



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:18 PM UTC

PDB ID : 5EPI / pdb_00005epi
Title : CRYSTAL STRUCTURE OF INFLUENZA B POLYMERASE WITH
BOUND 5' CRNA EXHIBITS A NOVEL DOMAIN ARRANGEMENT
Authors : Guilligay, D.; Cusack, S.
Deposited on : 2015-11-11
Resolution : 4.10 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:

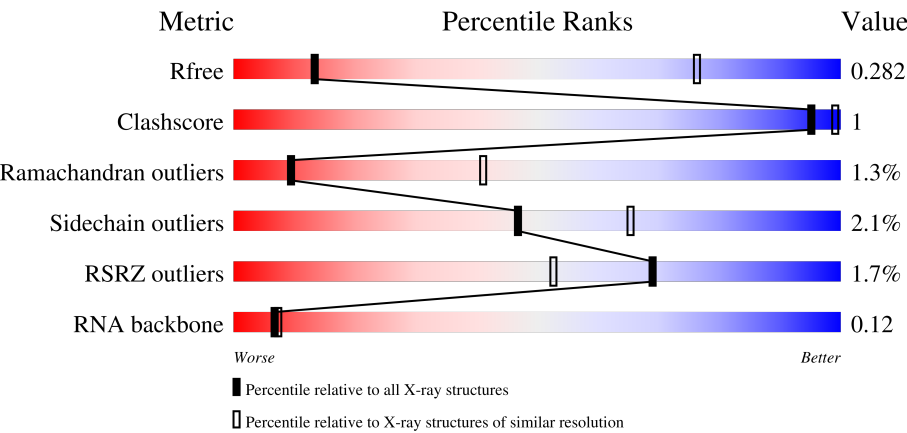
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.10 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.



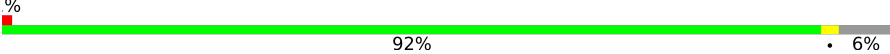
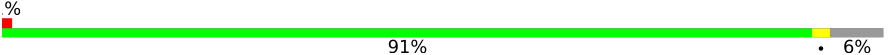
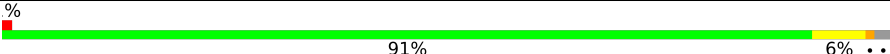
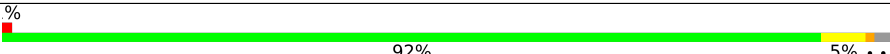
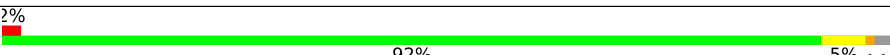
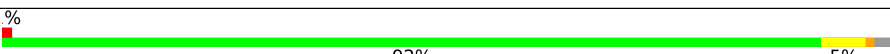
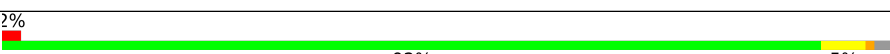
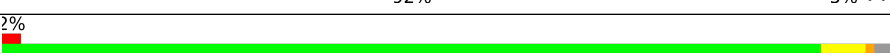
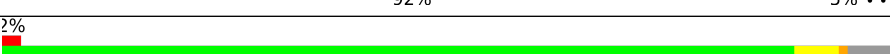
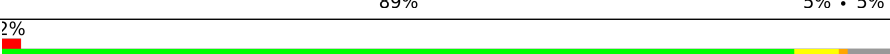
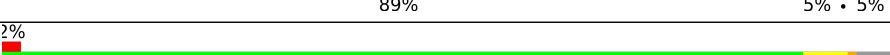
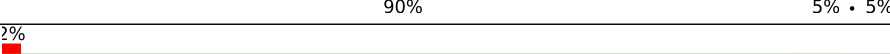
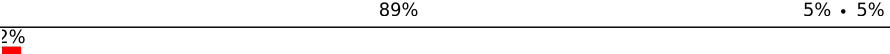
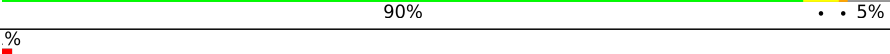
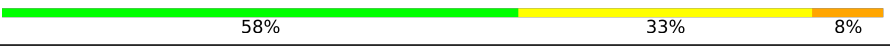
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)
RNA backbone	3983	1026 (5.04-3.10)

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	751	2% 91% 6%
1	E	751	2% 91% 6%
1	I	751	2% 91% 6%
1	M	751	% 92% 6%

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Mol	Chain	Length	Quality of chain
1	Q	751	 92% • 6%
1	U	751	 91% • 6%
2	B	772	 91% 6% ••
2	F	772	 92% 5% ••
2	J	772	 92% 5% ••
2	N	772	 92% 5% ••
2	R	772	 92% 5% ••
2	V	772	 92% 5% ••
3	C	798	 89% 5% • 5%
3	G	798	 89% 5% • 5%
3	K	798	 90% 5% • 5%
3	O	798	 89% 5% • 5%
3	S	798	 90% • • 5%
3	W	798	 71% 5% • 23%
4	D	12	 58% 42%
4	H	12	 58% 33% 8%
4	L	12	 50% 42% 8%
4	P	12	 58% 33% 8%
4	T	12	 58% 33% 8%
4	X	12	 50% 42% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 106314 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	703	Total	C	N	O	S	0	0	0
			5646	3590	946	1070	40			
1	E	703	Total	C	N	O	S	0	0	0
			5646	3590	946	1070	40			
1	I	708	Total	C	N	O	S	0	0	0
			5685	3613	951	1080	41			
1	M	703	Total	C	N	O	S	0	0	0
			5646	3590	946	1070	40			
1	Q	703	Total	C	N	O	S	0	0	0
			5646	3590	946	1070	40			
1	U	703	Total	C	N	O	S	0	0	0
			5646	3590	946	1070	40			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	GLY	-	expression tag	UNP Q5V8Z9
A	-12	SER	-	expression tag	UNP Q5V8Z9
A	-11	HIS	-	expression tag	UNP Q5V8Z9
A	-10	HIS	-	expression tag	UNP Q5V8Z9
A	-9	HIS	-	expression tag	UNP Q5V8Z9
A	-8	HIS	-	expression tag	UNP Q5V8Z9
A	-7	HIS	-	expression tag	UNP Q5V8Z9
A	-6	HIS	-	expression tag	UNP Q5V8Z9
A	-5	HIS	-	expression tag	UNP Q5V8Z9
A	-4	HIS	-	expression tag	UNP Q5V8Z9
A	-3	GLY	-	expression tag	UNP Q5V8Z9
A	-2	SER	-	expression tag	UNP Q5V8Z9
A	-1	GLY	-	expression tag	UNP Q5V8Z9
A	0	SER	-	expression tag	UNP Q5V8Z9
A	727	GLY	-	expression tag	UNP Q5V8Z9
A	728	SER	-	expression tag	UNP Q5V8Z9
A	729	GLY	-	expression tag	UNP Q5V8Z9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	730	SER	-	expression tag	UNP Q5V8Z9
A	731	GLY	-	expression tag	UNP Q5V8Z9
A	732	GLU	-	expression tag	UNP Q5V8Z9
A	733	ASN	-	expression tag	UNP Q5V8Z9
A	734	LEU	-	expression tag	UNP Q5V8Z9
A	735	TYR	-	expression tag	UNP Q5V8Z9
A	736	PHE	-	expression tag	UNP Q5V8Z9
A	737	GLN	-	expression tag	UNP Q5V8Z9
E	-13	GLY	-	expression tag	UNP Q5V8Z9
E	-12	SER	-	expression tag	UNP Q5V8Z9
E	-11	HIS	-	expression tag	UNP Q5V8Z9
E	-10	HIS	-	expression tag	UNP Q5V8Z9
E	-9	HIS	-	expression tag	UNP Q5V8Z9
E	-8	HIS	-	expression tag	UNP Q5V8Z9
E	-7	HIS	-	expression tag	UNP Q5V8Z9
E	-6	HIS	-	expression tag	UNP Q5V8Z9
E	-5	HIS	-	expression tag	UNP Q5V8Z9
E	-4	HIS	-	expression tag	UNP Q5V8Z9
E	-3	GLY	-	expression tag	UNP Q5V8Z9
E	-2	SER	-	expression tag	UNP Q5V8Z9
E	-1	GLY	-	expression tag	UNP Q5V8Z9
E	0	SER	-	expression tag	UNP Q5V8Z9
E	727	GLY	-	expression tag	UNP Q5V8Z9
E	728	SER	-	expression tag	UNP Q5V8Z9
E	729	GLY	-	expression tag	UNP Q5V8Z9
E	730	SER	-	expression tag	UNP Q5V8Z9
E	731	GLY	-	expression tag	UNP Q5V8Z9
E	732	GLU	-	expression tag	UNP Q5V8Z9
E	733	ASN	-	expression tag	UNP Q5V8Z9
E	734	LEU	-	expression tag	UNP Q5V8Z9
E	735	TYR	-	expression tag	UNP Q5V8Z9
E	736	PHE	-	expression tag	UNP Q5V8Z9
E	737	GLN	-	expression tag	UNP Q5V8Z9
I	-13	GLY	-	expression tag	UNP Q5V8Z9
I	-12	SER	-	expression tag	UNP Q5V8Z9
I	-11	HIS	-	expression tag	UNP Q5V8Z9
I	-10	HIS	-	expression tag	UNP Q5V8Z9
I	-9	HIS	-	expression tag	UNP Q5V8Z9
I	-8	HIS	-	expression tag	UNP Q5V8Z9
I	-7	HIS	-	expression tag	UNP Q5V8Z9
I	-6	HIS	-	expression tag	UNP Q5V8Z9
I	-5	HIS	-	expression tag	UNP Q5V8Z9

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-4	HIS	-	expression tag	UNP Q5V8Z9
I	-3	GLY	-	expression tag	UNP Q5V8Z9
I	-2	SER	-	expression tag	UNP Q5V8Z9
I	-1	GLY	-	expression tag	UNP Q5V8Z9
I	0	SER	-	expression tag	UNP Q5V8Z9
I	727	GLY	-	expression tag	UNP Q5V8Z9
I	728	SER	-	expression tag	UNP Q5V8Z9
I	729	GLY	-	expression tag	UNP Q5V8Z9
I	730	SER	-	expression tag	UNP Q5V8Z9
I	731	GLY	-	expression tag	UNP Q5V8Z9
I	732	GLU	-	expression tag	UNP Q5V8Z9
I	733	ASN	-	expression tag	UNP Q5V8Z9
I	734	LEU	-	expression tag	UNP Q5V8Z9
I	735	TYR	-	expression tag	UNP Q5V8Z9
I	736	PHE	-	expression tag	UNP Q5V8Z9
I	737	GLN	-	expression tag	UNP Q5V8Z9
M	-13	GLY	-	expression tag	UNP Q5V8Z9
M	-12	SER	-	expression tag	UNP Q5V8Z9
M	-11	HIS	-	expression tag	UNP Q5V8Z9
M	-10	HIS	-	expression tag	UNP Q5V8Z9
M	-9	HIS	-	expression tag	UNP Q5V8Z9
M	-8	HIS	-	expression tag	UNP Q5V8Z9
M	-7	HIS	-	expression tag	UNP Q5V8Z9
M	-6	HIS	-	expression tag	UNP Q5V8Z9
M	-5	HIS	-	expression tag	UNP Q5V8Z9
M	-4	HIS	-	expression tag	UNP Q5V8Z9
M	-3	GLY	-	expression tag	UNP Q5V8Z9
M	-2	SER	-	expression tag	UNP Q5V8Z9
M	-1	GLY	-	expression tag	UNP Q5V8Z9
M	0	SER	-	expression tag	UNP Q5V8Z9
M	727	GLY	-	expression tag	UNP Q5V8Z9
M	728	SER	-	expression tag	UNP Q5V8Z9
M	729	GLY	-	expression tag	UNP Q5V8Z9
M	730	SER	-	expression tag	UNP Q5V8Z9
M	731	GLY	-	expression tag	UNP Q5V8Z9
M	732	GLU	-	expression tag	UNP Q5V8Z9
M	733	ASN	-	expression tag	UNP Q5V8Z9
M	734	LEU	-	expression tag	UNP Q5V8Z9
M	735	TYR	-	expression tag	UNP Q5V8Z9
M	736	PHE	-	expression tag	UNP Q5V8Z9
M	737	GLN	-	expression tag	UNP Q5V8Z9
Q	-13	GLY	-	expression tag	UNP Q5V8Z9

