



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:56 am BST

PDB ID : 6EVJ
Title : Crystal structure of bat influenza A/H17N10 polymerase with viral RNA promoter and capped RNA primer
Authors : Pflug, A.; Cusack, S.
Deposited on : 2017-11-01
Resolution : 3.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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

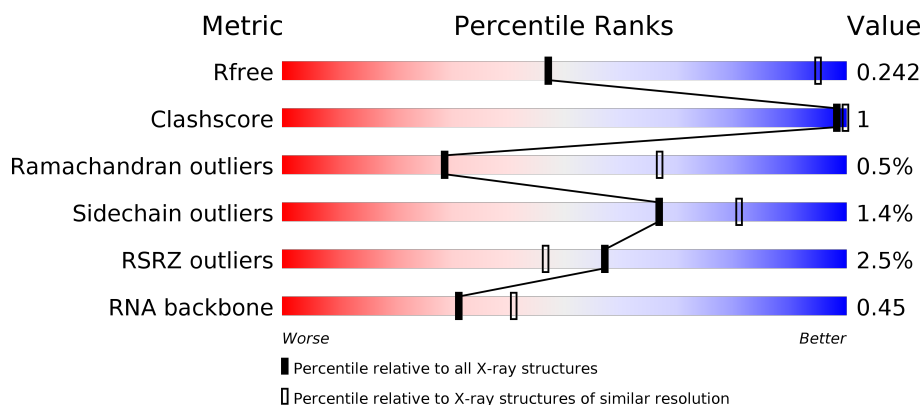
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)
RNA backbone	3102	1040 (4.76-3.00)

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 ≥ 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	738	<div> <div>2%</div> <div>93%</div> </div>
1	D	738	<div> <div>2%</div> <div>94%</div> </div>
2	B	776	<div> <div>4%</div> <div>93%</div> </div>
2	E	776	<div> <div>5%</div> <div>92%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	809	<div><div></div><div>90%</div><div></div><div></div><div>8%</div></div>
3	F	809	<div><div></div><div>89%</div><div></div><div></div><div>8%</div></div>
4	M	13	<div><div></div><div>15%</div><div>8%</div><div>23%</div><div></div><div>69%</div></div>
4	N	13	<div><div></div><div>15%</div><div>8%</div><div>23%</div><div></div><div>69%</div></div>
5	R	18	<div><div></div><div>6%</div><div></div><div>67%</div><div></div><div>6%</div><div>28%</div></div>
5	S	18	<div><div></div><div>6%</div><div></div><div>67%</div><div></div><div>6%</div><div>28%</div></div>
6	U	16	<div><div></div><div>56%</div><div></div><div>38%</div><div></div><div>6%</div></div>
6	V	16	<div><div></div><div>50%</div><div></div><div>44%</div><div></div><div>6%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36717 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	709	Total	C	N	O	S	0	0	0
			5775	3671	974	1093	37			
1	D	708	Total	C	N	O	S	0	0	0
			5769	3668	974	1090	37			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	GLY	-	expression tag	UNP H6QM92
A	-12	SER	-	expression tag	UNP H6QM92
A	-11	HIS	-	expression tag	UNP H6QM92
A	-10	HIS	-	expression tag	UNP H6QM92
A	-9	HIS	-	expression tag	UNP H6QM92
A	-8	HIS	-	expression tag	UNP H6QM92
A	-7	HIS	-	expression tag	UNP H6QM92
A	-6	HIS	-	expression tag	UNP H6QM92
A	-5	HIS	-	expression tag	UNP H6QM92
A	-4	HIS	-	expression tag	UNP H6QM92
A	-3	GLY	-	expression tag	UNP H6QM92
A	-2	SER	-	expression tag	UNP H6QM92
A	-1	GLY	-	expression tag	UNP H6QM92
A	0	SER	-	expression tag	UNP H6QM92
A	714	GLY	-	expression tag	UNP H6QM92
A	715	SER	-	expression tag	UNP H6QM92
A	716	GLY	-	expression tag	UNP H6QM92
A	717	SER	-	expression tag	UNP H6QM92
A	718	GLY	-	expression tag	UNP H6QM92
A	719	GLU	-	expression tag	UNP H6QM92
A	720	ASN	-	expression tag	UNP H6QM92
A	721	LEU	-	expression tag	UNP H6QM92
A	722	TYR	-	expression tag	UNP H6QM92
A	723	PHE	-	expression tag	UNP H6QM92
A	724	GLN	-	expression tag	UNP H6QM92

