



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:30 am BST

PDB ID : 5J09  
Title : Crystal structure of decameric BFDV Capsid Protein  
Authors : Sarker, S.; Raidal, S.; Aragao, D.; Forwood, J.K.  
Deposited on : 2016-03-28  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

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

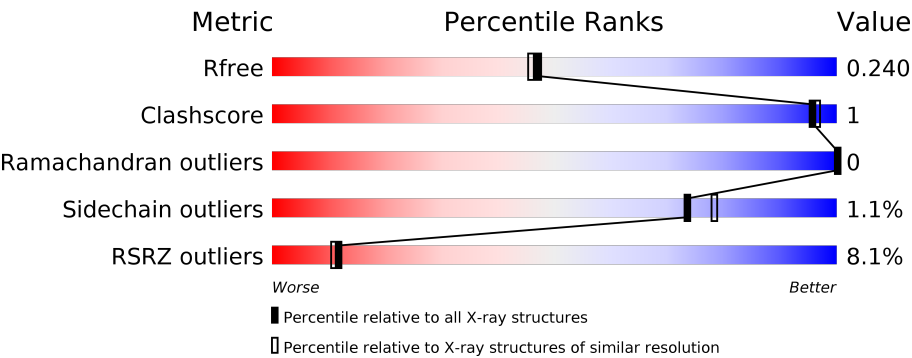
MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	A	257	<div><div>6%</div><div>66%</div><div>33%</div></div>
1	B	257	<div><div>5%</div><div>64%</div><div>34%</div></div>
1	C	257	<div><div>5%</div><div>61%</div><div>34%</div></div>
1	D	257	<div><div>5%</div><div>64%</div><div>33%</div></div>
1	E	257	<div><div>5%</div><div>63%</div><div>34%</div></div>
1	F	257	<div><div>5%</div><div>65%</div><div>34%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	257	<div><div><div>6%</div><div></div><div>63%</div><div></div><div>34%</div></div></div>
1	H	257	<div><div><div>4%</div><div></div><div>61%</div><div>5%</div><div>34%</div></div></div>
1	I	257	<div><div><div>7%</div><div></div><div>64%</div><div></div><div>34%</div></div></div>
1	J	257	<div><div><div>6%</div><div></div><div>64%</div><div></div><div>34%</div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29115 atoms, of which 13843 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 Beak and feather disease virus capsid protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	171	Total	C	H	N	O	S	0	0	0
			2783	899	1390	246	246	2			
1	B	169	Total	C	H	N	O	S	0	0	0
			2762	893	1380	244	243	2			
1	C	169	Total	C	H	N	O	S	0	0	0
			2762	893	1380	244	243	2			
1	D	171	Total	C	H	N	O	S	0	0	0
			2789	901	1393	247	246	2			
1	E	170	Total	C	H	N	O	S	0	0	0
			2772	896	1385	245	244	2			
1	F	170	Total	C	H	N	O	S	0	0	0
			2772	896	1385	245	244	2			
1	G	170	Total	C	H	N	O	S	0	0	0
			2772	896	1385	245	244	2			
1	H	169	Total	C	H	N	O	S	0	0	0
			2762	893	1380	244	243	2			
1	I	169	Total	C	H	N	O	S	0	0	0
			2762	893	1380	244	243	2			
1	J	170	Total	C	H	N	O	S	0	0	0
			2772	896	1385	245	244	2			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP A0A023R6W2
A	-8	HIS	-	expression tag	UNP A0A023R6W2
A	-7	HIS	-	expression tag	UNP A0A023R6W2
A	-6	HIS	-	expression tag	UNP A0A023R6W2
A	-5	HIS	-	expression tag	UNP A0A023R6W2
A	-4	HIS	-	expression tag	UNP A0A023R6W2
A	-3	HIS	-	expression tag	UNP A0A023R6W2
A	-2	SER	-	expression tag	UNP A0A023R6W2
A	-1	SER	-	expression tag	UNP A0A023R6W2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A0A023R6W2
A	1	VAL	-	expression tag	UNP A0A023R6W2