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-12	SER	-	expression tag	UNP Q5V8Z9
Q	-11	HIS	-	expression tag	UNP Q5V8Z9
Q	-10	HIS	-	expression tag	UNP Q5V8Z9
Q	-9	HIS	-	expression tag	UNP Q5V8Z9
Q	-8	HIS	-	expression tag	UNP Q5V8Z9
Q	-7	HIS	-	expression tag	UNP Q5V8Z9
Q	-6	HIS	-	expression tag	UNP Q5V8Z9
Q	-5	HIS	-	expression tag	UNP Q5V8Z9
Q	-4	HIS	-	expression tag	UNP Q5V8Z9
Q	-3	GLY	-	expression tag	UNP Q5V8Z9
Q	-2	SER	-	expression tag	UNP Q5V8Z9
Q	-1	GLY	-	expression tag	UNP Q5V8Z9
Q	0	SER	-	expression tag	UNP Q5V8Z9
Q	727	GLY	-	expression tag	UNP Q5V8Z9
Q	728	SER	-	expression tag	UNP Q5V8Z9
Q	729	GLY	-	expression tag	UNP Q5V8Z9
Q	730	SER	-	expression tag	UNP Q5V8Z9
Q	731	GLY	-	expression tag	UNP Q5V8Z9
Q	732	GLU	-	expression tag	UNP Q5V8Z9
Q	733	ASN	-	expression tag	UNP Q5V8Z9
Q	734	LEU	-	expression tag	UNP Q5V8Z9
Q	735	TYR	-	expression tag	UNP Q5V8Z9
Q	736	PHE	-	expression tag	UNP Q5V8Z9
Q	737	GLN	-	expression tag	UNP Q5V8Z9
U	-13	GLY	-	expression tag	UNP Q5V8Z9
U	-12	SER	-	expression tag	UNP Q5V8Z9
U	-11	HIS	-	expression tag	UNP Q5V8Z9
U	-10	HIS	-	expression tag	UNP Q5V8Z9
U	-9	HIS	-	expression tag	UNP Q5V8Z9
U	-8	HIS	-	expression tag	UNP Q5V8Z9
U	-7	HIS	-	expression tag	UNP Q5V8Z9
U	-6	HIS	-	expression tag	UNP Q5V8Z9
U	-5	HIS	-	expression tag	UNP Q5V8Z9
U	-4	HIS	-	expression tag	UNP Q5V8Z9
U	-3	GLY	-	expression tag	UNP Q5V8Z9
U	-2	SER	-	expression tag	UNP Q5V8Z9
U	-1	GLY	-	expression tag	UNP Q5V8Z9
U	0	SER	-	expression tag	UNP Q5V8Z9
U	727	GLY	-	expression tag	UNP Q5V8Z9
U	728	SER	-	expression tag	UNP Q5V8Z9
U	729	GLY	-	expression tag	UNP Q5V8Z9
U	730	SER	-	expression tag	UNP Q5V8Z9

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Chain	Residue	Modelled	Actual	Comment	Reference
U	731	GLY	-	expression tag	UNP Q5V8Z9
U	732	GLU	-	expression tag	UNP Q5V8Z9
U	733	ASN	-	expression tag	UNP Q5V8Z9
U	734	LEU	-	expression tag	UNP Q5V8Z9
U	735	TYR	-	expression tag	UNP Q5V8Z9
U	736	PHE	-	expression tag	UNP Q5V8Z9
U	737	GLN	-	expression tag	UNP Q5V8Z9

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	756	Total	C	N	O	S	0	0	0
			5927	3741	1022	1112	52			
2	F	756	Total	C	N	O	S	0	0	0
			5927	3741	1022	1112	52			
2	J	756	Total	C	N	O	S	0	0	0
			5927	3741	1022	1112	52			
2	N	756	Total	C	N	O	S	0	0	0
			5927	3741	1022	1112	52			
2	R	756	Total	C	N	O	S	0	0	0
			5927	3741	1022	1112	52			
2	V	756	Total	C	N	O	S	0	0	0
			5927	3741	1022	1112	52			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP Q5V8Y6
B	-7	SER	-	expression tag	UNP Q5V8Y6
B	-6	GLY	-	expression tag	UNP Q5V8Y6
B	-5	SER	-	expression tag	UNP Q5V8Y6
B	-4	GLY	-	expression tag	UNP Q5V8Y6
B	-3	SER	-	expression tag	UNP Q5V8Y6
B	-2	GLY	-	expression tag	UNP Q5V8Y6
B	-1	SER	-	expression tag	UNP Q5V8Y6
B	0	GLY	-	expression tag	UNP Q5V8Y6
B	753	GLY	-	expression tag	UNP Q5V8Y6
B	754	SER	-	expression tag	UNP Q5V8Y6
B	755	GLY	-	expression tag	UNP Q5V8Y6
B	756	SER	-	expression tag	UNP Q5V8Y6
B	757	GLY	-	expression tag	UNP Q5V8Y6
B	758	GLU	-	expression tag	UNP Q5V8Y6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	759	ASN	-	expression tag	UNP Q5V8Y6
B	760	LEU	-	expression tag	UNP Q5V8Y6
B	761	TYR	-	expression tag	UNP Q5V8Y6
B	762	PHE	-	expression tag	UNP Q5V8Y6
B	763	GLN	-	expression tag	UNP Q5V8Y6
F	-8	GLY	-	expression tag	UNP Q5V8Y6
F	-7	SER	-	expression tag	UNP Q5V8Y6
F	-6	GLY	-	expression tag	UNP Q5V8Y6
F	-5	SER	-	expression tag	UNP Q5V8Y6
F	-4	GLY	-	expression tag	UNP Q5V8Y6
F	-3	SER	-	expression tag	UNP Q5V8Y6
F	-2	GLY	-	expression tag	UNP Q5V8Y6
F	-1	SER	-	expression tag	UNP Q5V8Y6
F	0	GLY	-	expression tag	UNP Q5V8Y6
F	753	GLY	-	expression tag	UNP Q5V8Y6
F	754	SER	-	expression tag	UNP Q5V8Y6
F	755	GLY	-	expression tag	UNP Q5V8Y6
F	756	SER	-	expression tag	UNP Q5V8Y6
F	757	GLY	-	expression tag	UNP Q5V8Y6
F	758	GLU	-	expression tag	UNP Q5V8Y6
F	759	ASN	-	expression tag	UNP Q5V8Y6
F	760	LEU	-	expression tag	UNP Q5V8Y6
F	761	TYR	-	expression tag	UNP Q5V8Y6
F	762	PHE	-	expression tag	UNP Q5V8Y6
F	763	GLN	-	expression tag	UNP Q5V8Y6
J	-8	GLY	-	expression tag	UNP Q5V8Y6
J	-7	SER	-	expression tag	UNP Q5V8Y6
J	-6	GLY	-	expression tag	UNP Q5V8Y6
J	-5	SER	-	expression tag	UNP Q5V8Y6
J	-4	GLY	-	expression tag	UNP Q5V8Y6
J	-3	SER	-	expression tag	UNP Q5V8Y6
J	-2	GLY	-	expression tag	UNP Q5V8Y6
J	-1	SER	-	expression tag	UNP Q5V8Y6
J	0	GLY	-	expression tag	UNP Q5V8Y6
J	753	GLY	-	expression tag	UNP Q5V8Y6
J	754	SER	-	expression tag	UNP Q5V8Y6
J	755	GLY	-	expression tag	UNP Q5V8Y6
J	756	SER	-	expression tag	UNP Q5V8Y6
J	757	GLY	-	expression tag	UNP Q5V8Y6
J	758	GLU	-	expression tag	UNP Q5V8Y6
J	759	ASN	-	expression tag	UNP Q5V8Y6
J	760	LEU	-	expression tag	UNP Q5V8Y6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	761	TYR	-	expression tag	UNP Q5V8Y6
J	762	PHE	-	expression tag	UNP Q5V8Y6
J	763	GLN	-	expression tag	UNP Q5V8Y6
N	-8	GLY	-	expression tag	UNP Q5V8Y6
N	-7	SER	-	expression tag	UNP Q5V8Y6
N	-6	GLY	-	expression tag	UNP Q5V8Y6
N	-5	SER	-	expression tag	UNP Q5V8Y6
N	-4	GLY	-	expression tag	UNP Q5V8Y6
N	-3	SER	-	expression tag	UNP Q5V8Y6
N	-2	GLY	-	expression tag	UNP Q5V8Y6
N	-1	SER	-	expression tag	UNP Q5V8Y6
N	0	GLY	-	expression tag	UNP Q5V8Y6
N	753	GLY	-	expression tag	UNP Q5V8Y6
N	754	SER	-	expression tag	UNP Q5V8Y6
N	755	GLY	-	expression tag	UNP Q5V8Y6
N	756	SER	-	expression tag	UNP Q5V8Y6
N	757	GLY	-	expression tag	UNP Q5V8Y6
N	758	GLU	-	expression tag	UNP Q5V8Y6
N	759	ASN	-	expression tag	UNP Q5V8Y6
N	760	LEU	-	expression tag	UNP Q5V8Y6
N	761	TYR	-	expression tag	UNP Q5V8Y6
N	762	PHE	-	expression tag	UNP Q5V8Y6
N	763	GLN	-	expression tag	UNP Q5V8Y6
R	-8	GLY	-	expression tag	UNP Q5V8Y6
R	-7	SER	-	expression tag	UNP Q5V8Y6
R	-6	GLY	-	expression tag	UNP Q5V8Y6
R	-5	SER	-	expression tag	UNP Q5V8Y6
R	-4	GLY	-	expression tag	UNP Q5V8Y6
R	-3	SER	-	expression tag	UNP Q5V8Y6
R	-2	GLY	-	expression tag	UNP Q5V8Y6
R	-1	SER	-	expression tag	UNP Q5V8Y6
R	0	GLY	-	expression tag	UNP Q5V8Y6
R	753	GLY	-	expression tag	UNP Q5V8Y6
R	754	SER	-	expression tag	UNP Q5V8Y6
R	755	GLY	-	expression tag	UNP Q5V8Y6
R	756	SER	-	expression tag	UNP Q5V8Y6
R	757	GLY	-	expression tag	UNP Q5V8Y6
R	758	GLU	-	expression tag	UNP Q5V8Y6
R	759	ASN	-	expression tag	UNP Q5V8Y6
R	760	LEU	-	expression tag	UNP Q5V8Y6
R	761	TYR	-	expression tag	UNP Q5V8Y6
R	762	PHE	-	expression tag	UNP Q5V8Y6