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-13	GLY	-	expression tag	UNP H6QM92
D	-12	SER	-	expression tag	UNP H6QM92
D	-11	HIS	-	expression tag	UNP H6QM92
D	-10	HIS	-	expression tag	UNP H6QM92
D	-9	HIS	-	expression tag	UNP H6QM92
D	-8	HIS	-	expression tag	UNP H6QM92
D	-7	HIS	-	expression tag	UNP H6QM92
D	-6	HIS	-	expression tag	UNP H6QM92
D	-5	HIS	-	expression tag	UNP H6QM92
D	-4	HIS	-	expression tag	UNP H6QM92
D	-3	GLY	-	expression tag	UNP H6QM92
D	-2	SER	-	expression tag	UNP H6QM92
D	-1	GLY	-	expression tag	UNP H6QM92
D	0	SER	-	expression tag	UNP H6QM92
D	714	GLY	-	expression tag	UNP H6QM92
D	715	SER	-	expression tag	UNP H6QM92
D	716	GLY	-	expression tag	UNP H6QM92
D	717	SER	-	expression tag	UNP H6QM92
D	718	GLY	-	expression tag	UNP H6QM92
D	719	GLU	-	expression tag	UNP H6QM92
D	720	ASN	-	expression tag	UNP H6QM92
D	721	LEU	-	expression tag	UNP H6QM92
D	722	TYR	-	expression tag	UNP H6QM92
D	723	PHE	-	expression tag	UNP H6QM92
D	724	GLN	-	expression tag	UNP H6QM92

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	752	Total	C	N	O	S	0	0	0
			5999	3772	1067	1120	40			
2	E	749	Total	C	N	O	S	0	0	0
			5972	3756	1061	1115	40			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP H6QM91
B	-7	SER	-	expression tag	UNP H6QM91
B	-6	GLY	-	expression tag	UNP H6QM91
B	-5	SER	-	expression tag	UNP H6QM91
B	-4	GLY	-	expression tag	UNP H6QM91

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	SER	-	expression tag	UNP H6QM91
B	-2	GLY	-	expression tag	UNP H6QM91
B	-1	SER	-	expression tag	UNP H6QM91
B	0	GLY	-	expression tag	UNP H6QM91
B	757	GLY	-	expression tag	UNP H6QM91
B	758	SER	-	expression tag	UNP H6QM91
B	759	GLY	-	expression tag	UNP H6QM91
B	760	SER	-	expression tag	UNP H6QM91
B	761	GLY	-	expression tag	UNP H6QM91
B	762	GLU	-	expression tag	UNP H6QM91
B	763	ASN	-	expression tag	UNP H6QM91
B	764	LEU	-	expression tag	UNP H6QM91
B	765	TYR	-	expression tag	UNP H6QM91
B	766	PHE	-	expression tag	UNP H6QM91
B	767	GLN	-	expression tag	UNP H6QM91
E	-8	GLY	-	expression tag	UNP H6QM91
E	-7	SER	-	expression tag	UNP H6QM91
E	-6	GLY	-	expression tag	UNP H6QM91
E	-5	SER	-	expression tag	UNP H6QM91
E	-4	GLY	-	expression tag	UNP H6QM91
E	-3	SER	-	expression tag	UNP H6QM91
E	-2	GLY	-	expression tag	UNP H6QM91
E	-1	SER	-	expression tag	UNP H6QM91
E	0	GLY	-	expression tag	UNP H6QM91
E	757	GLY	-	expression tag	UNP H6QM91
E	758	SER	-	expression tag	UNP H6QM91
E	759	GLY	-	expression tag	UNP H6QM91
E	760	SER	-	expression tag	UNP H6QM91
E	761	GLY	-	expression tag	UNP H6QM91
E	762	GLU	-	expression tag	UNP H6QM91
E	763	ASN	-	expression tag	UNP H6QM91
E	764	LEU	-	expression tag	UNP H6QM91
E	765	TYR	-	expression tag	UNP H6QM91
E	766	PHE	-	expression tag	UNP H6QM91
E	767	GLN	-	expression tag	UNP H6QM91

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	748	Total	C	N	O	S	0	0	0
			5937	3742	1049	1114	32			
3	F	746	Total	C	N	O	S	0	0	0
			5926	3736	1049	1109	32			