A	2	ASP	-	expression tag	UNP A0A023R6W2
A	3	LEU	-	expression tag	UNP A0A023R6W2
A	4	GLY	-	expression tag	UNP A0A023R6W2
A	5	THR	-	expression tag	UNP A0A023R6W2
A	6	GLU	-	expression tag	UNP A0A023R6W2
A	7	ASN	-	expression tag	UNP A0A023R6W2
A	8	LEU	-	expression tag	UNP A0A023R6W2
A	9	TYR	-	expression tag	UNP A0A023R6W2
A	10	PHE	-	expression tag	UNP A0A023R6W2
A	11	GLN	-	expression tag	UNP A0A023R6W2
A	12	SER	-	expression tag	UNP A0A023R6W2
A	13	ASN	-	expression tag	UNP A0A023R6W2
A	14	ALA	-	expression tag	UNP A0A023R6W2
B	-9	MET	-	initiating methionine	UNP A0A023R6W2
B	-8	HIS	-	expression tag	UNP A0A023R6W2
B	-7	HIS	-	expression tag	UNP A0A023R6W2
B	-6	HIS	-	expression tag	UNP A0A023R6W2
B	-5	HIS	-	expression tag	UNP A0A023R6W2
B	-4	HIS	-	expression tag	UNP A0A023R6W2
B	-3	HIS	-	expression tag	UNP A0A023R6W2
B	-2	SER	-	expression tag	UNP A0A023R6W2
B	-1	SER	-	expression tag	UNP A0A023R6W2
B	0	GLY	-	expression tag	UNP A0A023R6W2
B	1	VAL	-	expression tag	UNP A0A023R6W2
B	2	ASP	-	expression tag	UNP A0A023R6W2
B	3	LEU	-	expression tag	UNP A0A023R6W2
B	4	GLY	-	expression tag	UNP A0A023R6W2
B	5	THR	-	expression tag	UNP A0A023R6W2
B	6	GLU	-	expression tag	UNP A0A023R6W2
B	7	ASN	-	expression tag	UNP A0A023R6W2
B	8	LEU	-	expression tag	UNP A0A023R6W2
B	9	TYR	-	expression tag	UNP A0A023R6W2
B	10	PHE	-	expression tag	UNP A0A023R6W2
B	11	GLN	-	expression tag	UNP A0A023R6W2
B	12	SER	-	expression tag	UNP A0A023R6W2
B	13	ASN	-	expression tag	UNP A0A023R6W2
B	14	ALA	-	expression tag	UNP A0A023R6W2
C	-9	MET	-	initiating methionine	UNP A0A023R6W2
C	-8	HIS	-	expression tag	UNP A0A023R6W2
C	-7	HIS	-	expression tag	UNP A0A023R6W2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	HIS	-	expression tag	UNP A0A023R6W2
C	-5	HIS	-	expression tag	UNP A0A023R6W2
C	-4	HIS	-	expression tag	UNP A0A023R6W2
C	-3	HIS	-	expression tag	UNP A0A023R6W2
C	-2	SER	-	expression tag	UNP A0A023R6W2
C	-1	SER	-	expression tag	UNP A0A023R6W2
C	0	GLY	-	expression tag	UNP A0A023R6W2
C	1	VAL	-	expression tag	UNP A0A023R6W2
C	2	ASP	-	expression tag	UNP A0A023R6W2
C	3	LEU	-	expression tag	UNP A0A023R6W2
C	4	GLY	-	expression tag	UNP A0A023R6W2
C	5	THR	-	expression tag	UNP A0A023R6W2
C	6	GLU	-	expression tag	UNP A0A023R6W2
C	7	ASN	-	expression tag	UNP A0A023R6W2
C	8	LEU	-	expression tag	UNP A0A023R6W2
C	9	TYR	-	expression tag	UNP A0A023R6W2
C	10	PHE	-	expression tag	UNP A0A023R6W2
C	11	GLN	-	expression tag	UNP A0A023R6W2
C	12	SER	-	expression tag	UNP A0A023R6W2
C	13	ASN	-	expression tag	UNP A0A023R6W2
C	14	ALA	-	expression tag	UNP A0A023R6W2
