wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 07:27 AM EDT

PDB ID	:	5EPI
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

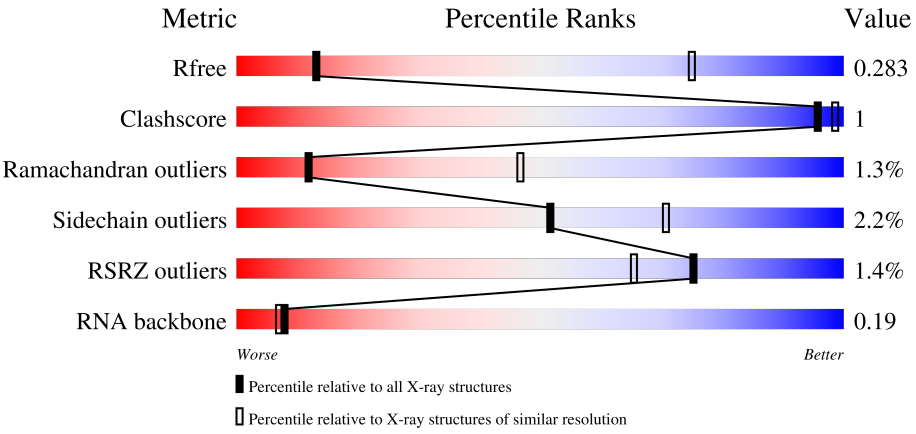
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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}	130704	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)
RNA backbone	3102	1049 (5.04-3.00)

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 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 <=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	% 92% • 6%
1	I	751	2% 91% • 6%
1	M	751	2% 92% • 6%

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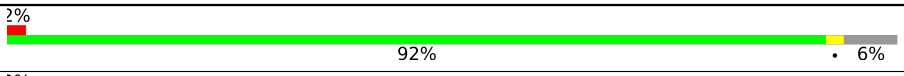
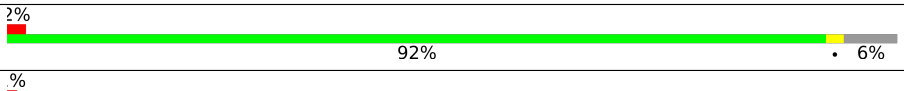
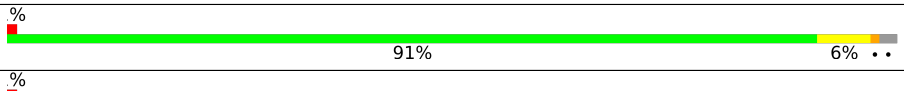
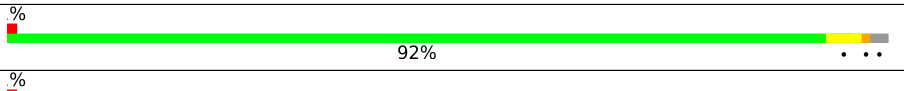
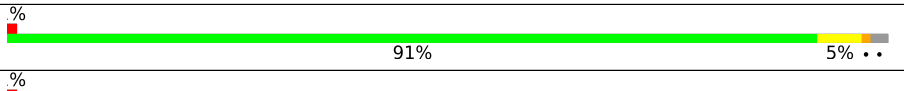
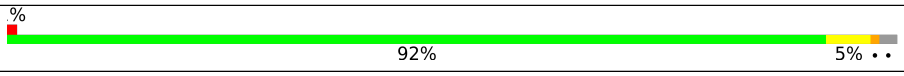
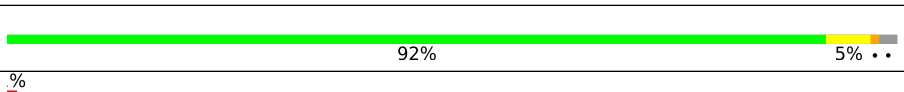
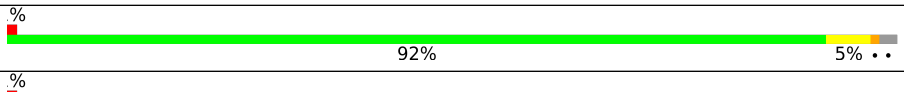
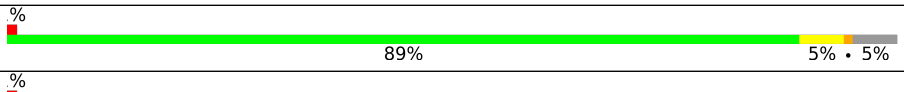
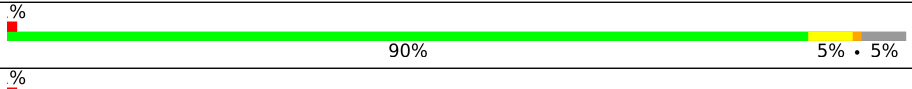
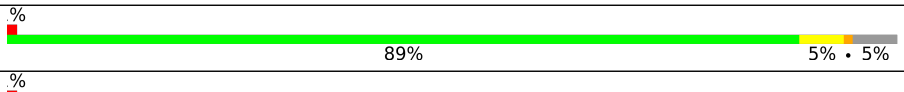
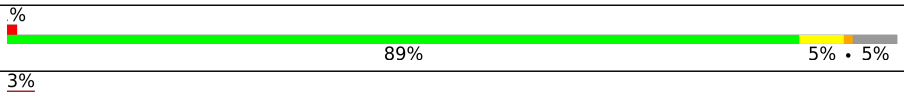
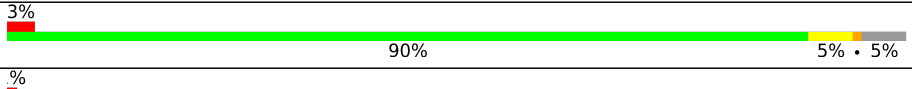
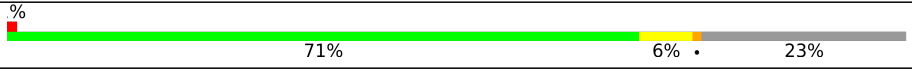
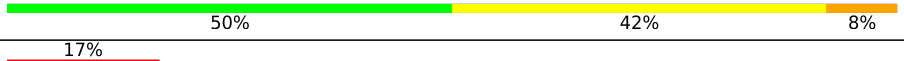
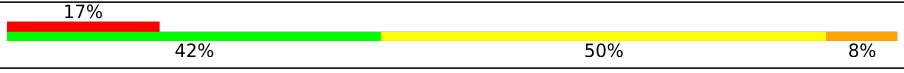
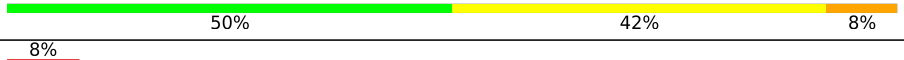
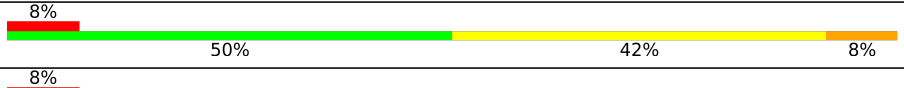
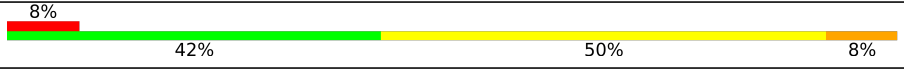
Mol	Chain	Length	Quality of chain
1	Q	751	
1	U	751	
2	B	772	
2	F	772	
2	J	772	
2	N	772	
2	R	772	
2	V	772	
3	C	798	
3	G	798	
3	K	798	
3	O	798	
3	S	798	
3	W	798	
4	D	12	
4	H	12	
4	L	12	
4	P	12	
4	T	12	
4	X	12	