There are 98 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLY	-	expression tag	UNP H6QM90
C	-7	SER	-	expression tag	UNP H6QM90
C	-6	GLY	-	expression tag	UNP H6QM90
C	-5	SER	-	expression tag	UNP H6QM90
C	-4	GLY	-	expression tag	UNP H6QM90
C	-3	SER	-	expression tag	UNP H6QM90
C	-2	GLY	-	expression tag	UNP H6QM90
C	-1	SER	-	expression tag	UNP H6QM90
C	0	GLY	-	expression tag	UNP H6QM90
C	761	GLY	-	expression tag	UNP H6QM90
C	762	TRP	-	expression tag	UNP H6QM90
C	763	SER	-	expression tag	UNP H6QM90
C	764	HIS	-	expression tag	UNP H6QM90
C	765	PRO	-	expression tag	UNP H6QM90
C	766	GLN	-	expression tag	UNP H6QM90
C	767	PHE	-	expression tag	UNP H6QM90
C	768	GLU	-	expression tag	UNP H6QM90
C	769	LYS	-	expression tag	UNP H6QM90
C	770	GLY	-	expression tag	UNP H6QM90
C	771	GLY	-	expression tag	UNP H6QM90
C	772	GLY	-	expression tag	UNP H6QM90
C	773	SER	-	expression tag	UNP H6QM90
C	774	GLY	-	expression tag	UNP H6QM90
C	775	GLY	-	expression tag	UNP H6QM90
C	776	GLY	-	expression tag	UNP H6QM90
C	777	SER	-	expression tag	UNP H6QM90
C	778	GLY	-	expression tag	UNP H6QM90
C	779	GLY	-	expression tag	UNP H6QM90
C	780	SER	-	expression tag	UNP H6QM90
C	781	ALA	-	expression tag	UNP H6QM90
C	782	TRP	-	expression tag	UNP H6QM90
C	783	SER	-	expression tag	UNP H6QM90
C	784	HIS	-	expression tag	UNP H6QM90
C	785	PRO	-	expression tag	UNP H6QM90
C	786	GLN	-	expression tag	UNP H6QM90
C	787	PHE	-	expression tag	UNP H6QM90
C	788	GLU	-	expression tag	UNP H6QM90
C	789	LYS	-	expression tag	UNP H6QM90
C	790	GLY	-	expression tag	UNP H6QM90
C	791	ARG	-	expression tag	UNP H6QM90
C	792	SER	-	expression tag	UNP H6QM90
C	793	GLY	-	expression tag	UNP H6QM90

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	794	GLY	-	expression tag	UNP H6QM90
C	795	GLU	-	expression tag	UNP H6QM90
C	796	ASN	-	expression tag	UNP H6QM90
C	797	LEU	-	expression tag	UNP H6QM90
C	798	TYR	-	expression tag	UNP H6QM90
C	799	PHE	-	expression tag	UNP H6QM90
C	800	GLN	-	expression tag	UNP H6QM90
F	-8	GLY	-	expression tag	UNP H6QM90
F	-7	SER	-	expression tag	UNP H6QM90
F	-6	GLY	-	expression tag	UNP H6QM90
F	-5	SER	-	expression tag	UNP H6QM90
F	-4	GLY	-	expression tag	UNP H6QM90
F	-3	SER	-	expression tag	UNP H6QM90
F	-2	GLY	-	expression tag	UNP H6QM90
F	-1	SER	-	expression tag	UNP H6QM90
F	0	GLY	-	expression tag	UNP H6QM90
F	761	GLY	-	expression tag	UNP H6QM90
F	762	TRP	-	expression tag	UNP H6QM90
F	763	SER	-	expression tag	UNP H6QM90
F	764	HIS	-	expression tag	UNP H6QM90
F	765	PRO	-	expression tag	UNP H6QM90
F	766	GLN	-	expression tag	UNP H6QM90
F	767	PHE	-	expression tag	UNP H6QM90
F	768	GLU	-	expression tag	UNP H6QM90
F	769	LYS	-	expression tag	UNP H6QM90
F	770	GLY	-	expression tag	UNP H6QM90
F	771	GLY	-	expression tag	UNP H6QM90
F	772	GLY	-	expression tag	UNP H6QM90
F	773	SER	-	expression tag	UNP H6QM90
F	774	GLY	-	expression tag	UNP H6QM90
F	775	GLY	-	expression tag	UNP H6QM90
F	776	GLY	-	expression tag	UNP H6QM90
F	777	SER	-	expression tag	UNP H6QM90
F	778	GLY	-	expression tag	UNP H6QM90
F	779	GLY	-	expression tag	UNP H6QM90
F	780	SER	-	expression tag	UNP H6QM90
F	781	ALA	-	expression tag	UNP H6QM90
F	782	TRP	-	expression tag	UNP H6QM90
F	783	SER	-	expression tag	UNP H6QM90
F	784	HIS	-	expression tag	UNP H6QM90
F	785	PRO	-	expression tag	UNP H6QM90
F	786	GLN	-	expression tag	UNP H6QM90