D	-9	MET	-	initiating methionine	UNP A0A023R6W2
D	-8	HIS	-	expression tag	UNP A0A023R6W2
D	-7	HIS	-	expression tag	UNP A0A023R6W2
D	-6	HIS	-	expression tag	UNP A0A023R6W2
D	-5	HIS	-	expression tag	UNP A0A023R6W2
D	-4	HIS	-	expression tag	UNP A0A023R6W2
D	-3	HIS	-	expression tag	UNP A0A023R6W2
D	-2	SER	-	expression tag	UNP A0A023R6W2
D	-1	SER	-	expression tag	UNP A0A023R6W2
D	0	GLY	-	expression tag	UNP A0A023R6W2
D	1	VAL	-	expression tag	UNP A0A023R6W2
D	2	ASP	-	expression tag	UNP A0A023R6W2
D	3	LEU	-	expression tag	UNP A0A023R6W2
D	4	GLY	-	expression tag	UNP A0A023R6W2
D	5	THR	-	expression tag	UNP A0A023R6W2
D	6	GLU	-	expression tag	UNP A0A023R6W2
D	7	ASN	-	expression tag	UNP A0A023R6W2
D	8	LEU	-	expression tag	UNP A0A023R6W2
D	9	TYR	-	expression tag	UNP A0A023R6W2
D	10	PHE	-	expression tag	UNP A0A023R6W2
D	11	GLN	-	expression tag	UNP A0A023R6W2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	12	SER	-	expression tag	UNP A0A023R6W2
D	13	ASN	-	expression tag	UNP A0A023R6W2
D	14	ALA	-	expression tag	UNP A0A023R6W2
E	-9	MET	-	initiating methionine	UNP A0A023R6W2
E	-8	HIS	-	expression tag	UNP A0A023R6W2
E	-7	HIS	-	expression tag	UNP A0A023R6W2
E	-6	HIS	-	expression tag	UNP A0A023R6W2
E	-5	HIS	-	expression tag	UNP A0A023R6W2
E	-4	HIS	-	expression tag	UNP A0A023R6W2
E	-3	HIS	-	expression tag	UNP A0A023R6W2
E	-2	SER	-	expression tag	UNP A0A023R6W2
E	-1	SER	-	expression tag	UNP A0A023R6W2
E	0	GLY	-	expression tag	UNP A0A023R6W2
E	1	VAL	-	expression tag	UNP A0A023R6W2
E	2	ASP	-	expression tag	UNP A0A023R6W2
E	3	LEU	-	expression tag	UNP A0A023R6W2
E	4	GLY	-	expression tag	UNP A0A023R6W2
E	5	THR	-	expression tag	UNP A0A023R6W2
E	6	GLU	-	expression tag	UNP A0A023R6W2
E	7	ASN	-	expression tag	UNP A0A023R6W2
E	8	LEU	-	expression tag	UNP A0A023R6W2
E	9	TYR	-	expression tag	UNP A0A023R6W2
E	10	PHE	-	expression tag	UNP A0A023R6W2
E	11	GLN	-	expression tag	UNP A0A023R6W2
E	12	SER	-	expression tag	UNP A0A023R6W2
E	13	ASN	-	expression tag	UNP A0A023R6W2
E	14	ALA	-	expression tag	UNP A0A023R6W2
F	-9	MET	-	initiating methionine	UNP A0A023R6W2
F	-8	HIS	-	expression tag	UNP A0A023R6W2
F	-7	HIS	-	expression tag	UNP A0A023R6W2
F	-6	HIS	-	expression tag	UNP A0A023R6W2
F	-5	HIS	-	expression tag	UNP A0A023R6W2
F	-4	HIS	-	expression tag	UNP A0A023R6W2
F	-3	HIS	-	expression tag	UNP A0A023R6W2
F	-2	SER	-	expression tag	UNP A0A023R6W2
F	-1	SER	-	expression tag	UNP A0A023R6W2
F	0	GLY	-	expression tag	UNP A0A023R6W2
F	1	VAL	-	expression tag	UNP A0A023R6W2
F	2	ASP	-	expression tag	UNP A0A023R6W2
