



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:37 PM UTC

PDB ID : 5J09 / pdb_00005j09
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

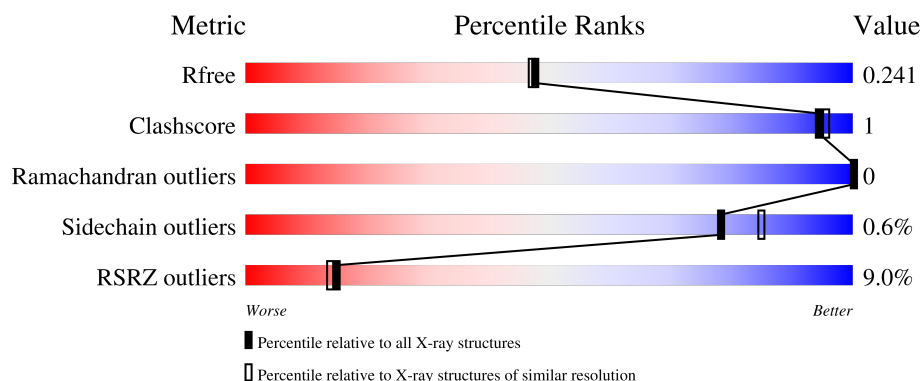
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



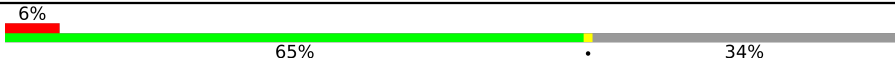
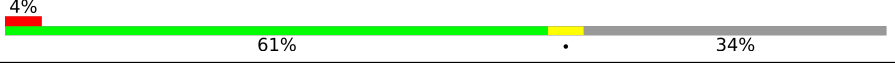
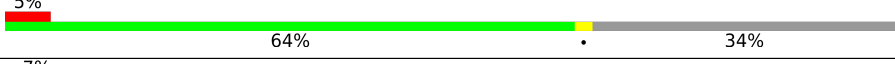
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	257	5% 66% 33%
1	B	257	6% 63% 34%
1	C	257	5% 61% 34%
1	D	257	7% 64% 33%
1	E	257	6% 63% 34%

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Mol	Chain	Length	Quality of chain
1	F	257	
1	G	257	
1	H	257	
1	I	257	
1	J	257	

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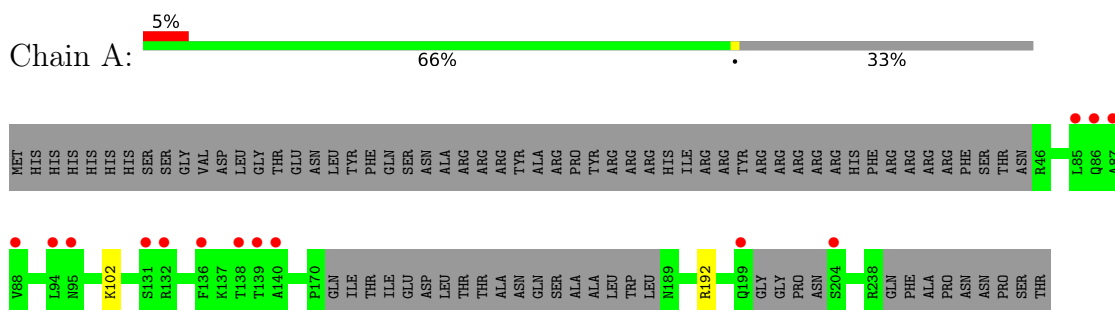
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	J	134	Total 134	O 134	0	0