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	787	PHE	-	expression tag	UNP H6QM90
F	788	GLU	-	expression tag	UNP H6QM90
F	789	LYS	-	expression tag	UNP H6QM90
F	790	GLY	-	expression tag	UNP H6QM90
F	791	ARG	-	expression tag	UNP H6QM90
F	792	SER	-	expression tag	UNP H6QM90
F	793	GLY	-	expression tag	UNP H6QM90
F	794	GLY	-	expression tag	UNP H6QM90
F	795	GLU	-	expression tag	UNP H6QM90
F	796	ASN	-	expression tag	UNP H6QM90
F	797	LEU	-	expression tag	UNP H6QM90
F	798	TYR	-	expression tag	UNP H6QM90
F	799	PHE	-	expression tag	UNP H6QM90
F	800	GLN	-	expression tag	UNP H6QM90

- Molecule 4 is a RNA chain called RNA (5'-D(*(GDM))-R(P*AP*AP*U)-3').

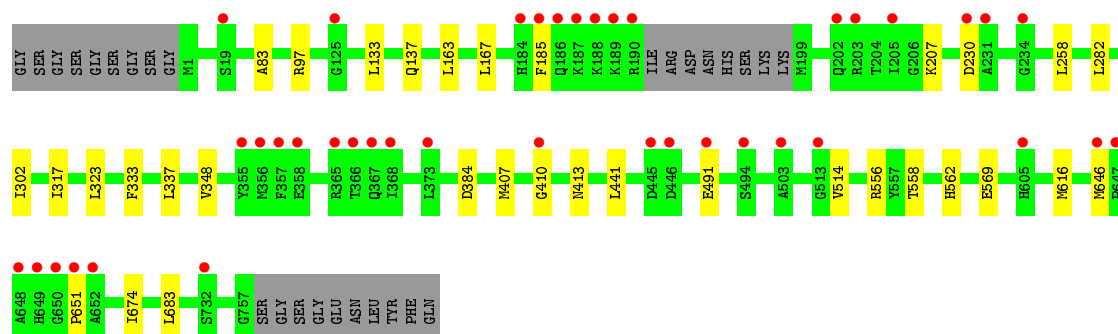
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	4	Total 93	C 40	N 17	O 31	P 5	0	0	0
4	M	4	Total 93	C 40	N 17	O 31	P 5	0	0	0

- Molecule 5 is a RNA chain called RNA (5'-R(*UP*AP*UP*AP*CP*CP*UP*CP*UP*GP*CP*UP*U)-3').

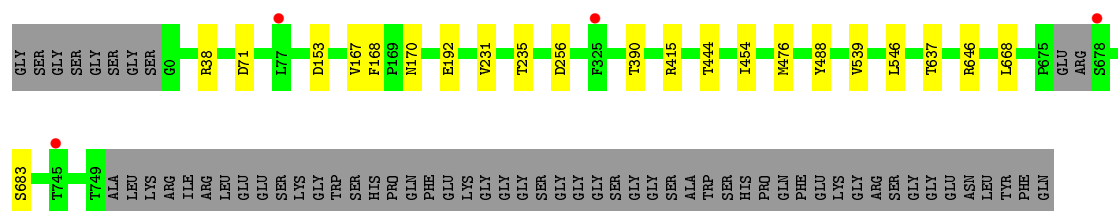
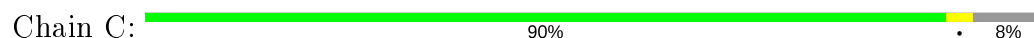
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	R	13	Total 246	C 111	N 37	O 86	P 12	0	0	0
5	S	13	Total 247	C 111	N 37	O 87	P 12	0	0	0

- Molecule 6 is a RNA chain called RNA (5'-R(P*AP*GP*UP*AP*GP*UP*AP*AP*CP*AP*AP*GP*AP*GP*G)-3').