F	3	LEU	-	expression tag	UNP A0A023R6W2
F	4	GLY	-	expression tag	UNP A0A023R6W2
F	5	THR	-	expression tag	UNP A0A023R6W2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	6	GLU	-	expression tag	UNP A0A023R6W2
F	7	ASN	-	expression tag	UNP A0A023R6W2
F	8	LEU	-	expression tag	UNP A0A023R6W2
F	9	TYR	-	expression tag	UNP A0A023R6W2
F	10	PHE	-	expression tag	UNP A0A023R6W2
F	11	GLN	-	expression tag	UNP A0A023R6W2
F	12	SER	-	expression tag	UNP A0A023R6W2
F	13	ASN	-	expression tag	UNP A0A023R6W2
F	14	ALA	-	expression tag	UNP A0A023R6W2
G	-9	MET	-	initiating methionine	UNP A0A023R6W2
G	-8	HIS	-	expression tag	UNP A0A023R6W2
G	-7	HIS	-	expression tag	UNP A0A023R6W2
G	-6	HIS	-	expression tag	UNP A0A023R6W2
G	-5	HIS	-	expression tag	UNP A0A023R6W2
G	-4	HIS	-	expression tag	UNP A0A023R6W2
G	-3	HIS	-	expression tag	UNP A0A023R6W2
G	-2	SER	-	expression tag	UNP A0A023R6W2
G	-1	SER	-	expression tag	UNP A0A023R6W2
G	0	GLY	-	expression tag	UNP A0A023R6W2
G	1	VAL	-	expression tag	UNP A0A023R6W2
G	2	ASP	-	expression tag	UNP A0A023R6W2
G	3	LEU	-	expression tag	UNP A0A023R6W2
G	4	GLY	-	expression tag	UNP A0A023R6W2
G	5	THR	-	expression tag	UNP A0A023R6W2
G	6	GLU	-	expression tag	UNP A0A023R6W2
G	7	ASN	-	expression tag	UNP A0A023R6W2
G	8	LEU	-	expression tag	UNP A0A023R6W2
G	9	TYR	-	expression tag	UNP A0A023R6W2
G	10	PHE	-	expression tag	UNP A0A023R6W2
G	11	GLN	-	expression tag	UNP A0A023R6W2
G	12	SER	-	expression tag	UNP A0A023R6W2
G	13	ASN	-	expression tag	UNP A0A023R6W2
G	14	ALA	-	expression tag	UNP A0A023R6W2
H	-9	MET	-	initiating methionine	UNP A0A023R6W2
H	-8	HIS	-	expression tag	UNP A0A023R6W2
H	-7	HIS	-	expression tag	UNP A0A023R6W2
H	-6	HIS	-	expression tag	UNP A0A023R6W2
H	-5	HIS	-	expression tag	UNP A0A023R6W2
H	-4	HIS	-	expression tag	UNP A0A023R6W2
H	-3	HIS	-	expression tag	UNP A0A023R6W2
H	-2	SER	-	expression tag	UNP A0A023R6W2
H	-1	SER	-	expression tag	UNP A0A023R6W2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	0	GLY	-	expression tag	UNP A0A023R6W2
H	1	VAL	-	expression tag	UNP A0A023R6W2
H	2	ASP	-	expression tag	UNP A0A023R6W2
H	3	LEU	-	expression tag	UNP A0A023R6W2
H	4	GLY	-	expression tag	UNP A0A023R6W2
H	5	THR	-	expression tag	UNP A0A023R6W2
H	6	GLU	-	expression tag	UNP A0A023R6W2
H	7	ASN	-	expression tag	UNP A0A023R6W2
H	8	LEU	-	expression tag	UNP A0A023R6W2
H	9	TYR	-	expression tag	UNP A0A023R6W2
H	10	PHE	-	expression tag	UNP A0A023R6W2
H	11	GLN	-	expression tag	UNP A0A023R6W2
H	12	SER	-	expression tag	UNP A0A023R6W2
H	13	ASN	-	expression tag	UNP A0A023R6W2
H	14	ALA	-	expression tag	UNP A0A023R6W2