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Chain	Residue	Modelled	Actual	Comment	Reference
R	763	GLN	-	expression tag	UNP Q5V8Y6
V	-8	GLY	-	expression tag	UNP Q5V8Y6
V	-7	SER	-	expression tag	UNP Q5V8Y6
V	-6	GLY	-	expression tag	UNP Q5V8Y6
V	-5	SER	-	expression tag	UNP Q5V8Y6
V	-4	GLY	-	expression tag	UNP Q5V8Y6
V	-3	SER	-	expression tag	UNP Q5V8Y6
V	-2	GLY	-	expression tag	UNP Q5V8Y6
V	-1	SER	-	expression tag	UNP Q5V8Y6
V	0	GLY	-	expression tag	UNP Q5V8Y6
V	753	GLY	-	expression tag	UNP Q5V8Y6
V	754	SER	-	expression tag	UNP Q5V8Y6
V	755	GLY	-	expression tag	UNP Q5V8Y6
V	756	SER	-	expression tag	UNP Q5V8Y6
V	757	GLY	-	expression tag	UNP Q5V8Y6
V	758	GLU	-	expression tag	UNP Q5V8Y6
V	759	ASN	-	expression tag	UNP Q5V8Y6
V	760	LEU	-	expression tag	UNP Q5V8Y6
V	761	TYR	-	expression tag	UNP Q5V8Y6
V	762	PHE	-	expression tag	UNP Q5V8Y6
V	763	GLN	-	expression tag	UNP Q5V8Y6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	761	Total	C	N	O	S	0	0	0
			6078	3863	1063	1111	41			
3	G	759	Total	C	N	O	S	0	0	0
			6061	3852	1059	1109	41			
3	K	759	Total	C	N	O	S	0	0	0
			6061	3852	1059	1109	41			
3	O	759	Total	C	N	O	S	0	0	0
			6061	3852	1059	1109	41			
3	S	759	Total	C	N	O	S	0	0	0
			6061	3852	1059	1109	41			
3	W	618	Total	C	N	O	S	0	0	0
			4925	3115	872	906	32			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLY	-	expression tag	UNP Q5V8X3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	SER	-	expression tag	UNP Q5V8X3
C	-6	GLY	-	expression tag	UNP Q5V8X3
C	-5	SER	-	expression tag	UNP Q5V8X3
C	-4	GLY	-	expression tag	UNP Q5V8X3
C	-3	SER	-	expression tag	UNP Q5V8X3
C	-2	GLY	-	expression tag	UNP Q5V8X3
C	-1	SER	-	expression tag	UNP Q5V8X3
C	0	ALA	-	expression tag	UNP Q5V8X3
C	771	GLY	-	expression tag	UNP Q5V8X3
C	772	TRP	-	expression tag	UNP Q5V8X3
C	773	SER	-	expression tag	UNP Q5V8X3
C	774	HIS	-	expression tag	UNP Q5V8X3
C	775	PRO	-	expression tag	UNP Q5V8X3
C	776	GLN	-	expression tag	UNP Q5V8X3
C	777	PHE	-	expression tag	UNP Q5V8X3
C	778	GLU	-	expression tag	UNP Q5V8X3
C	779	LYS	-	expression tag	UNP Q5V8X3
C	780	GLY	-	expression tag	UNP Q5V8X3
C	781	SER	-	expression tag	UNP Q5V8X3
C	782	GLY	-	expression tag	UNP Q5V8X3
C	783	SER	-	expression tag	UNP Q5V8X3
C	784	GLU	-	expression tag	UNP Q5V8X3
C	785	ASN	-	expression tag	UNP Q5V8X3
C	786	LEU	-	expression tag	UNP Q5V8X3
C	787	TYR	-	expression tag	UNP Q5V8X3
C	788	PHE	-	expression tag	UNP Q5V8X3
C	789	GLN	-	expression tag	UNP Q5V8X3
G	-8	GLY	-	expression tag	UNP Q5V8X3
G	-7	SER	-	expression tag	UNP Q5V8X3
G	-6	GLY	-	expression tag	UNP Q5V8X3
G	-5	SER	-	expression tag	UNP Q5V8X3
G	-4	GLY	-	expression tag	UNP Q5V8X3
G	-3	SER	-	expression tag	UNP Q5V8X3
G	-2	GLY	-	expression tag	UNP Q5V8X3
G	-1	SER	-	expression tag	UNP Q5V8X3
G	0	ALA	-	expression tag	UNP Q5V8X3
G	771	GLY	-	expression tag	UNP Q5V8X3
G	772	TRP	-	expression tag	UNP Q5V8X3
G	773	SER	-	expression tag	UNP Q5V8X3
G	774	HIS	-	expression tag	UNP Q5V8X3
G	775	PRO	-	expression tag	UNP Q5V8X3
G	776	GLN	-	expression tag	UNP Q5V8X3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	777	PHE	-	expression tag	UNP Q5V8X3
G	778	GLU	-	expression tag	UNP Q5V8X3
G	779	LYS	-	expression tag	UNP Q5V8X3
G	780	GLY	-	expression tag	UNP Q5V8X3
G	781	SER	-	expression tag	UNP Q5V8X3
G	782	GLY	-	expression tag	UNP Q5V8X3
G	783	SER	-	expression tag	UNP Q5V8X3
G	784	GLU	-	expression tag	UNP Q5V8X3
G	785	ASN	-	expression tag	UNP Q5V8X3
G	786	LEU	-	expression tag	UNP Q5V8X3
G	787	TYR	-	expression tag	UNP Q5V8X3
G	788	PHE	-	expression tag	UNP Q5V8X3
G	789	GLN	-	expression tag	UNP Q5V8X3
K	-8	GLY	-	expression tag	UNP Q5V8X3
K	-7	SER	-	expression tag	UNP Q5V8X3
K	-6	GLY	-	expression tag	UNP Q5V8X3
K	-5	SER	-	expression tag	UNP Q5V8X3
K	-4	GLY	-	expression tag	UNP Q5V8X3
K	-3	SER	-	expression tag	UNP Q5V8X3
K	-2	GLY	-	expression tag	UNP Q5V8X3
K	-1	SER	-	expression tag	UNP Q5V8X3
K	0	ALA	-	expression tag	UNP Q5V8X3
K	771	GLY	-	expression tag	UNP Q5V8X3
K	772	TRP	-	expression tag	UNP Q5V8X3
K	773	SER	-	expression tag	UNP Q5V8X3
K	774	HIS	-	expression tag	UNP Q5V8X3
K	775	PRO	-	expression tag	UNP Q5V8X3
K	776	GLN	-	expression tag	UNP Q5V8X3
K	777	PHE	-	expression tag	UNP Q5V8X3
K	778	GLU	-	expression tag	UNP Q5V8X3
K	779	LYS	-	expression tag	UNP Q5V8X3
K	780	GLY	-	expression tag	UNP Q5V8X3
K	781	SER	-	expression tag	UNP Q5V8X3
K	782	GLY	-	expression tag	UNP Q5V8X3
K	783	SER	-	expression tag	UNP Q5V8X3
K	784	GLU	-	expression tag	UNP Q5V8X3
K	785	ASN	-	expression tag	UNP Q5V8X3
K	786	LEU	-	expression tag	UNP Q5V8X3
K	787	TYR	-	expression tag	UNP Q5V8X3
K	788	PHE	-	expression tag	UNP Q5V8X3
K	789	GLN	-	expression tag	UNP Q5V8X3
O	-8	GLY	-	expression tag	UNP Q5V8X3

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-7	SER	-	expression tag	UNP Q5V8X3
O	-6	GLY	-	expression tag	UNP Q5V8X3
O	-5	SER	-	expression tag	UNP Q5V8X3
O	-4	GLY	-	expression tag	UNP Q5V8X3
O	-3	SER	-	expression tag	UNP Q5V8X3
O	-2	GLY	-	expression tag	UNP Q5V8X3
O	-1	SER	-	expression tag	UNP Q5V8X3
O	0	ALA	-	expression tag	UNP Q5V8X3
O	771	GLY	-	expression tag	UNP Q5V8X3
O	772	TRP	-	expression tag	UNP Q5V8X3
O	773	SER	-	expression tag	UNP Q5V8X3
O	774	HIS	-	expression tag	UNP Q5V8X3
O	775	PRO	-	expression tag	UNP Q5V8X3
O	776	GLN	-	expression tag	UNP Q5V8X3
O	777	PHE	-	expression tag	UNP Q5V8X3
O	778	GLU	-	expression tag	UNP Q5V8X3
O	779	LYS	-	expression tag	UNP Q5V8X3
O	780	GLY	-	expression tag	UNP Q5V8X3
O	781	SER	-	expression tag	UNP Q5V8X3
O	782	GLY	-	expression tag	UNP Q5V8X3
O	783	SER	-	expression tag	UNP Q5V8X3
O	784	GLU	-	expression tag	UNP Q5V8X3
O	785	ASN	-	expression tag	UNP Q5V8X3
O	786	LEU	-	expression tag	UNP Q5V8X3
O	787	TYR	-	expression tag	UNP Q5V8X3
O	788	PHE	-	expression tag	UNP Q5V8X3
O	789	GLN	-	expression tag	UNP Q5V8X3
S	-8	GLY	-	expression tag	UNP Q5V8X3
S	-7	SER	-	expression tag	UNP Q5V8X3
S	-6	GLY	-	expression tag	UNP Q5V8X3
S	-5	SER	-	expression tag	UNP Q5V8X3
S	-4	GLY	-	expression tag	UNP Q5V8X3
S	-3	SER	-	expression tag	UNP Q5V8X3
S	-2	GLY	-	expression tag	UNP Q5V8X3
S	-1	SER	-	expression tag	UNP Q5V8X3
S	0	ALA	-	expression tag	UNP Q5V8X3
S	771	GLY	-	expression tag	UNP Q5V8X3
S	772	TRP	-	expression tag	UNP Q5V8X3
S	773	SER	-	expression tag	UNP Q5V8X3
S	774	HIS	-	expression tag	UNP Q5V8X3
S	775	PRO	-	expression tag	UNP Q5V8X3
S	776	GLN	-	expression tag	UNP Q5V8X3

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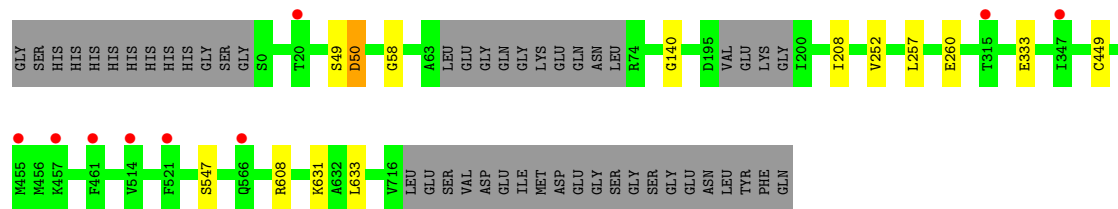
Chain	Residue	Modelled	Actual	Comment	Reference
S	777	PHE	-	expression tag	UNP Q5V8X3
S	778	GLU	-	expression tag	UNP Q5V8X3
S	779	LYS	-	expression tag	UNP Q5V8X3
S	780	GLY	-	expression tag	UNP Q5V8X3
S	781	SER	-	expression tag	UNP Q5V8X3
S	782	GLY	-	expression tag	UNP Q5V8X3
S	783	SER	-	expression tag	UNP Q5V8X3
S	784	GLU	-	expression tag	UNP Q5V8X3
S	785	ASN	-	expression tag	UNP Q5V8X3
S	786	LEU	-	expression tag	UNP Q5V8X3
S	787	TYR	-	expression tag	UNP Q5V8X3
S	788	PHE	-	expression tag	UNP Q5V8X3
S	789	GLN	-	expression tag	UNP Q5V8X3
W	-8	GLY	-	expression tag	UNP Q5V8X3
W	-7	SER	-	expression tag	UNP Q5V8X3
W	-6	GLY	-	expression tag	UNP Q5V8X3
W	-5	SER	-	expression tag	UNP Q5V8X3
W	-4	GLY	-	expression tag	UNP Q5V8X3
W	-3	SER	-	expression tag	UNP Q5V8X3
W	-2	GLY	-	expression tag	UNP Q5V8X3
W	-1	SER	-	expression tag	UNP Q5V8X3
W	0	ALA	-	expression tag	UNP Q5V8X3
W	771	GLY	-	expression tag	UNP Q5V8X3
W	772	TRP	-	expression tag	UNP Q5V8X3
W	773	SER	-	expression tag	UNP Q5V8X3
W	774	HIS	-	expression tag	UNP Q5V8X3
W	775	PRO	-	expression tag	UNP Q5V8X3
W	776	GLN	-	expression tag	UNP Q5V8X3
W	777	PHE	-	expression tag	UNP Q5V8X3
W	778	GLU	-	expression tag	UNP Q5V8X3
W	779	LYS	-	expression tag	UNP Q5V8X3
W	780	GLY	-	expression tag	UNP Q5V8X3
W	781	SER	-	expression tag	UNP Q5V8X3
W	782	GLY	-	expression tag	UNP Q5V8X3
W	783	SER	-	expression tag	UNP Q5V8X3
W	784	GLU	-	expression tag	UNP Q5V8X3
W	785	ASN	-	expression tag	UNP Q5V8X3
W	786	LEU	-	expression tag	UNP Q5V8X3
W	787	TYR	-	expression tag	UNP Q5V8X3
W	788	PHE	-	expression tag	UNP Q5V8X3
W	789	GLN	-	expression tag	UNP Q5V8X3

- Molecule 4 is a RNA chain called CRNA 5' END.

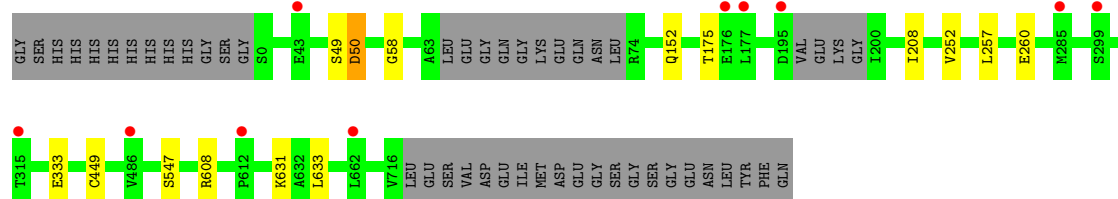
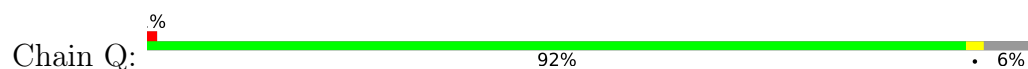
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	12	Total 265	C 118	N 56	O 79	P 12	0	0	0
4	H	12	Total 265	C 118	N 56	O 79	P 12	0	0	0
4	L	12	Total 265	C 118	N 56	O 79	P 12	0	0	0
4	P	12	Total 265	C 118	N 56	O 79	P 12	0	0	0
4	T	12	Total 265	C 118	N 56	O 79	P 12	0	0	0
4	X	12	Total 265	C 118	N 56	O 79	P 12	0	0	0