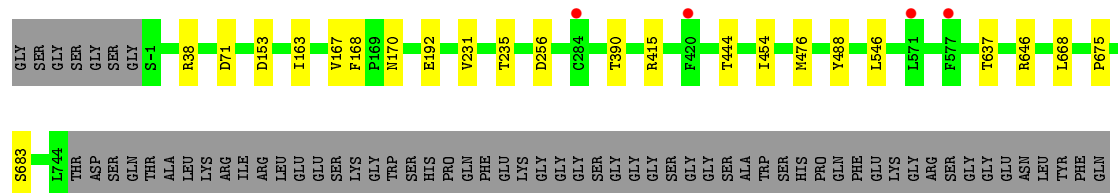
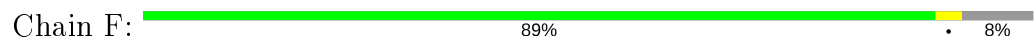
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	U	15	Total 330	C 147	N 67	O 101	P 15	0	0	0
6	V	15	Total 330	C 147	N 67	O 101	P 15	0	0	0



- Molecule 3: Polymerase basic protein 2



- Molecule 3: Polymerase basic protein 2



- Molecule 4: RNA (5'-D*(GDM))-R(P*AP*AP*U)-3')

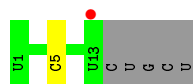


- Molecule 4: RNA (5'-D*(GDM))-R(P*AP*AP*U)-3')

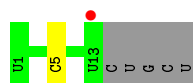


- Molecule 5: RNA (5'-R(*UP*AP*UP*AP*CP*CP*UP*CP*UP*GP*CP*UP*U)-3')





- Molecule 5: RNA (5'-R(*UP*AP*UP*AP*CP*CP*UP*CP*UP*GP*CP*UP*U)-3')



- Molecule 6: RNA (5'-R(P*AP*GP*UP*AP*GP*UP*AP*AP*CP*AP*AP*GP*AP*GP*G)-3')



- Molecule 6: RNA (5'-R(P*AP*GP*UP*AP*GP*UP*AP*AP*CP*AP*AP*GP*AP*GP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.46Å 286.17Å 171.93Å 90.00° 93.27° 90.00°	Depositor
Resolution (Å)	50.00 – 3.90 48.96 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-3.90) 99.8 (48.96-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.207 , 0.245 0.206 , 0.242	Depositor DCC
R_{free} test set	4018 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	158.6	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 124.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	36717	wwPDB-VP
Average B, all atoms (Å ²)	186.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 8NK

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	0.38	0/5897	0.52	0/7939
1	D	0.38	0/5891	0.52	0/7931
2	B	0.38	0/6115	0.55	0/8252
2	E	0.38	0/6088	0.55	0/8216
3	C	0.38	0/6038	0.55	0/8152
3	F	0.38	0/6028	0.55	0/8138
4	M	0.35	0/71	0.87	0/108
4	N	0.33	0/71	0.88	0/108
5	R	0.22	0/272	0.66	0/420
5	S	0.21	0/273	0.67	0/421
6	U	0.56	1/371 (0.3%)	0.65	0/576
6	V	0.56	1/371 (0.3%)	0.64	0/576
All	All	0.38	2/37486 (0.0%)	0.55	0/50837

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	1	A	OP3-P	-10.16	1.49	1.61
6	U	1	A	OP3-P	-10.12	1.49	1.61