I	-9	MET	-	initiating methionine	UNP A0A023R6W2
I	-8	HIS	-	expression tag	UNP A0A023R6W2
I	-7	HIS	-	expression tag	UNP A0A023R6W2
I	-6	HIS	-	expression tag	UNP A0A023R6W2
I	-5	HIS	-	expression tag	UNP A0A023R6W2
I	-4	HIS	-	expression tag	UNP A0A023R6W2
I	-3	HIS	-	expression tag	UNP A0A023R6W2
I	-2	SER	-	expression tag	UNP A0A023R6W2
I	-1	SER	-	expression tag	UNP A0A023R6W2
I	0	GLY	-	expression tag	UNP A0A023R6W2
I	1	VAL	-	expression tag	UNP A0A023R6W2
I	2	ASP	-	expression tag	UNP A0A023R6W2
I	3	LEU	-	expression tag	UNP A0A023R6W2
I	4	GLY	-	expression tag	UNP A0A023R6W2
I	5	THR	-	expression tag	UNP A0A023R6W2
I	6	GLU	-	expression tag	UNP A0A023R6W2
I	7	ASN	-	expression tag	UNP A0A023R6W2
I	8	LEU	-	expression tag	UNP A0A023R6W2
I	9	TYR	-	expression tag	UNP A0A023R6W2
I	10	PHE	-	expression tag	UNP A0A023R6W2
I	11	GLN	-	expression tag	UNP A0A023R6W2
I	12	SER	-	expression tag	UNP A0A023R6W2
I	13	ASN	-	expression tag	UNP A0A023R6W2
I	14	ALA	-	expression tag	UNP A0A023R6W2
J	-9	MET	-	initiating methionine	UNP A0A023R6W2
J	-8	HIS	-	expression tag	UNP A0A023R6W2
J	-7	HIS	-	expression tag	UNP A0A023R6W2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-6	HIS	-	expression tag	UNP A0A023R6W2
J	-5	HIS	-	expression tag	UNP A0A023R6W2
J	-4	HIS	-	expression tag	UNP A0A023R6W2
J	-3	HIS	-	expression tag	UNP A0A023R6W2
J	-2	SER	-	expression tag	UNP A0A023R6W2
J	-1	SER	-	expression tag	UNP A0A023R6W2
J	0	GLY	-	expression tag	UNP A0A023R6W2
J	1	VAL	-	expression tag	UNP A0A023R6W2
J	2	ASP	-	expression tag	UNP A0A023R6W2
J	3	LEU	-	expression tag	UNP A0A023R6W2
J	4	GLY	-	expression tag	UNP A0A023R6W2
J	5	THR	-	expression tag	UNP A0A023R6W2
J	6	GLU	-	expression tag	UNP A0A023R6W2
J	7	ASN	-	expression tag	UNP A0A023R6W2
J	8	LEU	-	expression tag	UNP A0A023R6W2
J	9	TYR	-	expression tag	UNP A0A023R6W2
J	10	PHE	-	expression tag	UNP A0A023R6W2
J	11	GLN	-	expression tag	UNP A0A023R6W2
J	12	SER	-	expression tag	UNP A0A023R6W2
J	13	ASN	-	expression tag	UNP A0A023R6W2
J	14	ALA	-	expression tag	UNP A0A023R6W2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	146	Total O 146 146	0	0
2	B	134	Total O 134 134	0	0
2	C	137	Total O 137 137	0	0
2	D	139	Total O 139 139	0	0
2	E	134	Total O 134 134	0	0
2	F	139	Total O 139 139	0	0
2	G	139	Total O 139 139	0	0
2	H	163	Total O 163 163	0	0
2	I	142	Total O 142 142	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	J	134	Total	O	0	0
			134	134		

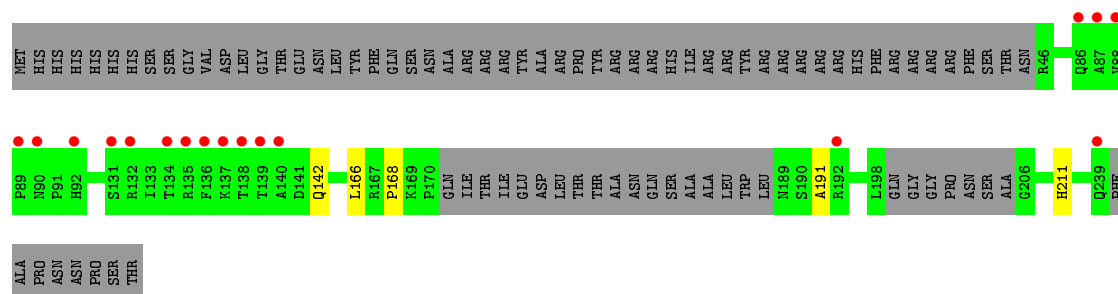


- Molecule 1: Beak and feather disease virus capsid protein

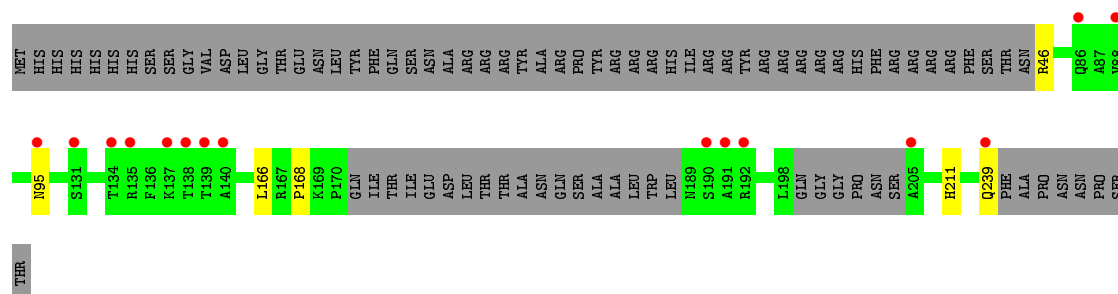