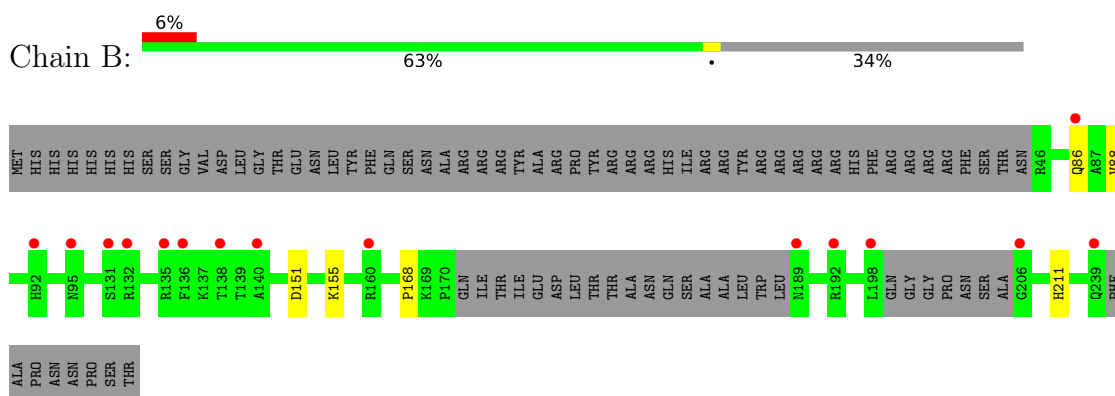
3 Residue-property plots

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.

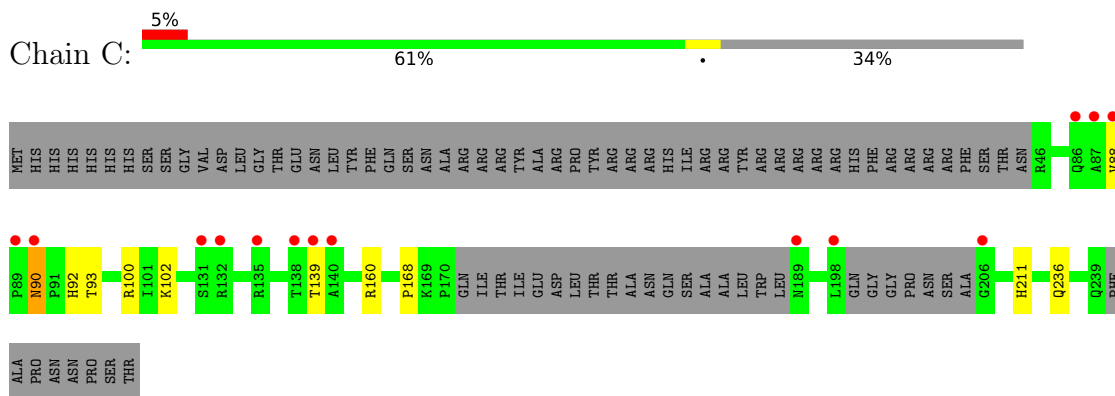
- Molecule 1: Beak and feather disease virus capsid protein



- Molecule 1: Beak and feather disease virus capsid protein



- Molecule 1: Beak and feather disease virus capsid protein



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.10pre_2104: ???)	Depositor
R, R_{free}	0.208 , 0.239 0.211 , 0.241	Depositor DCC
R_{free} test set	7445 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	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 ²)	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.*

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 [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	0.13	0/1429	0.34	0/1934
1	B	0.13	0/1418	0.33	0/1919
1	C	0.13	0/1418	0.32	0/1919
1	D	0.13	0/1432	0.32	0/1938
1	E	0.12	0/1423	0.33	0/1926
1	F	0.13	0/1423	0.32	0/1926
1	G	0.13	0/1423	0.33	0/1926
1	H	0.14	0/1418	0.33	0/1919
1	I	0.12	0/1418	0.32	0/1919
1	J	0.13	0/1423	0.33	0/1926
All	All	0.13	0/14225	0.33	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	2	0
1	B	1382	1380	1377	2	0
1	C	1382	1380	1377	6	0
1	D	1396	1393	1390	5	0
1	E	1387	1385	1382	6	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	7	0
1	I	1382	1380	1377	3	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	1	0
2	F	139	0	0	0	0
2	G	139	0	0	1	0
2	H	163	0	0	1	0
2	I	142	0	0	0	0
2	J	134	0	0	2	0
All	All	15272	13843	13813	35	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 (35) 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:D:94:LEU:C	1:D:96:PHE:H	2.29	0.41
1:G:168:PRO:HB2	1:G:211:HIS:HB3	2.02	0.41
1:C:168:PRO:HB2	1:C:211:HIS:HB3	2.03	0.41
1:H:62:LYS:NZ	2:H:308:HOH:O	2.53	0.41
1:H:192:ARG:CZ	1:H:192:ARG:HB3	2.51	0.41
1:A:102:LYS:NZ	1:I:151:ASP:OD1	2.53	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:E:59:LYS:NZ	2:E:313:HOH:O	2.54	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	149 (100%)	0	100	100
1	B	148/226 (66%)	145 (98%)	3 (2%)	48	54
1	C	148/226 (66%)	145 (98%)	3 (2%)	48	54
1	D	149/226 (66%)	148 (99%)	1 (1%)	76	82
1	E	148/226 (66%)	148 (100%)	0	100	100
1	F	148/226 (66%)	148 (100%)	0	100	100
1	G	148/226 (66%)	148 (100%)	0	100	100
1	H	148/226 (66%)	147 (99%)	1 (1%)	76	82
1	I	148/226 (66%)	147 (99%)	1 (1%)	76	82
1	J	148/226 (66%)	148 (100%)	0	100	100
All	All	1482/2260 (66%)	1473 (99%)	9 (1%)	78	85