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	5775	0	5690	7	0
1	D	5769	0	5692	7	0
2	B	5999	0	6011	10	0
2	E	5972	0	5983	10	0
3	C	5937	0	6053	6	0
3	F	5926	0	6047	7	0
4	M	93	0	33	0	0
4	N	93	0	33	0	0
5	R	246	0	125	0	0
5	S	247	0	128	0	0
6	U	330	0	164	1	0
6	V	330	0	164	0	0
All	All	36717	0	36123	45	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 (45) 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)
3:C:546:LEU:HD12	3:C:668:LEU:HD11	1.79	0.65
3:F:546:LEU:HD12	3:F:668:LEU:HD11	1.79	0.64
2:B:258:LEU:HD22	2:B:337:LEU:HD13	1.88	0.55
2:E:258:LEU:HD22	2:E:337:LEU:HD13	1.88	0.55
1:D:265:ILE:HG22	1:D:678:LEU:HD21	1.90	0.54
1:A:265:ILE:HG22	1:A:678:LEU:HD21	1.90	0.53
1:A:506:LEU:HD13	1:A:567:LYS:HG3	1.93	0.50
1:D:506:LEU:HD13	1:D:567:LYS:HG3	1.93	0.50
2:B:83:ALA:HB3	2:B:317:ILE:HD11	1.96	0.48
3:C:167:VAL:HG23	3:C:168:PHE:CD2	2.49	0.48
3:C:231:VAL:HG23	3:C:235:THR:HG23	1.96	0.48
2:E:83:ALA:HB3	2:E:317:ILE:HD11	1.96	0.48
3:F:231:VAL:HG23	3:F:235:THR:HG23	1.96	0.47
3:F:167:VAL:HG23	3:F:168:PHE:CD2	2.49	0.47
1:D:370:ALA:HB2	6:U:10:A:H3'	1.98	0.46
2:E:333:PHE:CZ	2:E:337:LEU:HD11	2.51	0.46
2:B:333:PHE:CZ	2:B:337:LEU:HD11	2.51	0.46
2:E:133:LEU:HD12	2:E:137:GLN:HE21	1.81	0.46
3:C:415:ARG:CG	3:C:444:THR:HG21	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:LEU:HD12	2:B:137:GLN:HE21	1.81	0.45
3:C:637:THR:HG22	3:C:646:ARG:HG2	1.98	0.45
2:B:83:ALA:CB	2:B:317:ILE:HD11	2.47	0.44
2:E:83:ALA:CB	2:E:317:ILE:HD11	2.47	0.44
1:A:230:LYS:HG3	2:B:323:LEU:HD22	1.98	0.44
3:F:415:ARG:CG	3:F:444:THR:HG21	2.47	0.44
1:D:230:LYS:HG3	2:E:323:LEU:HD22	2.00	0.44
3:F:637:THR:HG22	3:F:646:ARG:HG2	1.99	0.43
2:E:674:ILE:HG23	2:E:683:LEU:HD11	2.01	0.43
2:B:674:ILE:HG23	2:B:683:LEU:HD11	2.01	0.42
1:A:506:LEU:HD13	1:A:567:LYS:CG	2.49	0.42
2:B:282:LEU:HG	2:B:441:LEU:HD22	2.01	0.42
1:A:610:ARG:HD2	1:A:627:THR:HG21	2.01	0.42
2:B:514:VAL:HG11	2:B:558:THR:HG21	2.02	0.42
2:B:556:ARG:HD3	2:B:562:HIS:HA	2.02	0.42
1:D:610:ARG:HD2	1:D:627:THR:HG21	2.02	0.42
2:E:514:VAL:HG11	2:E:558:THR:HG21	2.02	0.42
1:D:506:LEU:HD13	1:D:567:LYS:CG	2.50	0.41
2:E:282:LEU:HG	2:E:441:LEU:HD22	2.02	0.41
3:C:415:ARG:HG3	3:C:444:THR:HG21	2.03	0.41
1:D:610:ARG:HG3	1:D:627:THR:HG21	2.03	0.41
2:E:556:ARG:HD3	2:E:562:HIS:HA	2.02	0.40
3:F:163:ILE:O	3:F:167:VAL:HG22	2.21	0.40
1:A:610:ARG:HG3	1:A:627:THR:HG21	2.03	0.40
3:F:415:ARG:HG3	3:F:444:THR:HG21	2.03	0.40
1:A:506:LEU:HD11	1:A:513:VAL:CG2	2.51	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	703/738 (95%)	677 (96%)	23 (3%)	3 (0%)	34	71
1	D	702/738 (95%)	675 (96%)	25 (4%)	2 (0%)	41	75
2	B	748/776 (96%)	710 (95%)	35 (5%)	3 (0%)	34	71
2	E	745/776 (96%)	706 (95%)	36 (5%)	3 (0%)	34	71
3	C	744/809 (92%)	701 (94%)	39 (5%)	4 (0%)	29	67
3	F	744/809 (92%)	703 (94%)	36 (5%)	5 (1%)	22	60
All	All	4386/4646 (94%)	4172 (95%)	194 (4%)	20 (0%)	29	67