- Molecule 1: Polymerase acidic protein

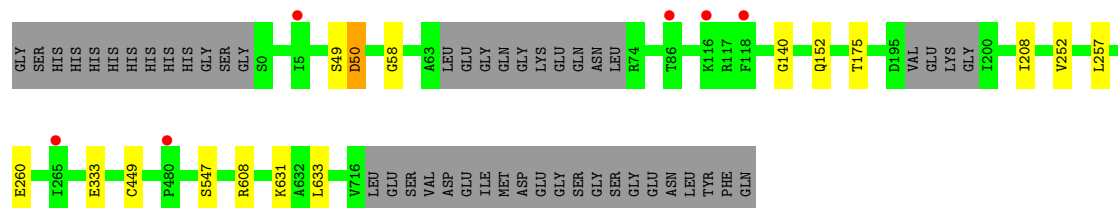
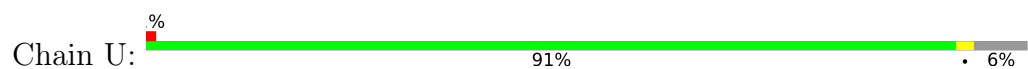




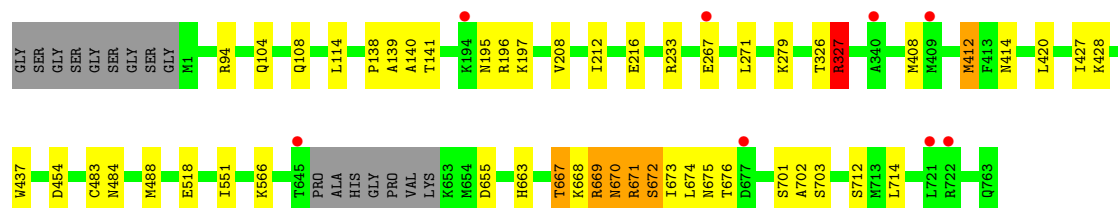
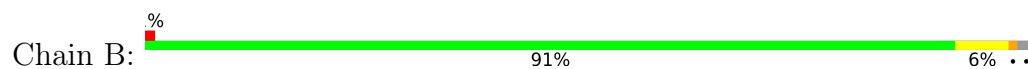
• Molecule 1: Polymerase acidic protein



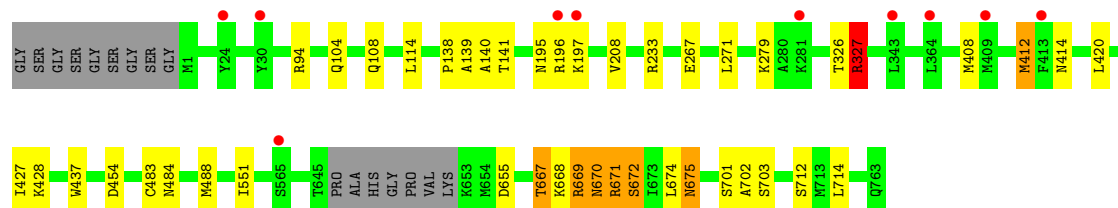
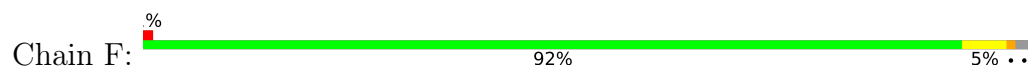
• Molecule 1: Polymerase acidic protein



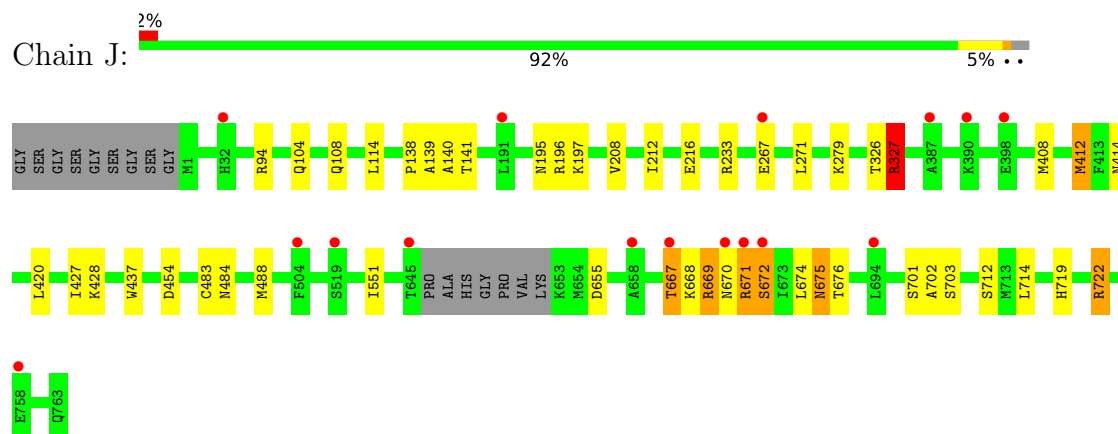
• Molecule 2: RNA-directed RNA polymerase catalytic subunit



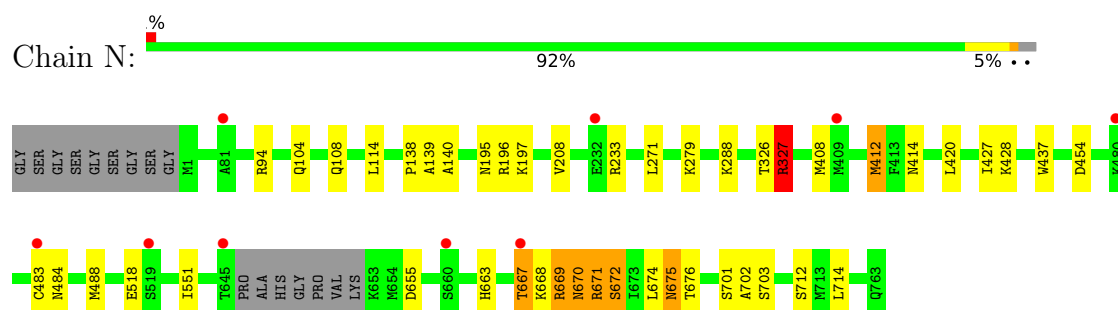
• Molecule 2: RNA-directed RNA polymerase catalytic subunit



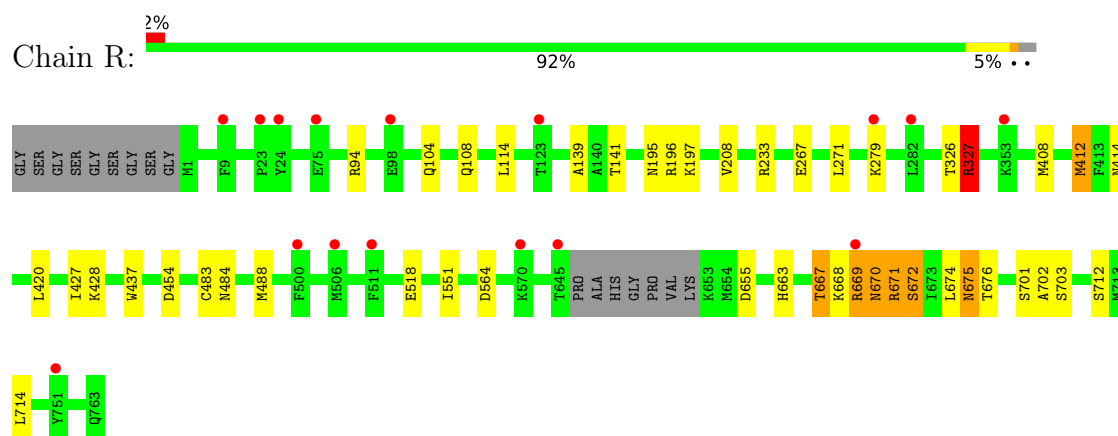
- Molecule 2: RNA-directed RNA polymerase catalytic subunit



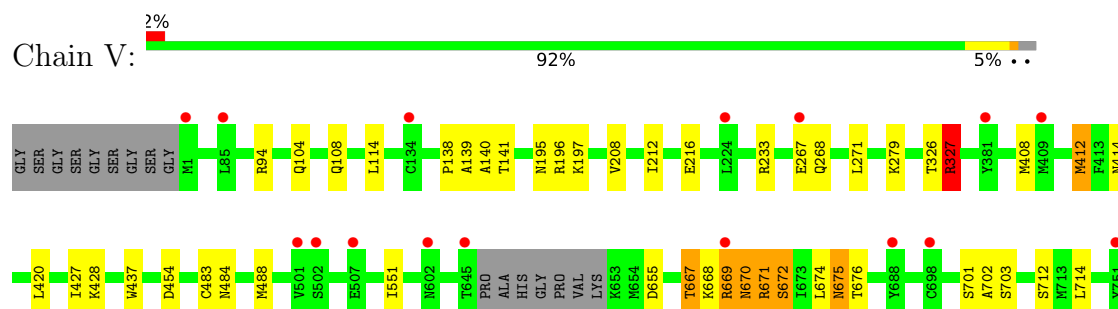
- Molecule 2: RNA-directed RNA polymerase catalytic subunit



- Molecule 2: RNA-directed RNA polymerase catalytic subunit

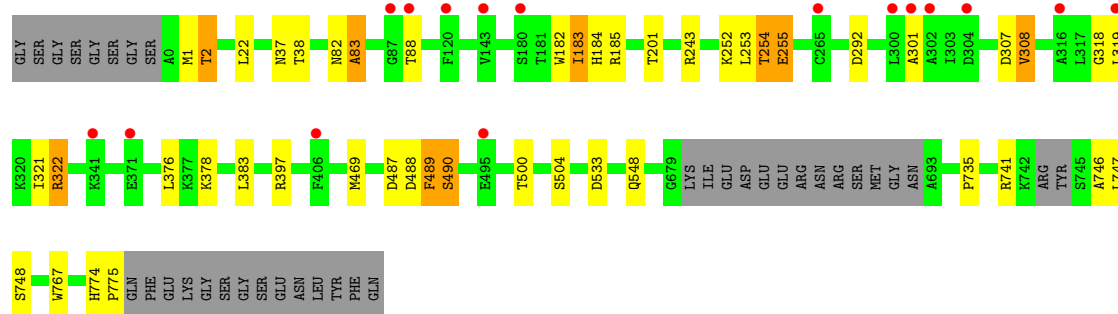
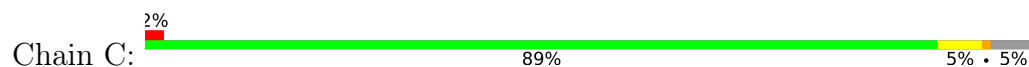


- Molecule 2: RNA-directed RNA polymerase catalytic subunit

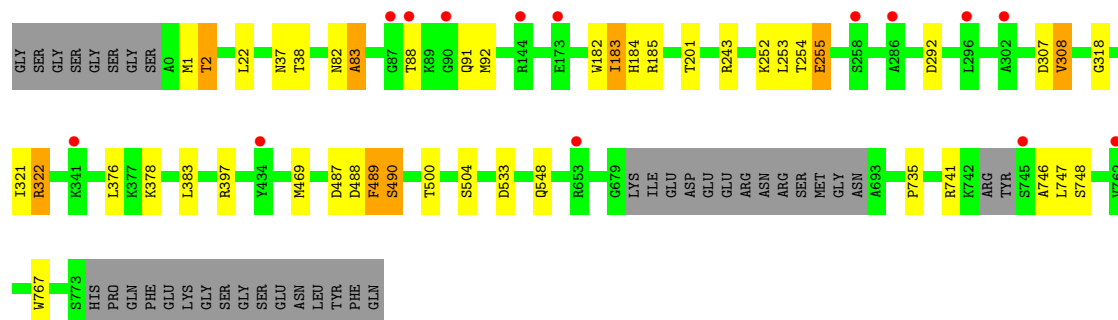
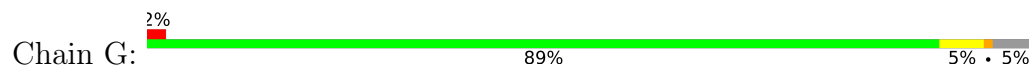




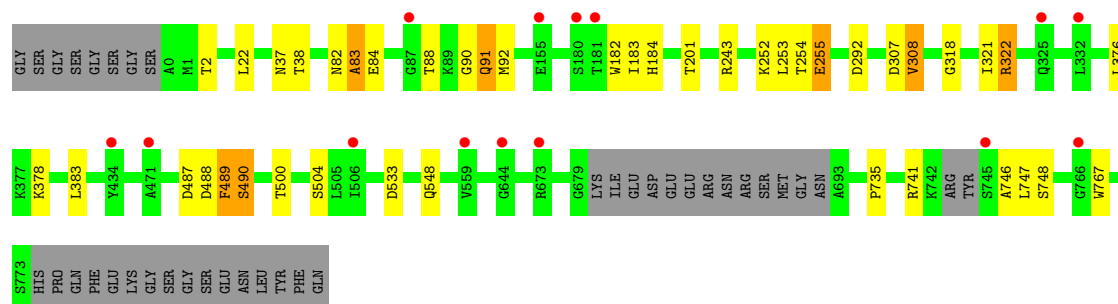
• Molecule 3: Polymerase basic protein 2