- Molecule 1: Beak and feather disease virus capsid protein



- Molecule 1: Beak and feather disease virus capsid protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.79Å 148.37Å 188.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 2.00 29.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.99-2.00) 95.4 (29.99-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.10pre_2104: ???)	Depositor
R, $R_{free}$	0.208 , 0.239 0.211 , 0.240	Depositor DCC
$R_{free}$ test set	7445 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 55.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	29115	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.6779e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/1429	0.48	0/1934
1	B	0.26	0/1418	0.47	0/1919
1	C	0.26	0/1418	0.46	0/1919
1	D	0.26	0/1432	0.47	0/1938
1	E	0.26	0/1423	0.47	0/1926
1	F	0.26	0/1423	0.47	0/1926
1	G	0.26	0/1423	0.46	0/1926
1	H	0.26	0/1418	0.47	0/1919
1	I	0.26	0/1418	0.47	0/1919
1	J	0.26	0/1423	0.47	0/1926
All	All	0.26	0/14225	0.47	0/19252

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1393	1390	1387	1	0
1	B	1382	1380	1377	2	0
1	C	1382	1380	1377	6	0
1	D	1396	1393	1390	4	0
1	E	1387	1385	1382	5	0
1	F	1387	1385	1382	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1387	1385	1382	4	0
1	H	1382	1380	1377	6	0
1	I	1382	1380	1377	2	0
1	J	1387	1385	1382	4	0
2	A	146	0	0	0	0
2	B	134	0	0	0	0
2	C	137	0	0	1	0
2	D	139	0	0	2	0
2	E	134	0	0	0	0
2	F	139	0	0	0	0
2	G	139	0	0	1	0
2	H	163	0	0	0	0
2	I	142	0	0	0	0
2	J	134	0	0	2	0
All	All	15272	13843	13813	31	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:GLN:NE2	2:D:301:HOH:O	2.15	0.79
1:J:239:GLN:OE1	2:J:301:HOH:O	2.04	0.74
1:H:83:ASP:OD2	1:H:210:ARG:NH2	2.24	0.70
1:G:46:ARG:N	2:G:1301:HOH:O	2.32	0.63
1:C:93:THR:OG1	1:D:239:GLN:NE2	2.33	0.62
1:H:138:THR:OG1	1:H:140:ALA:O	2.23	0.56
1:E:102:LYS:HE2	1:F:151:ASP:OD2	2.12	0.50
1:D:189:ASN:N	2:D:304:HOH:O	2.44	0.50
1:H:73:ASN:HA	1:H:138:THR:HG21	1.95	0.49
1:C:90:ASN:OD1	1:C:92:HIS:ND1	2.36	0.48
1:B:151:ASP:OD2	1:C:102:LYS:HE2	2.13	0.47
1:J:46:ARG:N	2:J:307:HOH:O	2.48	0.46
1:E:137:LYS:HB3	1:E:138:THR:HA	1.98	0.45
1:B:168:PRO:HB2	1:B:211:HIS:HB3	1.99	0.45
1:F:90:ASN:OD1	1:F:92:HIS:ND1	2.41	0.43
1:H:94:LEU:HD23	1:J:95:ASN:HB3	2.01	0.43
1:E:137:LYS:HB3	1:E:138:THR:CA	2.49	0.43
1:E:128:ILE:HG23	1:E:132:ARG:HE	1.83	0.42
1:D:101:ILE:HD12	1:D:211:HIS:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ARG:NH2	1:C:236:GLN:OE1	2.52	0.42
1:G:138:THR:HG22	1:G:140:ALA:H	1.84	0.42
1:J:168:PRO:HB2	1:J:211:HIS:HB3	2.01	0.42