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	413	ASN
3	C	683	SER
2	E	413	ASN
3	F	675	PRO
2	B	410	GLY
3	C	153	ASP
3	C	488	TYR
2	E	410	GLY
3	F	153	ASP
3	F	488	TYR
3	F	683	SER
2	B	651	PRO
3	C	476	MET
2	E	651	PRO
3	F	476	MET
1	A	389	LYS
1	D	389	LYS
1	A	670	ASN
1	D	299	GLY
1	A	299	GLY

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	633/657 (96%)	625 (99%)	8 (1%)	69	82
1	D	633/657 (96%)	627 (99%)	6 (1%)	78	87
2	B	659/676 (98%)	646 (98%)	13 (2%)	55	74
2	E	656/676 (97%)	642 (98%)	14 (2%)	53	73
3	C	663/706 (94%)	655 (99%)	8 (1%)	71	83
3	F	661/706 (94%)	654 (99%)	7 (1%)	73	84
All	All	3905/4078 (96%)	3849 (99%)	56 (1%)	67	81

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	29	GLN
1	A	55	ASP
1	A	219	LEU
1	A	375	ASP
1	A	507	ARG
1	A	551	THR
1	A	561	ARG
2	B	97	ARG
2	B	163	LEU
2	B	167	LEU
2	B	185	PHE
2	B	230	ASP
2	B	302	ILE
2	B	348	VAL
2	B	384	ASP
2	B	407	MET
2	B	491	GLU
2	B	569	GLU
2	B	616	MET
2	B	646	MET
3	C	38	ARG
3	C	71	ASP
3	C	170	ASN
3	C	192	GLU
3	C	256	ASP
3	C	390	THR
3	C	454	ILE
3	C	539	VAL
1	D	29	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	219	LEU
1	D	375	ASP
1	D	507	ARG
1	D	551	THR
1	D	561	ARG
2	E	97	ARG
2	E	163	LEU
2	E	167	LEU
2	E	185	PHE
2	E	207	LYS
2	E	230	ASP
2	E	302	ILE
2	E	348	VAL
2	E	384	ASP
2	E	407	MET
2	E	491	GLU
2	E	569	GLU
2	E	616	MET
2	E	646	MET
3	F	38	ARG
3	F	71	ASP
3	F	170	ASN
3	F	192	GLU
3	F	256	ASP
3	F	390	THR
3	F	454	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	142	ASN
2	B	137	GLN
2	B	346	ASN
2	B	460	GLN
2	B	464	ASN
2	B	485	ASN
2	B	537	ASN
3	C	13	ASN
3	C	482	GLN
3	C	530	ASN
3	C	532	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	632	GLN
1	D	10	ASN
1	D	142	ASN
1	D	387	GLN
2	E	137	GLN
2	E	346	ASN
2	E	428	GLN
2	E	460	GLN
2	E	464	ASN
2	E	485	ASN
3	F	13	ASN
3	F	482	GLN
3	F	530	ASN
3	F	532	ASN
3	F	632	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	M	3/13 (23%)	2 (66%)	1 (33%)
4	N	3/13 (23%)	2 (66%)	1 (33%)
5	R	11/18 (61%)	1 (9%)	0
5	S	11/18 (61%)	1 (9%)	0
6	U	14/16 (87%)	3 (21%)	1 (7%)
6	V	14/16 (87%)	5 (35%)	1 (7%)
All	All	56/94 (59%)	14 (25%)	4 (7%)

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	N	2	A
4	N	3	U
5	R	5	C
5	S	5	C
4	M	2	A
4	M	3	U
6	U	7	A
6	U	11	A
6	U	15	G
6	V	6	U
6	V	7	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	V	8	A
6	V	11	A
6	V	15	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	N	1	A
4	M	1	A
6	U	5	G
6	V	5	G