• Molecule 3: Polymerase basic protein 2



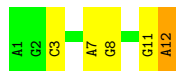
• Molecule 3: Polymerase basic protein 2



• Molecule 3: Polymerase basic protein 2



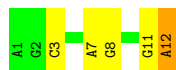
● Molecule 4: CRNA 5' END

Chain H:  58% 33% 8%

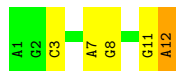
● Molecule 4: CRNA 5' END

Chain L:  50% 42% 8%

● Molecule 4: CRNA 5' END

Chain P:  58% 33% 8%

● Molecule 4: CRNA 5' END

Chain T:  58% 33% 8%

● Molecule 4: CRNA 5' END

Chain X:  50% 42% 8%

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	193.73Å 209.98Å 210.60Å 117.71° 92.81° 113.68°	Depositor
Resolution (Å)	49.95 – 4.10 49.95 – 4.10	Depositor EDS
% Data completeness (in resolution range)	93.2 (49.95-4.10) 93.1 (49.95-4.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 4.14Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.257 , 0.287 0.257 , 0.282	Depositor DCC
R_{free} test set	7765 reflections (3.84%)	wwPDB-VP
Wilson B-factor (Å ²)	154.8	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 135.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.040 for -h,h+k+l,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	106314	wwPDB-VP
Average B, all atoms (Å ²)	191.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.06% 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	A	0.12	0/5761	0.28	0/7768
1	E	0.11	0/5761	0.27	0/7768
1	I	0.13	0/5799	0.28	0/7818
1	M	0.11	0/5761	0.27	0/7768
1	Q	0.11	0/5761	0.27	0/7768
1	U	0.11	0/5761	0.27	0/7768
2	B	0.14	0/6042	0.32	0/8143
2	F	0.13	0/6042	0.32	0/8143
2	J	0.14	0/6042	0.32	0/8143
2	N	0.14	0/6042	0.32	0/8143
2	R	0.13	0/6042	0.32	0/8143
2	V	0.13	0/6042	0.32	0/8143
3	C	0.14	0/6184	0.34	0/8314
3	G	0.14	0/6165	0.33	0/8287
3	K	0.14	0/6165	0.34	0/8287
3	O	0.14	0/6165	0.34	0/8287
3	S	0.13	0/6165	0.34	0/8287
3	W	0.15	0/5003	0.36	0/6725
4	D	0.13	0/298	0.34	0/462
4	H	0.12	0/298	0.34	0/462
4	L	0.14	0/298	0.35	0/462
4	P	0.14	0/298	0.34	0/462
4	T	0.13	0/298	0.36	0/462
4	X	0.14	0/298	0.35	0/462
All	All	0.13	0/108491	0.31	0/146475

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 ⓘ

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	5646	0	5621	7	1
1	E	5646	0	5621	3	0
1	I	5685	0	5661	12	1
1	M	5646	0	5621	2	0
1	Q	5646	0	5621	3	0
1	U	5646	0	5621	2	0
2	B	5927	0	5929	21	0
2	F	5927	0	5929	18	0
2	J	5927	0	5929	21	0
2	N	5927	0	5929	21	0
2	R	5927	0	5929	19	0
2	V	5927	0	5929	21	0
3	C	6078	0	6240	22	0
3	G	6061	0	6226	20	0
3	K	6061	0	6226	18	0
3	O	6061	0	6226	22	0
3	S	6061	0	6226	19	0
3	W	4925	0	5071	19	0
4	D	265	0	133	0	0
4	H	265	0	133	1	0
4	L	265	0	133	1	0
4	P	265	0	133	1	0
4	T	265	0	133	1	0
4	X	265	0	133	1	0
All	All	106314	0	106353	250	1

