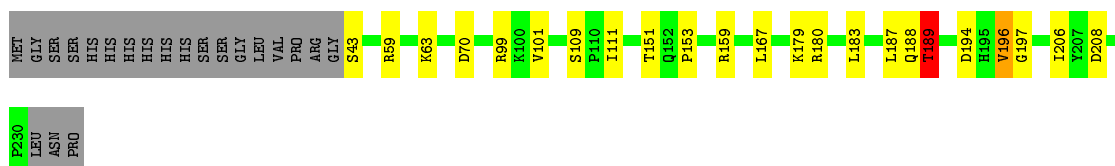
- Molecule 1: Capsid protein

Chain f: 82% 7% 10%



- Molecule 1: Capsid protein

Chain g: 79% 10% 10%



- Molecule 1: Capsid protein


Chain h: 82% 8% 10%




- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|
| MET | GLY | SER | SER | SER | HIS | HIS | HIS | HIS | HIS | HIS | HIS | SER | SER | GLY | LEU | VAL | PRO | ARG | ARG | GLY | S43 | H44 | R59 | D70 | R89 | S90 | V91 | R97 | I98 | R99 | R116 | D139 | T151 | R159 | L167 | K179 | R180 | L183 | R186 | L187 | V196 | G197 | I206 | E223 | P230 | LEU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|

ASN
PRO


- Molecule 1: Capsid protein

Chain o:  79% 8% 10%P230
LEU
ASN
PRO


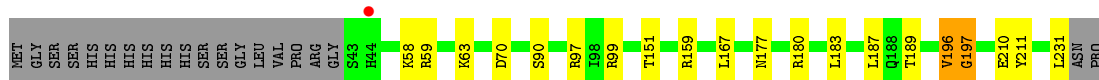
- Molecule 1: Capsid protein

Chain p:  81% 8% 10%

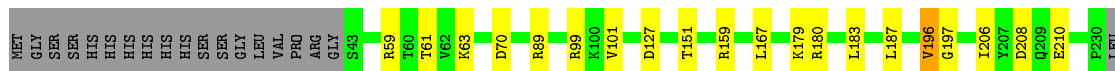
- Molecule 1: Capsid protein

Chain q:  79% 9% 10%P230
LEU
ASN
PRO


- Molecule 1: Capsid protein

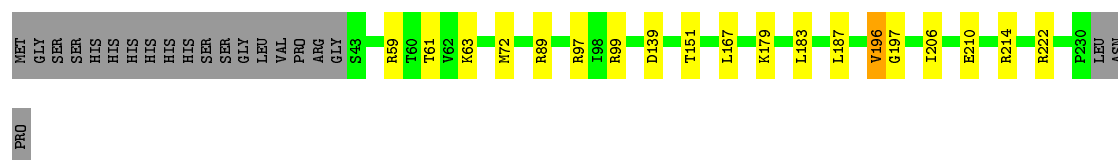
Chain r:  81% 9% 10%

- Molecule 1: Capsid protein


Chain s:  80% 9% 10%ASN
PRO

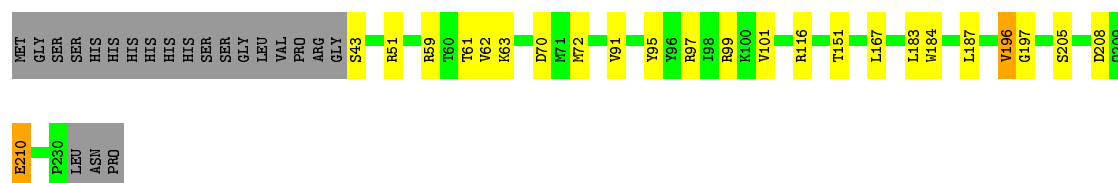
- Molecule 1: Capsid protein

Chain t:  81% 9% 10%




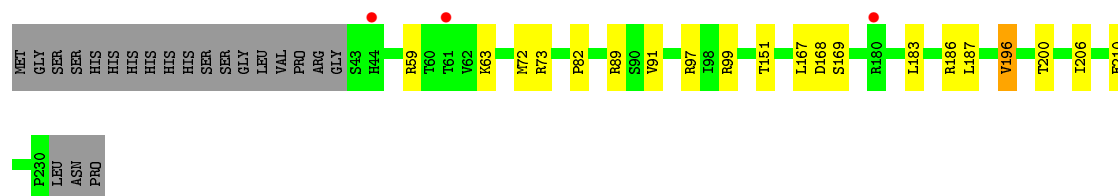
- Molecule 1: Capsid protein

Chain u:  78% 11% 10%




- Molecule 1: Capsid protein

Chain v:  80% 9% 10%




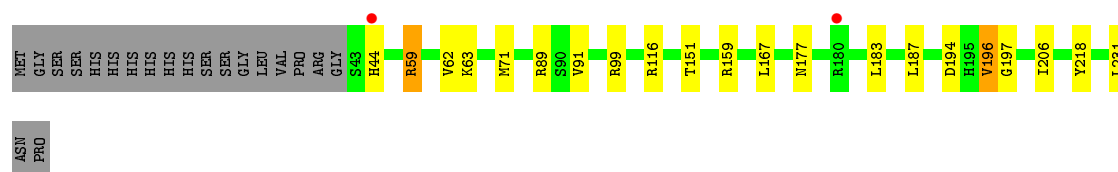
- Molecule 1: Capsid protein

Chain w:  81% 7% 10%



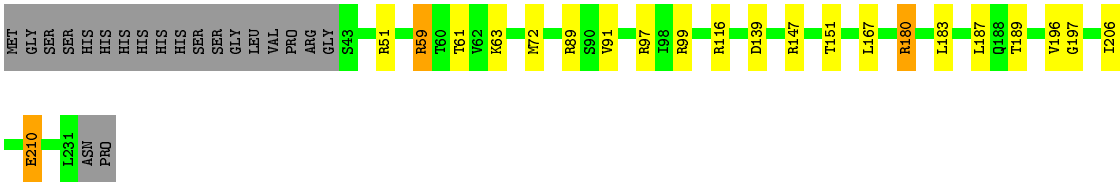
- Molecule 1: Capsid protein

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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.163 , 0.224 0.167 , 0.222	Depositor DCC
R_{free} test set	21255 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l 0.000 for k,h,-l 0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	97686	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	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

Continued on next page...

Continued from previous page...

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:

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 ⓘ

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	1	167	LEU
1	8	179	LYS
1	u	91	VAL
1	2	167	LEU
1	5	59	ARG

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

Mol	Chain	Res	Type
1	Z	44	HIS
1	6	181	ASN
1	t	178	ASN
1	Z	212	ASN
1	3	177	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	188/209 (89%)	-0.44	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, 37, 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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	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.