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, 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	709/738 (96%)	0.00	15 (2%) 63 53	138, 185, 225, 263	0
1	D	708/738 (95%)	-0.00	14 (1%) 65 55	155, 192, 230, 291	0
2	B	752/776 (96%)	0.12	28 (3%) 41 32	123, 174, 223, 264	0
2	E	749/776 (96%)	0.17	40 (5%) 26 22	139, 178, 227, 273	0
3	C	748/809 (92%)	-0.11	4 (0%) 91 85	145, 184, 221, 255	0
3	F	746/809 (92%)	-0.15	4 (0%) 91 85	138, 184, 222, 249	0
4	M	3/13 (23%)	2.79	2 (66%) 0 0	232, 232, 259, 281	0
4	N	3/13 (23%)	2.49	2 (66%) 0 0	219, 219, 262, 272	0
5	R	13/18 (72%)	-0.03	1 (7%) 13 10	164, 184, 216, 220	0
5	S	13/18 (72%)	0.31	1 (7%) 13 10	179, 195, 220, 232	0
6	U	15/16 (93%)	-0.15	0 100 100	175, 188, 208, 215	0
6	V	15/16 (93%)	-0.04	0 100 100	165, 175, 190, 192	0
All	All	4474/4740 (94%)	0.01	111 (2%) 57 47	123, 183, 225, 291	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	650	GLY	9.4
2	B	650	GLY	7.1
2	E	651	PRO	6.5
2	B	651	PRO	5.4
2	E	190	ARG	5.1
2	E	647	PRO	4.9
2	E	186	GLN	4.8
5	S	13	U	4.7
2	E	203	ARG	4.6
2	E	652	ALA	4.4
2	B	358	GLU	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	188	LYS	4.3
2	E	368	ILE	4.3
2	B	649	HIS	4.0
2	B	186	GLN	3.9
3	C	678	SER	3.9
2	E	367	GLN	3.8
2	E	184	HIS	3.7
1	A	374	MET	3.6
4	M	2	A	3.5
2	E	185	PHE	3.4
2	B	199	MET	3.4
2	B	652	ALA	3.4
2	B	647	PRO	3.3
4	M	3	U	3.2
2	E	355	TYR	3.2
2	E	365	ARG	3.2
2	E	187	LYS	3.2
2	B	357	PHE	3.2
4	N	3	U	3.1
4	N	2	A	3.0
2	B	190	ARG	3.0
2	E	202	GLN	3.0
2	B	410	GLY	2.9
3	C	745	THR	2.9
2	E	356	MET	2.9
2	B	445	ASP	2.9
1	A	146	HIS	2.9
1	A	66	ASP	2.9
1	D	388	TYR	2.9
2	B	188	LYS	2.9
1	A	48	TYR	2.9
5	R	13	U	2.9
2	E	230	ASP	2.8
2	E	648	ALA	2.8
2	E	649	HIS	2.8
1	A	9	PHE	2.8
2	E	646	MET	2.8
2	E	503	ALA	2.8
2	B	646	MET	2.8
1	D	376	PHE	2.7
2	E	19	SER	2.7
2	B	202	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	605	HIS	2.6
2	E	373	LEU	2.6
1	D	150	PHE	2.6
1	A	39	SER	2.6
2	E	446	ASP	2.6
1	D	112	TYR	2.5
1	D	374	MET	2.5
2	E	445	ASP	2.5
2	E	513	GLY	2.5
2	B	365	ARG	2.5
1	A	144	TYR	2.5
2	E	491	GLU	2.4
2	E	357	PHE	2.4
1	A	514	ASN	2.4
2	B	648	ALA	2.4
2	B	663	THR	2.4
2	E	494	SER	2.4
2	B	185	PHE	2.4
2	E	358	GLU	2.4
3	C	325	PHE	2.4
2	B	513	GLY	2.3
1	D	514	ASN	2.3
1	A	334	TYR	2.3
2	E	366	THR	2.3
1	D	48	TYR	2.3
1	D	146	HIS	2.3
2	E	732	SER	2.3
2	E	410	GLY	2.3
3	F	420	PHE	2.3
2	E	205	ILE	2.3
3	F	571	LEU	2.3
2	B	201	THR	2.3
2	B	444	SER	2.2
2	B	364	LEU	2.2
1	A	35	PHE	2.2
2	E	231	ALA	2.2
3	F	577	PHE	2.2
2	E	189	LYS	2.2
1	D	373	LYS	2.2
2	B	359	SER	2.2
1	D	148	PHE	2.2
2	B	184	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	376	PHE	2.2
3	F	284	CYS	2.2
1	D	77	GLU	2.1
2	B	200	ILE	2.1
1	D	696	LEU	2.1
1	A	76	PHE	2.1
2	B	230	ASP	2.1
2	B	203	ARG	2.1
1	A	150	PHE	2.1
2	E	125	GLY	2.1
3	C	77	LEU	2.1
1	A	75	ARG	2.1
1	A	536	CYS	2.0
2	E	234	GLY	2.0
1	D	276	CYS	2.0
1	D	365	LEU	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.