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 (250) 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:I:671:ARG:NH1	1:I:721:ASP:OD2	2.20	0.75
1:I:671:ARG:NH2	1:I:721:ASP:OD2	2.27	0.68
1:I:723:ILE:HG13	1:I:724:MET:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:397:ARG:HE	3:G:469:MET:HG3	1.61	0.66
2:J:701:SER:O	2:J:703:SER:N	2.30	0.65
3:C:397:ARG:HE	3:C:469:MET:HG3	1.61	0.64
2:B:701:SER:O	2:B:703:SER:N	2.31	0.64
2:R:701:SER:O	2:R:703:SER:N	2.31	0.63
3:W:746:ALA:O	3:W:748:SER:N	2.31	0.63
2:N:701:SER:O	2:N:703:SER:N	2.31	0.63
2:V:701:SER:O	2:V:703:SER:N	2.32	0.62
2:F:701:SER:O	2:F:703:SER:N	2.32	0.62
1:I:136:LYS:NZ	1:I:141:ASN:OD1	2.33	0.60
3:W:487:ASP:OD1	3:W:488:ASP:N	2.36	0.58
3:S:487:ASP:OD1	3:S:488:ASP:N	2.37	0.58
3:K:376:LEU:HD11	3:K:383:LEU:CD1	2.34	0.58
3:C:376:LEU:HD11	3:C:383:LEU:CD1	2.34	0.57
3:W:376:LEU:HD11	3:W:383:LEU:CD1	2.35	0.57
3:S:376:LEU:HD11	3:S:383:LEU:CD1	2.35	0.57
3:G:376:LEU:HD11	3:G:383:LEU:CD1	2.34	0.56
3:O:376:LEU:HD11	3:O:383:LEU:CD1	2.35	0.56
1:I:719:SER:O	1:I:723:ILE:HG12	2.06	0.56
2:F:667:THR:HG22	2:F:668:LYS:H	1.72	0.55
3:O:91:GLN:O	3:O:92:MET:HG3	2.06	0.55
3:O:84:GLU:HA	3:O:90:GLY:O	2.07	0.55
1:I:720:VAL:HA	1:I:723:ILE:HD11	1.88	0.54
3:K:487:ASP:OD1	3:K:488:ASP:N	2.41	0.54
3:C:487:ASP:OD1	3:C:488:ASP:N	2.40	0.54
3:K:182:TRP:O	3:K:184:HIS:N	2.41	0.54
2:J:667:THR:HG22	2:J:668:LYS:H	1.72	0.54
3:O:182:TRP:O	3:O:184:HIS:N	2.41	0.53
1:I:720:VAL:O	1:I:723:ILE:HG13	2.07	0.53
2:F:714:LEU:HB2	3:G:22:LEU:HB3	1.91	0.53
2:N:667:THR:HG22	2:N:668:LYS:H	1.73	0.53
3:O:487:ASP:OD1	3:O:488:ASP:N	2.42	0.53
2:J:714:LEU:HB2	3:K:22:LEU:HB3	1.91	0.52
2:R:667:THR:HG22	2:R:668:LYS:H	1.73	0.52
3:G:487:ASP:OD1	3:G:488:ASP:N	2.41	0.52
2:B:714:LEU:HB2	3:C:22:LEU:HB3	1.91	0.52
3:G:182:TRP:O	3:G:184:HIS:N	2.42	0.52
3:K:376:LEU:HD11	3:K:383:LEU:HD11	1.92	0.52
2:B:667:THR:HG22	2:B:668:LYS:H	1.73	0.52
2:V:667:THR:HG22	2:V:668:LYS:H	1.73	0.52
2:N:288:LYS:HZ2	3:O:335:ILE:HD12	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:714:LEU:HB2	3:O:22:LEU:HB3	1.91	0.52
1:I:671:ARG:CZ	1:I:721:ASP:OD2	2.57	0.52
3:C:182:TRP:O	3:C:184:HIS:N	2.43	0.51
3:G:397:ARG:CG	3:G:469:MET:HG3	2.41	0.51
1:I:712:GLU:O	1:I:716:VAL:HG23	2.11	0.50
2:R:714:LEU:HB2	3:S:22:LEU:HB3	1.92	0.50
3:G:489:PHE:O	3:G:490:SER:OG	2.28	0.50
2:B:674:LEU:C	2:B:676:THR:H	2.19	0.50
3:C:397:ARG:CG	3:C:469:MET:HG3	2.41	0.50
3:G:376:LEU:HD11	3:G:383:LEU:HD11	1.93	0.50
2:F:671:ARG:O	2:F:672:SER:CB	2.60	0.50
3:C:376:LEU:HD11	3:C:383:LEU:HD11	1.92	0.50
2:V:671:ARG:O	2:V:672:SER:CB	2.60	0.50
2:J:671:ARG:O	2:J:672:SER:CB	2.60	0.49
2:V:714:LEU:HB2	3:W:22:LEU:HB3	1.94	0.49
3:O:376:LEU:HD11	3:O:383:LEU:HD11	1.94	0.49
3:W:376:LEU:HD11	3:W:383:LEU:HD11	1.94	0.49
3:S:376:LEU:HD11	3:S:383:LEU:HD11	1.93	0.49
2:B:671:ARG:O	2:B:672:SER:CB	2.60	0.49
2:N:671:ARG:O	2:N:672:SER:CB	2.60	0.49
2:R:671:ARG:O	2:R:672:SER:CB	2.60	0.49
3:S:746:ALA:O	3:S:748:SER:N	2.46	0.49
2:R:668:LYS:O	2:R:669:ARG:HB2	2.13	0.49
2:B:668:LYS:O	2:B:669:ARG:CB	2.61	0.48
2:F:668:LYS:O	2:F:669:ARG:HB2	2.13	0.48
2:V:668:LYS:O	2:V:669:ARG:CB	2.61	0.48
2:R:668:LYS:O	2:R:669:ARG:CB	2.61	0.48
3:W:772:TRP:N	3:W:772:TRP:CD1	2.81	0.48
2:J:674:LEU:HD11	4:L:12:A:O2'	2.13	0.48
2:J:668:LYS:O	2:J:669:ARG:CB	2.62	0.48
2:J:668:LYS:O	2:J:669:ARG:HB2	2.14	0.48
2:N:668:LYS:O	2:N:669:ARG:HB2	2.14	0.48
2:B:668:LYS:O	2:B:669:ARG:HB2	2.13	0.47
2:N:668:LYS:O	2:N:669:ARG:CB	2.62	0.47
2:V:668:LYS:O	2:V:669:ARG:HB2	2.13	0.47
3:S:91:GLN:C	3:S:92:MET:HG3	2.39	0.47
3:C:82:ASN:O	3:C:83:ALA:C	2.58	0.47
3:W:253:LEU:O	3:W:255:GLU:N	2.47	0.47
1:I:716:VAL:O	1:I:719:SER:CB	2.63	0.47
1:A:299:SER:HB2	2:B:566:LYS:C	2.40	0.47
2:J:668:LYS:HE2	3:K:92:MET:SD	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:674:LEU:O	2:N:675:ASN:C	2.58	0.46
3:O:82:ASN:O	3:O:83:ALA:C	2.59	0.46
2:F:674:LEU:O	2:F:675:ASN:C	2.58	0.46
2:F:668:LYS:O	2:F:669:ARG:CB	2.63	0.46
3:C:489:PHE:O	3:C:490:SER:OG	2.29	0.46
3:G:82:ASN:O	3:G:83:ALA:C	2.58	0.46
3:K:91:GLN:O	3:K:92:MET:HG3	2.15	0.46
3:O:307:ASP:CG	3:O:308:VAL:N	2.74	0.46
2:J:674:LEU:O	2:J:675:ASN:C	2.58	0.46
2:R:674:LEU:O	2:R:675:ASN:C	2.58	0.46
2:V:141:THR:HG21	3:W:37:ASN:O	2.16	0.46
3:C:746:ALA:O	3:C:748:SER:N	2.49	0.46
3:S:253:LEU:O	3:S:255:GLU:N	2.48	0.46
2:V:674:LEU:O	2:V:675:ASN:C	2.59	0.46
3:C:253:LEU:O	3:C:255:GLU:N	2.48	0.46
3:S:82:ASN:O	3:S:83:ALA:C	2.59	0.46
3:S:489:PHE:O	3:S:490:SER:OG	2.31	0.46
2:V:195:ASN:O	2:V:197:LYS:N	2.49	0.46
3:C:774:HIS:HB3	3:C:775:PRO:HD3	1.98	0.46
3:K:746:ALA:O	3:K:748:SER:N	2.49	0.46
3:W:82:ASN:O	3:W:83:ALA:C	2.59	0.46
3:S:307:ASP:OD1	3:S:308:VAL:N	2.46	0.46
3:G:253:LEU:O	3:G:255:GLU:N	2.48	0.46
3:O:307:ASP:OD1	3:O:308:VAL:N	2.48	0.46
1:I:716:VAL:O	1:I:719:SER:OG	2.28	0.45
2:R:326:THR:O	2:R:327:ARG:C	2.59	0.45
2:R:195:ASN:O	2:R:197:LYS:N	2.49	0.45
3:O:253:LEU:O	3:O:255:GLU:N	2.49	0.45
3:W:307:ASP:OD1	3:W:308:VAL:N	2.47	0.45
2:B:326:THR:O	2:B:327:ARG:C	2.60	0.45
2:J:326:THR:O	2:J:327:ARG:C	2.60	0.45
1:Q:49:SER:O	1:Q:50:ASP:C	2.60	0.45
2:N:326:THR:O	2:N:327:ARG:C	2.59	0.45
3:G:746:ALA:O	3:G:748:SER:N	2.50	0.45
3:K:82:ASN:O	3:K:83:ALA:C	2.58	0.45
2:F:195:ASN:O	2:F:197:LYS:N	2.49	0.45
2:F:437:TRP:CD1	2:F:437:TRP:C	2.95	0.45
2:J:722:ARG:NH1	2:V:763:GLN:O	2.49	0.45
3:K:307:ASP:CG	3:K:308:VAL:N	2.75	0.45
3:W:307:ASP:CG	3:W:308:VAL:N	2.75	0.45
1:M:50:ASP:O	3:O:757:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ASN:O	2:B:197:LYS:N	2.50	0.45
2:V:326:THR:O	2:V:327:ARG:C	2.60	0.45
3:G:376:LEU:CD1	3:G:383:LEU:HD11	2.47	0.45
3:K:321:ILE:O	3:K:322:ARG:HB2	2.17	0.45
2:F:326:THR:O	2:F:327:ARG:C	2.60	0.45
2:N:195:ASN:O	2:N:197:LYS:N	2.49	0.45
3:C:307:ASP:CG	3:C:308:VAL:N	2.75	0.45
3:K:253:LEU:O	3:K:255:GLU:N	2.49	0.45
3:O:321:ILE:O	3:O:322:ARG:HB2	2.17	0.45
2:B:483:CYS:SG	2:B:484:ASN:N	2.91	0.44
2:B:673:ILE:O	2:B:674:LEU:HB2	2.16	0.44
3:S:307:ASP:CG	3:S:308:VAL:N	2.74	0.44
1:E:49:SER:O	1:E:50:ASP:C	2.61	0.44
3:C:376:LEU:CD1	3:C:383:LEU:HD11	2.47	0.44
2:V:483:CYS:SG	2:V:484:ASN:N	2.90	0.44
3:S:321:ILE:O	3:S:322:ARG:CB	2.65	0.44
3:S:376:LEU:CD1	3:S:383:LEU:HD11	2.47	0.44
2:J:437:TRP:CD1	2:J:437:TRP:C	2.95	0.44
2:N:483:CYS:SG	2:N:484:ASN:N	2.91	0.44
2:V:674:LEU:HD11	4:X:12:A:O2'	2.17	0.44
3:K:376:LEU:CD1	3:K:383:LEU:HD11	2.47	0.44
3:W:712:LYS:HB3	3:W:716:GLU:HB3	2.00	0.44
2:J:195:ASN:O	2:J:197:LYS:N	2.51	0.44
2:R:437:TRP:CD1	2:R:437:TRP:C	2.96	0.44
3:K:321:ILE:O	3:K:322:ARG:CB	2.65	0.44
3:W:376:LEU:CD1	3:W:383:LEU:HD11	2.48	0.44
2:F:668:LYS:HE2	3:G:92:MET:SD	2.57	0.44
2:F:674:LEU:HD11	4:H:12:A:O2'	2.18	0.44
2:V:454:ASP:OD1	2:V:454:ASP:N	2.51	0.44
3:C:321:ILE:O	3:C:322:ARG:CB	2.65	0.44
3:G:307:ASP:CG	3:G:308:VAL:N	2.75	0.44
3:O:746:ALA:O	3:O:748:SER:N	2.49	0.44
3:W:321:ILE:O	3:W:322:ARG:CB	2.65	0.44
3:W:321:ILE:O	3:W:322:ARG:HB2	2.18	0.44
1:A:49:SER:O	1:A:50:ASP:C	2.60	0.44
1:I:49:SER:O	1:I:50:ASP:C	2.61	0.44
3:O:489:PHE:O	3:O:490:SER:OG	2.30	0.44
3:S:182:TRP:CZ3	3:S:729:LEU:HG	2.53	0.44
1:U:49:SER:O	1:U:50:ASP:C	2.61	0.43
2:N:437:TRP:CD1	2:N:437:TRP:C	2.95	0.43
2:V:437:TRP:CD1	2:V:437:TRP:C	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:321:ILE:O	3:G:322:ARG:CB	2.65	0.43
3:S:182:TRP:HB2	3:S:733:GLY:HA2	1.99	0.43
3:S:321:ILE:O	3:S:322:ARG:HB2	2.18	0.43
2:B:437:TRP:CD1	2:B:437:TRP:C	2.96	0.43
3:W:397:ARG:HG3	3:W:469:MET:SD	2.59	0.43
2:N:288:LYS:CE	3:O:335:ILE:HD12	2.47	0.43
1:A:252:VAL:O	1:A:253:THR:OG1	2.35	0.43
2:B:673:ILE:HG22	2:B:674:LEU:HG	2.01	0.43
3:O:376:LEU:CD1	3:O:383:LEU:HD11	2.48	0.43
2:B:670:ASN:O	2:B:672:SER:N	2.51	0.43
2:R:454:ASP:N	2:R:454:ASP:OD1	2.51	0.43
3:C:321:ILE:O	3:C:322:ARG:HB2	2.19	0.43
3:O:321:ILE:O	3:O:322:ARG:CB	2.65	0.43
1:M:49:SER:O	1:M:50:ASP:C	2.61	0.43
1:Q:152:GLN:OE1	1:Q:175:THR:OG1	2.36	0.43
3:G:321:ILE:O	3:G:322:ARG:HB2	2.18	0.43
3:O:1:MET:O	3:O:2:THR:C	2.62	0.43
2:F:454:ASP:OD1	2:F:454:ASP:N	2.52	0.43
3:C:307:ASP:OD1	3:C:308:VAL:N	2.50	0.42
2:F:483:CYS:SG	2:F:484:ASN:N	2.91	0.42
2:J:483:CYS:SG	2:J:484:ASN:N	2.92	0.42
2:R:141:THR:HG21	3:S:37:ASN:O	2.19	0.42
2:V:670:ASN:O	2:V:672:SER:N	2.52	0.42
3:K:489:PHE:O	3:K:490:SER:OG	2.29	0.42
1:A:152:GLN:OE1	1:A:175:THR:OG1	2.36	0.42
1:A:297:GLY:C	1:A:484:ARG:HH22	2.27	0.42
2:J:719:HIS:HA	2:J:722:ARG:HD2	2.01	0.42
2:J:674:LEU:O	2:J:676:THR:N	2.53	0.42
2:N:454:ASP:OD1	2:N:454:ASP:N	2.51	0.42
2:J:141:THR:HG21	3:K:37:ASN:O	2.20	0.42
2:J:454:ASP:OD1	2:J:454:ASP:N	2.51	0.42
2:R:427:ILE:O	2:R:428:LYS:HB2	2.20	0.42
2:B:454:ASP:OD1	2:B:454:ASP:N	2.52	0.42
2:B:518:GLU:OE1	2:B:663:HIS:ND1	2.52	0.42
2:J:427:ILE:O	2:J:428:LYS:HB2	2.20	0.42
2:N:668:LYS:HE2	3:O:92:MET:SD	2.60	0.42
1:E:152:GLN:OE1	1:E:175:THR:OG1	2.37	0.42
2:R:670:ASN:O	2:R:672:SER:N	2.53	0.42
2:V:674:LEU:O	2:V:676:THR:N	2.53	0.42
3:C:1:MET:O	3:C:2:THR:C	2.64	0.41
1:A:298:LYS:N	1:A:484:ARG:HH22	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:751:ILE:O	3:W:754:GLY:N	2.52	0.41
2:B:138:PRO:O	2:B:140:ALA:N	2.54	0.41
2:B:427:ILE:O	2:B:428:LYS:HB2	2.20	0.41
2:F:141:THR:HG21	3:G:37:ASN:O	2.20	0.41
2:R:674:LEU:HD11	4:T:12:A:O2'	2.20	0.41
3:C:301:ALA:HB2	3:C:319:LEU:HD13	2.03	0.41
3:G:1:MET:O	3:G:2:THR:C	2.63	0.41
2:B:141:THR:HG21	3:C:37:ASN:O	2.20	0.41
2:F:138:PRO:O	2:F:140:ALA:N	2.53	0.41
2:N:427:ILE:O	2:N:428:LYS:HB2	2.20	0.41
2:R:674:LEU:O	2:R:676:THR:N	2.54	0.41
2:V:427:ILE:O	2:V:428:LYS:HB2	2.20	0.41
3:W:488:ASP:O	3:W:489:PHE:C	2.64	0.41
1:A:297:GLY:C	1:A:484:ARG:NH2	2.79	0.41
1:E:125:LYS:NZ	1:E:190:LEU:O	2.50	0.41
2:N:674:LEU:HD11	4:P:12:A:O2'	2.21	0.41
3:C:253:LEU:C	3:C:254:THR:HG1	2.27	0.41
1:Q:50:ASP:O	3:S:757:ARG:NH1	2.53	0.41
2:B:212:ILE:HG23	2:B:216:GLU:HB2	2.03	0.41
2:F:427:ILE:O	2:F:428:LYS:HB2	2.20	0.41
2:N:138:PRO:O	2:N:140:ALA:N	2.54	0.41
2:V:212:ILE:HG23	2:V:216:GLU:HB2	2.03	0.41
2:N:518:GLU:OE1	2:N:663:HIS:ND1	2.54	0.41
2:N:670:ASN:O	2:N:672:SER:N	2.54	0.41
2:N:674:LEU:O	2:N:676:THR:N	2.54	0.41
2:R:483:CYS:SG	2:R:484:ASN:N	2.93	0.41
2:R:518:GLU:OE1	2:R:663:HIS:ND1	2.53	0.41
3:G:183:ILE:C	3:G:185:ARG:H	2.29	0.41
2:V:138:PRO:O	2:V:140:ALA:N	2.54	0.41
3:K:182:TRP:C	3:K:184:HIS:N	2.79	0.41
3:W:91:GLN:C	3:W:92:MET:HG3	2.46	0.41
2:F:670:ASN:O	2:F:672:SER:N	2.53	0.40
3:O:182:TRP:C	3:O:184:HIS:N	2.79	0.40
3:S:486:ILE:HG22	3:S:487:ASP:N	2.36	0.40
1:U:152:GLN:OE1	1:U:175:THR:OG1	2.39	0.40
2:J:138:PRO:O	2:J:140:ALA:N	2.54	0.40
2:J:212:ILE:HG23	2:J:216:GLU:HB2	2.03	0.40
2:R:564:ASP:OD1	2:R:564:ASP:N	2.54	0.40
2:V:674:LEU:O	2:V:676:THR:OG1	2.37	0.40
3:C:183:ILE:C	3:C:185:ARG:H	2.29	0.40
3:G:397:ARG:HG2	3:G:469:MET:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:84:GLU:HA	3:K:90:GLY:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:ASN:ND2	1:I:722:GLU:OE1[1_445]	2.13	0.07

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	A	697/751 (93%)	660 (95%)	34 (5%)	3 (0%)	30	65
1	E	697/751 (93%)	662 (95%)	31 (4%)	4 (1%)	21	58
1	I	702/751 (94%)	666 (95%)	31 (4%)	5 (1%)	18	55
1	M	697/751 (93%)	662 (95%)	31 (4%)	4 (1%)	21	58
1	Q	697/751 (93%)	662 (95%)	32 (5%)	3 (0%)	30	65
1	U	697/751 (93%)	662 (95%)	31 (4%)	4 (1%)	21	58
2	B	752/772 (97%)	692 (92%)	50 (7%)	10 (1%)	9	41
2	F	752/772 (97%)	693 (92%)	49 (6%)	10 (1%)	9	41
2	J	752/772 (97%)	693 (92%)	49 (6%)	10 (1%)	9	41
2	N	752/772 (97%)	694 (92%)	48 (6%)	10 (1%)	9	41
2	R	752/772 (97%)	693 (92%)	49 (6%)	10 (1%)	9	41
2	V	752/772 (97%)	694 (92%)	48 (6%)	10 (1%)	9	41
3	C	755/798 (95%)	681 (90%)	59 (8%)	15 (2%)	6	33
3	G	753/798 (94%)	679 (90%)	59 (8%)	15 (2%)	6	33
3	K	753/798 (94%)	677 (90%)	61 (8%)	15 (2%)	6	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O	753/798 (94%)	677 (90%)	61 (8%)	15 (2%)	6	33
3	S	753/798 (94%)	678 (90%)	62 (8%)	13 (2%)	7	36
3	W	612/798 (77%)	547 (89%)	52 (8%)	13 (2%)	5	32
All	All	13078/13926 (94%)	12072 (92%)	837 (6%)	169 (1%)	9	41