1:C:160:ARG:NH1	2:C:1508:HOH:O	2.52	0.41
1:G:136:PHE:HZ	1:G:150:PHE:CZ	2.38	0.41
1:A:192:ARG:HG2	1:I:191:ALA:HB1	2.03	0.41
1:G:168:PRO:HB2	1:G:211:HIS:HB3	2.02	0.41
1:H:192:ARG:CZ	1:H:192:ARG:HB3	2.51	0.41
1:C:168:PRO:HB2	1:C:211:HIS:HB3	2.03	0.41
1:E:168:PRO:HB2	1:E:211:HIS:HB3	2.03	0.41
1:H:168:PRO:HB2	1:H:211:HIS:HB3	2.03	0.40
1:I:168:PRO:HB2	1:I:211:HIS:HB3	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	165/257 (64%)	161 (98%)	4 (2%)	0	100	100
1	B	163/257 (63%)	160 (98%)	3 (2%)	0	100	100
1	C	163/257 (63%)	160 (98%)	3 (2%)	0	100	100
1	D	165/257 (64%)	161 (98%)	4 (2%)	0	100	100
1	E	164/257 (64%)	161 (98%)	3 (2%)	0	100	100
1	F	164/257 (64%)	161 (98%)	3 (2%)	0	100	100
1	G	164/257 (64%)	160 (98%)	4 (2%)	0	100	100
1	H	163/257 (63%)	160 (98%)	3 (2%)	0	100	100
1	I	163/257 (63%)	157 (96%)	6 (4%)	0	100	100
1	J	164/257 (64%)	161 (98%)	3 (2%)	0	100	100
All	All	1638/2570 (64%)	1602 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	149/226 (66%)	148 (99%)	1 (1%)	84	88
1	B	148/226 (66%)	146 (99%)	2 (1%)	67	72
1	C	148/226 (66%)	145 (98%)	3 (2%)	55	58
1	D	149/226 (66%)	147 (99%)	2 (1%)	69	74
1	E	148/226 (66%)	148 (100%)	0	100	100
1	F	148/226 (66%)	147 (99%)	1 (1%)	84	88
1	G	148/226 (66%)	147 (99%)	1 (1%)	84	88
1	H	148/226 (66%)	144 (97%)	4 (3%)	44	46
1	I	148/226 (66%)	146 (99%)	2 (1%)	67	72
1	J	148/226 (66%)	147 (99%)	1 (1%)	84	88
All	All	1482/2260 (66%)	1465 (99%)	17 (1%)	73	78

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	LEU
1	B	86	GLN
1	B	166	LEU
1	C	90	ASN
1	C	139	THR
1	C	166	LEU
1	D	86	GLN
1	D	166	LEU
1	F	166	LEU
1	G	166	LEU
1	H	88	VAL
1	H	137	LYS
1	H	166	LEU
1	H	189	ASN

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Mol	Chain	Res	Type
1	I	142	GLN
1	I	166	LEU
1	J	166	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	236	GLN
1	D	239	GLN
1	E	95	ASN
1	I	90	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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, 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	A	171/257 (66%)	0.18	15 (8%) 10 9	12, 22, 53, 73	0
1	B	169/257 (65%)	0.22	13 (7%) 13 12	15, 25, 57, 72	0
1	C	169/257 (65%)	0.17	12 (7%) 16 15	14, 23, 58, 75	0
1	D	171/257 (66%)	0.13	14 (8%) 11 11	11, 22, 59, 79	0
1	E	170/257 (66%)	0.26	13 (7%) 13 13	14, 25, 56, 68	0
1	F	170/257 (66%)	0.17	12 (7%) 16 15	14, 24, 54, 81	0
1	G	170/257 (66%)	0.24	16 (9%) 8 8	12, 22, 59, 68	0
1	H	169/257 (65%)	0.09	11 (6%) 18 18	12, 21, 51, 75	0
1	I	169/257 (65%)	0.31	17 (10%) 7 6	14, 23, 52, 66	0
1	J	170/257 (66%)	0.21	15 (8%) 10 9	12, 22, 54, 70	0