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	86	GLN
1	B	88	VAL
1	B	155	LYS
1	C	88	VAL
1	C	90	ASN

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Mol	Chain	Res	Type
1	C	139	THR
1	D	86	GLN
1	H	88	VAL
1	I	142	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	B	61	ASN
1	B	86	GLN
1	B	95	ASN
1	C	57	GLN
1	C	61	ASN
1	C	69	ASN
1	D	236	GLN
1	D	239	GLN
1	E	95	ASN
1	E	118	GLN
1	F	61	ASN
1	F	239	GLN
1	G	61	ASN
1	G	69	ASN
1	G	118	GLN
1	G	189	ASN
1	G	239	GLN
1	H	86	GLN
1	H	142	GLN
1	I	90	ASN
1	J	57	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	171/257 (66%)	0.13	14 (8%) 17 16	12, 25, 58, 81	0
1	B	169/257 (65%)	0.25	15 (8%) 15 14	16, 29, 64, 81	0
1	C	169/257 (65%)	0.25	14 (8%) 17 16	15, 26, 64, 82	0
1	D	171/257 (66%)	0.16	18 (10%) 11 10	12, 24, 64, 86	0
1	E	170/257 (66%)	0.32	16 (9%) 14 13	16, 29, 60, 74	0
1	F	170/257 (66%)	0.21	16 (9%) 14 13	15, 26, 62, 89	0
1	G	170/257 (66%)	0.17	18 (10%) 11 10	13, 25, 63, 76	0
1	H	169/257 (65%)	-0.01	11 (6%) 25 23	12, 23, 56, 84	0
1	I	169/257 (65%)	0.14	14 (8%) 17 16	15, 26, 57, 75	0
1	J	170/257 (66%)	0.15	17 (10%) 12 11	13, 24, 60, 80	0
All	All	1698/2570 (66%)	0.18	153 (9%) 15 14	12, 26, 62, 89	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	87	ALA	6.0
1	F	138	THR	5.5
1	C	131	SER	5.0
1	G	138	THR	5.0
1	A	131	SER	4.7
1	E	140	ALA	4.7
1	D	239	GLN	4.7
1	C	89	PRO	4.5
1	E	138	THR	4.4
1	I	139	THR	4.4
1	B	136	PHE	4.4
1	H	191	ALA	4.3
1	G	140	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	131	SER	4.3
1	C	87	ALA	4.0
1	B	140	ALA	4.0
1	B	86	GLN	4.0
1	J	191	ALA	3.9
1	J	205	ALA	3.9
1	A	85	LEU	3.9
1	C	189	ASN	3.9
1	G	136	PHE	3.8
1	G	131	SER	3.8
1	J	131	SER	3.8
1	D	136	PHE	3.8
1	I	131	SER	3.8
1	C	88	VAL	3.8
1	H	189	ASN	3.8
1	C	139	THR	3.8
1	J	88	VAL	3.8
1	F	139	THR	3.7
1	G	139	THR	3.7
1	D	86	GLN	3.6
1	J	239	GLN	3.6
1	A	139	THR	3.6
1	D	191	ALA	3.6
1	I	136	PHE	3.5
1	H	138	THR	3.5
1	F	198	LEU	3.5
1	A	87	ALA	3.5
1	H	131	SER	3.5
1	C	138	THR	3.4