All (169) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ASP
1	E	50	ASP
1	I	50	ASP
1	M	50	ASP
1	Q	50	ASP
1	U	50	ASP
2	B	139	ALA
2	B	669	ARG
2	B	670	ASN
2	B	671	ARG
2	B	702	ALA
2	F	139	ALA
2	F	669	ARG
2	F	670	ASN
2	F	671	ARG
2	F	675	ASN
2	F	702	ALA
2	J	139	ALA
2	J	669	ARG
2	J	670	ASN
2	J	671	ARG
2	J	675	ASN
2	J	702	ALA
2	N	139	ALA
2	N	669	ARG
2	N	670	ASN
2	N	671	ARG
2	N	675	ASN
2	N	702	ALA
2	R	139	ALA
2	R	669	ARG
2	R	670	ASN
2	R	671	ARG

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Mol	Chain	Res	Type
2	R	675	ASN
2	R	702	ALA
2	V	139	ALA
2	V	669	ARG
2	V	670	ASN
2	V	671	ARG
2	V	675	ASN
2	V	702	ALA
3	C	308	VAL
3	C	322	ARG
3	C	741	ARG
3	G	308	VAL
3	G	322	ARG
3	G	741	ARG
3	K	308	VAL
3	K	322	ARG
3	K	741	ARG
3	O	308	VAL
3	O	322	ARG
3	O	741	ARG
3	S	308	VAL
3	S	322	ARG
3	S	741	ARG
3	W	308	VAL
3	W	322	ARG
3	W	732	GLN
3	W	747	LEU
1	A	58	GLY
1	E	58	GLY
1	I	58	GLY
1	I	723	ILE
1	M	58	GLY
1	Q	58	GLY
1	U	58	GLY
3	C	83	ALA
3	C	489	PHE
3	G	83	ALA
3	G	489	PHE
3	K	83	ALA
3	K	489	PHE
3	O	2	THR
3	O	83	ALA

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Mol	Chain	Res	Type
3	O	489	PHE
3	S	83	ALA
3	S	489	PHE
3	W	83	ALA
3	W	489	PHE
2	B	196	ARG
2	B	327	ARG
2	B	412	MET
2	F	196	ARG
2	F	327	ARG
2	F	412	MET
2	F	672	SER
2	J	196	ARG
2	J	327	ARG
2	J	412	MET
2	J	672	SER
2	N	196	ARG
2	N	327	ARG
2	N	412	MET
2	N	672	SER
2	R	196	ARG
2	R	327	ARG
2	R	412	MET
2	R	672	SER
2	V	196	ARG
2	V	327	ARG
2	V	412	MET
2	V	672	SER
3	C	254	THR
3	G	254	THR
3	K	254	THR
3	O	254	THR
3	S	254	THR
3	W	254	THR
1	A	547	SER
1	E	547	SER
1	I	547	SER
1	M	547	SER
1	Q	547	SER
1	U	547	SER
2	B	672	SER
3	C	2	THR

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Mol	Chain	Res	Type
3	C	38	THR
3	C	292	ASP
3	C	747	LEU
3	G	2	THR
3	G	38	THR
3	G	292	ASP
3	G	747	LEU
3	K	2	THR
3	K	38	THR
3	K	292	ASP
3	K	747	LEU
3	O	38	THR
3	O	292	ASP
3	O	747	LEU
3	S	38	THR
3	S	292	ASP
3	S	490	SER
3	S	747	LEU
3	W	38	THR
3	W	292	ASP
3	W	490	SER
2	B	675	ASN
3	C	252	LYS
3	C	490	SER
3	G	252	LYS
3	G	490	SER
3	K	183	ILE
3	K	252	LYS
3	K	490	SER
3	O	252	LYS
3	O	490	SER
3	S	318	GLY
3	W	318	GLY
3	G	183	ILE
3	O	183	ILE
3	S	252	LYS
3	W	252	LYS
3	C	183	ILE
3	C	735	PRO
3	G	735	PRO
3	O	735	PRO
1	I	140	GLY

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Mol	Chain	Res	Type
3	K	735	PRO
3	S	735	PRO
3	C	318	GLY
3	W	735	PRO
3	G	318	GLY
3	K	318	GLY
3	O	318	GLY
1	E	140	GLY
1	M	140	GLY
1	U	140	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	625/664 (94%)	616 (99%)	9 (1%)	59	71
1	E	625/664 (94%)	616 (99%)	9 (1%)	59	71
1	I	631/664 (95%)	622 (99%)	9 (1%)	59	71
1	M	625/664 (94%)	616 (99%)	9 (1%)	59	71
1	Q	625/664 (94%)	616 (99%)	9 (1%)	59	71
1	U	625/664 (94%)	616 (99%)	9 (1%)	59	71
2	B	647/657 (98%)	628 (97%)	19 (3%)	37	58
2	F	647/657 (98%)	628 (97%)	19 (3%)	37	58
2	J	647/657 (98%)	627 (97%)	20 (3%)	35	56
2	N	647/657 (98%)	629 (97%)	18 (3%)	38	59
2	R	647/657 (98%)	628 (97%)	19 (3%)	37	58
2	V	647/657 (98%)	627 (97%)	20 (3%)	35	56
3	C	664/694 (96%)	654 (98%)	10 (2%)	57	70
3	G	662/694 (95%)	651 (98%)	11 (2%)	53	68
3	K	662/694 (95%)	651 (98%)	11 (2%)	53	68
3	O	662/694 (95%)	652 (98%)	10 (2%)	57	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	S	662/694 (95%)	650 (98%)	12 (2%)	51	67
3	W	538/694 (78%)	520 (97%)	18 (3%)	33	55
All	All	11488/12090 (95%)	11247 (98%)	241 (2%)	47	65

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	ILE
1	A	252	VAL
1	A	257	LEU
1	A	260	GLU
1	A	333	GLU
1	A	470	ASN
1	A	608	ARG
1	A	631	LYS
1	A	633	LEU
1	E	208	ILE
1	E	252	VAL
1	E	257	LEU
1	E	260	GLU
1	E	333	GLU
1	E	449	CYS
1	E	608	ARG
1	E	631	LYS
1	E	633	LEU
1	I	208	ILE
1	I	252	VAL
1	I	257	LEU
1	I	260	GLU
1	I	333	GLU
1	I	449	CYS
1	I	608	ARG
1	I	631	LYS
1	I	633	LEU
1	M	208	ILE
1	M	252	VAL
1	M	257	LEU
1	M	260	GLU
1	M	333	GLU
1	M	449	CYS
1	M	608	ARG

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Mol	Chain	Res	Type
1	M	631	LYS
1	M	633	LEU
1	Q	208	ILE
1	Q	252	VAL
1	Q	257	LEU
1	Q	260	GLU
1	Q	333	GLU
1	Q	449	CYS
1	Q	608	ARG
1	Q	631	LYS
1	Q	633	LEU
1	U	208	ILE
1	U	252	VAL
1	U	257	LEU
1	U	260	GLU
1	U	333	GLU
1	U	449	CYS
1	U	608	ARG
1	U	631	LYS
1	U	633	LEU
2	B	94	ARG
2	B	104	GLN
2	B	108	GLN
2	B	114	LEU
2	B	208	VAL
2	B	233	ARG
2	B	267	GLU
2	B	271	LEU
2	B	279	LYS
2	B	327	ARG
2	B	408	MET
2	B	412	MET
2	B	414	ASN
2	B	420	LEU
2	B	488	MET
2	B	551	ILE
2	B	655	ASP
2	B	667	THR
2	B	712	SER
2	F	94	ARG
2	F	104	GLN
2	F	108	GLN

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Mol	Chain	Res	Type
2	F	114	LEU
2	F	208	VAL
2	F	233	ARG
2	F	267	GLU
2	F	271	LEU
2	F	279	LYS
2	F	327	ARG
2	F	408	MET
2	F	412	MET
2	F	414	ASN
2	F	420	LEU
2	F	488	MET
2	F	551	ILE
2	F	655	ASP
2	F	667	THR
2	F	712	SER
2	J	94	ARG
2	J	104	GLN
2	J	108	GLN
2	J	114	LEU
2	J	208	VAL
2	J	233	ARG
2	J	267	GLU
2	J	271	LEU
2	J	279	LYS
2	J	327	ARG
2	J	408	MET
2	J	412	MET
2	J	414	ASN
2	J	420	LEU
2	J	488	MET
2	J	551	ILE
2	J	655	ASP
2	J	667	THR
2	J	712	SER
2	J	722	ARG
2	N	94	ARG
2	N	104	GLN
2	N	108	GLN
2	N	114	LEU
2	N	208	VAL
2	N	233	ARG

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Mol	Chain	Res	Type
2	N	271	LEU
2	N	279	LYS
2	N	327	ARG
2	N	408	MET
2	N	412	MET
2	N	414	ASN
2	N	420	LEU
2	N	488	MET
2	N	551	ILE
2	N	655	ASP
2	N	667	THR
2	N	712	SER
2	R	94	ARG
2	R	104	GLN
2	R	108	GLN
2	R	114	LEU
2	R	208	VAL
2	R	233	ARG
2	R	267	GLU
2	R	271	LEU
2	R	279	LYS
2	R	327	ARG
2	R	408	MET
2	R	412	MET
2	R	414	ASN
2	R	420	LEU
2	R	488	MET
2	R	551	ILE
2	R	655	ASP
2	R	667	THR
2	R	712	SER
2	V	94	ARG
2	V	104	GLN
2	V	108	GLN
2	V	114	LEU
2	V	208	VAL
2	V	233	ARG
2	V	267	GLU
2	V	268	GLN
2	V	271	LEU
2	V	279	LYS
2	V	327	ARG

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Mol	Chain	Res	Type
2	V	408	MET
2	V	412	MET
2	V	414	ASN
2	V	420	LEU
2	V	488	MET
2	V	551	ILE
2	V	655	ASP
2	V	667	THR
2	V	712	SER
3	C	88	THR
3	C	201	THR
3	C	243	ARG
3	C	255	GLU
3	C	378	LYS
3	C	500	THR
3	C	504	SER
3	C	533	ASP
3	C	548	GLN
3	C	767	TRP
3	G	88	THR
3	G	91	GLN
3	G	201	THR
3	G	243	ARG
3	G	255	GLU
3	G	378	LYS
3	G	500	THR
3	G	504	SER
3	G	533	ASP
3	G	548	GLN
3	G	767	TRP
3	K	88	THR
3	K	91	GLN
3	K	201	THR
3	K	243	ARG
3	K	255	GLU
3	K	378	LYS
3	K	500	THR
3	K	504	SER
3	K	533	ASP
3	K	548	GLN
3	K	767	TRP
3	O	88	THR

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Mol	Chain	Res	Type
3	O	201	THR
3	O	243	ARG
3	O	255	GLU
3	O	378	LYS
3	O	500	THR
3	O	504	SER
3	O	533	ASP
3	O	548	GLN
3	O	767	TRP
3	S	88	THR
3	S	91	GLN
3	S	92	MET
3	S	201	THR
3	S	243	ARG
3	S	255	GLU
3	S	378	LYS
3	S	500	THR
3	S	504	SER
3	S	533	ASP
3	S	548	GLN
3	S	767	TRP
3	W	88	THR
3	W	92	MET
3	W	201	THR
3	W	243	ARG
3	W	255	GLU
3	W	378	LYS
3	W	500	THR
3	W	504	SER
3	W	533	ASP
3	W	705	ASP
3	W	713	THR
3	W	727	ASN
3	W	729	LEU
3	W	731	TYR
3	W	736	VAL
3	W	756	LYS
3	W	767	TRP
3	W	772	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	52	ASN
1	A	467	ASN
1	A	506	HIS
1	A	643	HIS
1	E	10	GLN
1	E	52	ASN
1	E	470	ASN
1	E	506	HIS
1	I	10	GLN
1	I	52	ASN
1	I	242	ASN
1	I	467	ASN
1	I	506	HIS
1	I	666	GLN
1	M	52	ASN
1	M	467	ASN
1	M	470	ASN
1	M	506	HIS
1	M	643	HIS
1	M	698	GLN
1	Q	10	GLN
1	Q	41	HIS
1	Q	52	ASN
1	Q	242	ASN
1	Q	467	ASN
1	Q	470	ASN
1	Q	506	HIS
1	Q	643	HIS
1	Q	698	GLN
1	U	10	GLN
1	U	52	ASN
1	U	467	ASN
1	U	470	ASN
1	U	506	HIS
1	U	643	HIS
2	B	104	GLN
2	B	544	GLN
2	B	548	GLN
2	B	625	HIS
2	F	32	HIS
2	F	104	GLN
2	F	532	ASN