All	All	1698/2570 (66%)	0.20	138 (8%) 12 11	11, 23, 56, 81	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	139	THR	8.9
1	H	191	ALA	7.7
1	F	139	THR	7.7
1	I	139	THR	7.5
1	H	139	THR	6.3
1	J	139	THR	6.1
1	D	139	THR	6.1
1	A	139	THR	5.9
1	G	138	THR	5.8
1	J	191	ALA	5.7
1	G	139	THR	5.7
1	D	87	ALA	5.6
1	C	138	THR	5.3

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Mol	Chain	Res	Type	RSRZ
1	I	88	VAL	5.3
1	B	139	THR	5.3
1	C	88	VAL	5.0
1	G	131	SER	5.0
1	E	140	ALA	4.9
1	B	86	GLN	4.9
1	E	86	GLN	4.8
1	E	138	THR	4.7
1	A	204	SER	4.5
1	H	138	THR	4.5
1	G	87	ALA	4.4
1	D	131	SER	4.4
1	D	135	ARG	4.4
1	J	140	ALA	4.3
1	I	140	ALA	4.2
1	F	138	THR	4.2
1	D	239	GLN	4.2
1	D	86	GLN	4.2
1	C	131	SER	4.0
1	F	88	VAL	4.0
1	I	136	PHE	3.9
1	E	139	THR	3.9
1	I	131	SER	3.8
1	J	190	SER	3.8
1	J	205	ALA	3.8
1	I	92	HIS	3.8
1	B	135	ARG	3.7
1	I	87	ALA	3.7
1	B	138	THR	3.7
1	C	86	GLN	3.7
1	C	87	ALA	3.7
1	B	136	PHE	3.6
1	J	192	ARG	3.6
1	J	131	SER	3.6
1	D	136	PHE	3.5
1	G	86	GLN	3.5
1	A	140	ALA	3.5
1	I	137	LYS	3.5
1	G	137	LYS	3.4
1	F	189	ASN	3.4
1	G	92	HIS	3.3
1	H	131	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	90	ASN	3.3
1	J	138	THR	3.3
1	J	135	ARG	3.3
1	G	140	ALA	3.3
1	H	140	ALA	3.3
1	A	131	SER	3.3
1	E	137	LYS	3.3
1	J	137	LYS	3.3
1	B	140	ALA	3.3
1	B	92	HIS	3.2
1	B	239	GLN	3.2
1	F	191	ALA	3.2
1	I	135	ARG	3.1
1	F	190	SER	3.1
1	E	88	VAL	3.1
1	C	89	PRO	3.0
1	J	239	GLN	3.0
1	A	85	LEU	3.0
1	D	134	THR	2.9
1	G	191	ALA	2.9
1	J	88	VAL	2.9
1	C	189	ASN	2.9
1	B	131	SER	2.8
1	B	137	LYS	2.8
1	G	205	ALA	2.8
1	D	191	ALA	2.7
1	G	88	VAL	2.7
1	D	137	LYS	2.7
1	C	140	ALA	2.7
1	D	140	ALA	2.7
1	I	239	GLN	2.6
1	I	138	THR	2.6
1	E	95	ASN	2.6
1	A	189	ASN	2.6
1	A	86	GLN	2.6
1	F	192	ARG	2.5
1	C	132	ARG	2.5
1	A	136	PHE	2.5
1	E	189	ASN	2.5
1	H	132	ARG	2.5
1	B	87	ALA	2.5
1	C	191	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	192	ARG	2.5
1	H	190	SER	2.5
1	I	134	THR	2.4
1	F	131	SER	2.4
1	H	135	ARG	2.4
1	A	88	VAL	2.4
1	H	137	LYS	2.4
1	E	134	THR	2.4
1	D	199	GLN	2.4
1	G	239	GLN	2.4
1	B	134	THR	2.4
1	I	86	GLN	2.4
1	F	135	ARG	2.4
1	E	131	SER	2.4
1	E	239	GLN	2.3
1	J	134	THR	2.3
1	B	89	PRO	2.3
1	E	132	ARG	2.3
1	E	135	ARG	2.3
1	A	87	ALA	2.2
1	F	140	ALA	2.2
1	A	138	THR	2.2
1	F	132	ARG	2.2
1	G	189	ASN	2.2
1	I	89	PRO	2.2
1	A	132	ARG	2.2
1	G	136	PHE	2.1
1	A	191	ALA	2.1
1	C	190	SER	2.1
1	D	192	ARG	2.1
1	H	87	ALA	2.1
1	H	192	ARG	2.1
1	A	135	ARG	2.1
1	G	132	ARG	2.1
1	G	90	ASN	2.1
1	J	95	ASN	2.1
1	F	86	GLN	2.1
1	I	132	ARG	2.0
1	J	86	GLN	2.0
1	A	137	LYS	2.0
1	D	95	ASN	2.0



## 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 carbohydrates 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.