1	E	95	ASN	3.4
1	E	198	LEU	3.4
1	I	88	VAL	3.4
1	J	189	ASN	3.3
1	G	130	ASP	3.3
1	J	95	ASN	3.3
1	F	189	ASN	3.3
1	C	86	GLN	3.3
1	C	198	LEU	3.3
1	A	204	SER	3.2
1	B	138	THR	3.2
1	F	131	SER	3.2
1	G	92	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	88	VAL	3.1
1	J	192	ARG	3.1
1	D	138	THR	3.1
1	G	132	ARG	3.1
1	A	88	VAL	3.1
1	D	139	THR	3.0
1	B	239	GLN	3.0
1	D	140	ALA	3.0
1	A	136	PHE	3.0
1	E	132	ARG	3.0
1	C	132	ARG	2.9
1	I	140	ALA	2.9
1	E	137	LYS	2.9
1	A	86	GLN	2.9
1	E	142	GLN	2.9
1	H	198	LEU	2.9
1	J	137	LYS	2.9
1	G	198	LEU	2.9
1	J	140	ALA	2.9
1	J	139	THR	2.8
1	G	86	GLN	2.8
1	C	135	ARG	2.7
1	G	205	ALA	2.7
1	J	87	ALA	2.7
1	A	138	THR	2.7
1	D	134	THR	2.7
1	H	139	THR	2.7
1	D	95	ASN	2.7
1	D	189	ASN	2.7
1	E	189	ASN	2.7
1	F	239	GLN	2.7
1	I	132	ARG	2.7
1	D	199	GLN	2.6
1	G	87	ALA	2.6
1	I	89	PRO	2.6
1	J	190	SER	2.6
1	D	135	ARG	2.6
1	B	135	ARG	2.6
1	F	132	ARG	2.6
1	J	138	THR	2.6
1	A	94	LEU	2.6
1	C	206	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	95	ASN	2.5
1	G	95	ASN	2.5
1	E	86	GLN	2.5
1	G	239	GLN	2.5
1	B	95	ASN	2.5
1	C	90	ASN	2.5
1	I	130	ASP	2.5
1	A	199	GLN	2.5
1	E	131	SER	2.5
1	H	190	SER	2.5
1	G	189	ASN	2.5
1	F	140	ALA	2.5
1	F	88	VAL	2.4
1	D	94	LEU	2.4
1	B	132	ARG	2.4
1	I	192	ARG	2.4
1	J	135	ARG	2.4
1	I	189	ASN	2.4
1	D	130	ASP	2.4
1	B	206	GLY	2.4
1	B	131	SER	2.4
1	E	94	LEU	2.3
1	J	212	TYR	2.3
1	D	192	ARG	2.3
1	F	192	ARG	2.3
1	B	192	ARG	2.3
1	I	206	GLY	2.3
1	I	137	LYS	2.3
1	A	132	ARG	2.3
1	H	132	ARG	2.3
1	F	136	PHE	2.2
1	B	92	HIS	2.2
1	G	137	LYS	2.2
1	C	140	ALA	2.2
1	I	239	GLN	2.2
1	B	198	LEU	2.2
1	F	135	ARG	2.2
1	D	137	LYS	2.2
1	G	90	ASN	2.2
1	E	92	HIS	2.1
1	H	87	ALA	2.1
1	H	192	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	97	GLU	2.1
1	E	130	ASP	2.1
1	J	193	THR	2.1
1	E	239	GLN	2.1
1	F	86	GLN	2.1
1	B	160	ARG	2.1
1	G	97	GLU	2.1
1	F	223	GLN	2.1
1	F	191	ALA	2.1
1	I	191	ALA	2.1
1	H	88	VAL	2.0
1	A	140	ALA	2.0
1	B	189	ASN	2.0
1	F	137	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.