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Mol	Chain	Res	Type
2	F	544	GLN
2	F	625	HIS
2	F	670	ASN
2	J	104	GLN
2	J	136	ASN
2	J	544	GLN
2	J	625	HIS
2	N	104	GLN
2	N	544	GLN
2	N	625	HIS
2	R	104	GLN
2	R	544	GLN
2	R	548	GLN
2	R	625	HIS
2	V	104	GLN
2	V	136	ASN
2	V	544	GLN
2	V	625	HIS
3	C	29	GLN
3	C	31	ASN
3	C	150	ASN
3	C	244	GLN
3	C	251	ASN
3	C	259	GLN
3	C	366	HIS
3	C	484	ASN
3	C	517	ASN
3	C	564	GLN
3	G	31	ASN
3	G	150	ASN
3	G	163	ASN
3	G	244	GLN
3	G	251	ASN
3	G	484	ASN
3	G	517	ASN
3	G	564	GLN
3	K	31	ASN
3	K	150	ASN
3	K	163	ASN
3	K	235	HIS
3	K	244	GLN
3	K	251	ASN

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Mol	Chain	Res	Type
3	K	484	ASN
3	K	517	ASN
3	K	564	GLN
3	O	31	ASN
3	O	150	ASN
3	O	163	ASN
3	O	244	GLN
3	O	251	ASN
3	O	484	ASN
3	O	517	ASN
3	O	564	GLN
3	S	31	ASN
3	S	150	ASN
3	S	244	GLN
3	S	517	ASN
3	S	564	GLN
3	W	29	GLN
3	W	31	ASN
3	W	150	ASN
3	W	163	ASN
3	W	517	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	11/12 (91%)	5 (45%)	0
4	H	11/12 (91%)	5 (45%)	0
4	L	11/12 (91%)	5 (45%)	1 (9%)
4	P	11/12 (91%)	5 (45%)	0
4	T	11/12 (91%)	5 (45%)	0
4	X	11/12 (91%)	5 (45%)	1 (9%)
All	All	66/72 (91%)	30 (45%)	2 (3%)

All (30) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	3	C
4	D	7	A
4	D	8	G
4	D	11	G
4	D	12	A

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Mol	Chain	Res	Type
4	H	3	C
4	H	7	A
4	H	8	G
4	H	11	G
4	H	12	A
4	L	3	C
4	L	7	A
4	L	8	G
4	L	11	G
4	L	12	A
4	P	3	C
4	P	7	A
4	P	8	G
4	P	11	G
4	P	12	A
4	T	3	C
4	T	7	A
4	T	8	G
4	T	11	G
4	T	12	A
4	X	3	C
4	X	7	A
4	X	8	G
4	X	11	G
4	X	12	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	L	5	G
4	X	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	703/751 (93%)	0.16	13 (1%) 67 51	108, 190, 258, 348	0
1	E	703/751 (93%)	0.21	16 (2%) 61 46	115, 214, 280, 335	0
1	I	708/751 (94%)	0.14	15 (2%) 63 48	103, 198, 269, 354	0
1	M	703/751 (93%)	0.16	9 (1%) 75 58	111, 222, 292, 352	0
1	Q	703/751 (93%)	0.09	10 (1%) 73 56	105, 211, 278, 388	0
1	U	703/751 (93%)	0.08	6 (0%) 81 65	111, 213, 276, 338	0
2	B	756/772 (97%)	0.04	8 (1%) 78 61	103, 163, 216, 276	0
2	F	756/772 (97%)	0.13	10 (1%) 75 58	110, 182, 241, 298	0
2	J	756/772 (97%)	0.10	16 (2%) 63 48	88, 157, 228, 301	0
2	N	756/772 (97%)	0.14	9 (1%) 76 60	91, 181, 247, 297	0
2	R	756/772 (97%)	0.11	16 (2%) 63 48	100, 170, 231, 306	0
2	V	756/772 (97%)	0.12	16 (2%) 63 48	100, 172, 239, 302	0
3	C	761/798 (95%)	0.15	16 (2%) 63 48	97, 192, 261, 362	0
3	G	759/798 (95%)	0.18	14 (1%) 67 51	116, 203, 265, 391	0
3	K	759/798 (95%)	0.20	14 (1%) 67 51	106, 176, 256, 336	0
3	O	759/798 (95%)	0.17	15 (1%) 65 49	121, 188, 258, 353	0
3	S	759/798 (95%)	0.28	18 (2%) 59 45	104, 192, 296, 382	0
3	W	618/798 (77%)	0.25	10 (1%) 70 53	114, 188, 261, 361	0
4	D	12/12 (100%)	-0.32	0 100 100	163, 174, 202, 224	0
4	H	12/12 (100%)	-0.24	0 100 100	177, 206, 218, 219	0
4	L	12/12 (100%)	-0.21	0 100 100	151, 190, 224, 232	0
4	P	12/12 (100%)	-0.27	0 100 100	175, 208, 246, 251	0
4	T	12/12 (100%)	-0.28	0 100 100	187, 211, 225, 235	0
4	X	12/12 (100%)	-0.09	0 100 100	172, 202, 232, 233	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	13246/13998 (94%)	0.15	231 (1%)	69	52	88, 188, 266, 391	0

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	301	ALA	5.4
3	O	450	GLN	5.3
3	S	647	GLU	5.2
3	S	645	GLY	4.7
1	A	294	MET	4.4
1	I	514	VAL	4.4
3	K	180	SER	4.3
1	M	521	PHE	4.2
3	K	434	TYR	4.1
1	I	716	VAL	4.1
1	A	50	ASP	3.9
2	F	24	TYR	3.9
3	S	630	SER	3.8
3	K	559	VAL	3.8
2	J	672	SER	3.7
3	C	302	ALA	3.7
1	E	572	GLU	3.7
1	E	562	THR	3.7
2	B	645	THR	3.7
2	F	343	LEU	3.6
2	V	502	SER	3.5
3	K	745	SER	3.5
2	R	669	ARG	3.4
3	S	675	MET	3.3
1	U	116	LYS	3.3
2	N	667	THR	3.3
2	J	670	ASN	3.2
3	C	120	PHE	3.2
3	K	766	GLY	3.2
3	S	648	ASN	3.2
1	A	661	LEU	3.2
3	O	294	GLU	3.2
1	U	480	PRO	3.2
3	K	644	GLY	3.2
3	K	155	GLU	3.1
3	S	434	TYR	3.1
3	O	506	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	Q	177	LEU	3.1
2	R	279	LYS	3.1
1	I	562	THR	3.1
2	V	267	GLU	3.0
3	C	87	GLY	3.0
2	F	197	LYS	3.0
1	Q	662	LEU	3.0
3	G	286	ALA	3.0
2	F	413	PHE	3.0
3	G	173	GLU	3.0
3	O	87	GLY	3.0
3	S	347	LEU	2.9
2	F	30	TYR	2.9
2	N	645	THR	2.9
1	M	461	PHE	2.9
1	I	492	SER	2.9
3	C	319	LEU	2.9
1	M	514	VAL	2.8
1	I	45	CYS	2.8
1	I	512	ASP	2.8
1	I	485	VAL	2.8
3	O	41	ILE	2.8
2	J	645	THR	2.8
3	C	143	VAL	2.8
2	J	658	ALA	2.8
2	F	409	MET	2.8
2	V	134	CYS	2.8
3	K	325	GLN	2.8
3	S	618	LEU	2.8
3	W	695	LEU	2.7
1	Q	315	THR	2.7
3	K	673	ARG	2.7
2	R	75	GLU	2.7
2	J	667	THR	2.7
1	A	664	LEU	2.7
3	O	533	ASP	2.7
3	S	616	ILE	2.7
1	Q	195	ASP	2.7
3	S	341	LYS	2.7
2	B	721	LEU	2.7
3	W	373	ARG	2.6
3	C	495	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	R	645	THR	2.6
2	J	387	ALA	2.6
2	J	191	LEU	2.6
2	J	390	LYS	2.6
3	C	304	ASP	2.6
1	I	18	LYS	2.6
1	E	662	LEU	2.6
3	G	258	SER	2.6
2	R	9	PHE	2.6
3	O	510	GLY	2.6
3	O	638	LEU	2.6
3	W	319	LEU	2.6
3	W	414	GLN	2.6
3	K	506	ILE	2.6
2	R	23	PRO	2.6
1	M	347	ILE	2.6
2	N	232	GLU	2.6
1	I	513	VAL	2.6
2	V	381	TYR	2.6
3	O	293	THR	2.6
1	M	457	LYS	2.5
1	A	485	VAL	2.5
2	J	519	SER	2.5
1	M	455	MET	2.5
1	E	20	THR	2.5
2	B	267	GLU	2.5
2	J	694	LEU	2.5
2	V	698	CYS	2.5
2	F	196	ARG	2.5
1	E	60	ALA	2.5
1	M	315	THR	2.5
1	I	279	TYR	2.5
3	S	650	ILE	2.5
1	A	703	PHE	2.5
1	Q	43	GLU	2.5
2	N	480	LYS	2.5
1	A	282	PHE	2.4
3	C	300	LEU	2.4
1	Q	176	GLU	2.4
2	J	758	GLU	2.4
3	O	292	ASP	2.4
2	N	660	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	V	669	ARG	2.4
3	W	762	VAL	2.4
1	A	544	LEU	2.4
1	Q	299	SER	2.4
1	E	586	ALA	2.4
2	B	194	LYS	2.4
2	R	98	GLU	2.4
3	G	88	THR	2.4
2	N	519	SER	2.4
3	K	471	ALA	2.4
2	V	507	GLU	2.4
2	R	511	PHE	2.4
1	E	530	SER	2.3
3	G	762	VAL	2.3
2	J	398	GLU	2.3
3	S	646	GLY	2.3
3	C	88	THR	2.3
2	F	565	SER	2.3
3	G	296	LEU	2.3
3	S	159	ASP	2.3
1	A	32	PRO	2.3
1	E	374	LYS	2.3
2	V	409	MET	2.3
3	G	341	LYS	2.3
2	J	32	HIS	2.3
3	O	434	TYR	2.3
3	W	434	TYR	2.3
2	F	281	LYS	2.3
3	S	703	LYS	2.3
3	W	450	GLN	2.3
3	O	88	THR	2.3
2	B	722	ARG	2.3
2	V	1	MET	2.3
3	C	265	CYS	2.3
2	R	24	TYR	2.3
1	E	703	PHE	2.3
1	U	118	PHE	2.3
1	I	298	LYS	2.3
2	J	671	ARG	2.3
3	G	87	GLY	2.2
3	G	90	GLY	2.2
2	J	267	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	R	353	LYS	2.2
1	I	28	PRO	2.2
3	W	374	GLY	2.2
1	E	661	LEU	2.2
3	W	59	LEU	2.2
3	S	745	SER	2.2
1	E	15	GLN	2.2
2	V	224	LEU	2.2
3	G	653	ARG	2.2
2	V	645	THR	2.2
3	S	559	VAL	2.2
2	R	500	PHE	2.2
2	V	85	LEU	2.2
2	N	409	MET	2.2
2	R	506	MET	2.2
1	E	282	PHE	2.2
2	R	282	LEU	2.2
3	C	316	ALA	2.1
3	K	87	GLY	2.1
2	R	570	LYS	2.1
2	V	602	ASN	2.1
2	V	688	TYR	2.1
1	A	285	MET	2.1
1	Q	612	PRO	2.1
1	U	265	ILE	2.1
1	Q	486	VAL	2.1
3	O	326	ARG	2.1
1	I	60	ALA	2.1
3	S	649	PHE	2.1
1	A	280	ASN	2.1
1	U	86	THR	2.1
2	R	751	TYR	2.1
1	A	533	TRP	2.1
3	C	341	LYS	2.1
3	S	545	GLU	2.1
1	A	265	ILE	2.1
1	E	375	ILE	2.1
3	C	406	PHE	2.1
2	N	483	CYS	2.1
1	Q	285	MET	2.1
1	E	535	LYS	2.1
3	G	745	SER	2.1

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Mol	Chain	Res	Type	RSRZ
3	O	745	SER	2.1
1	I	280	ASN	2.1
1	M	20	THR	2.1
2	J	504	PHE	2.1
1	I	278	PRO	2.1
3	C	180	SER	2.1
2	B	677	ASP	2.1
2	F	364	LEU	2.1
3	K	332	LEU	2.1
1	U	5	ILE	2.1
3	K	181	THR	2.1
2	B	409	MET	2.0
3	G	144	ARG	2.0
2	V	751	TYR	2.0
3	G	434	TYR	2.0
1	M	566	GLN	2.0
2	V	501	VAL	2.0
2	B	340	ALA	2.0
2	N	81	ALA	2.0
1	E	43	GLU	2.0
1	E	482	THR	2.0
3	C	371	GLU	2.0
3	G	302	ALA	2.0
3	W	83	ALA	2.0
2	R	123	THR	2.0
3	O	341	LYS	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 oligosaccharides 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.