2 Entry composition (i)

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.

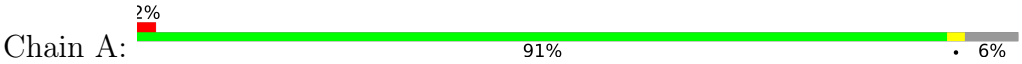
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	12	Total	C	N	O	P	0	0	0
			265	118	56	79	12			
4	H	12	Total	C	N	O	P	0	0	0
			265	118	56	79	12			
4	L	12	Total	C	N	O	P	0	0	0
			265	118	56	79	12			
4	P	12	Total	C	N	O	P	0	0	0
			265	118	56	79	12			
4	T	12	Total	C	N	O	P	0	0	0
			265	118	56	79	12			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

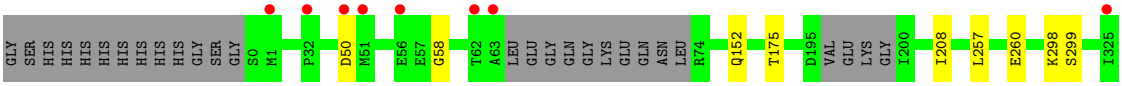
3 Residue-property plots (i)

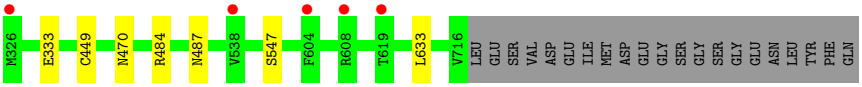
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Polymerase acidic protein

Chain A:

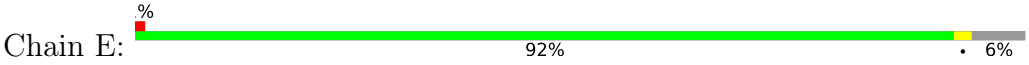


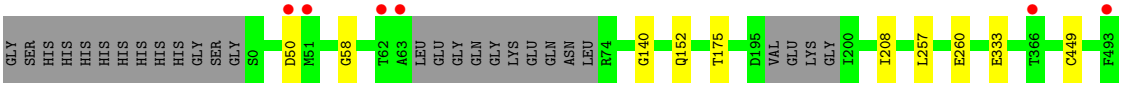


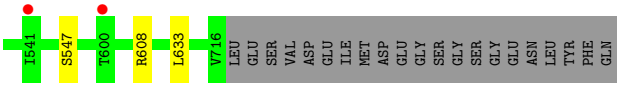


• Molecule 1: Polymerase acidic protein

Chain E:

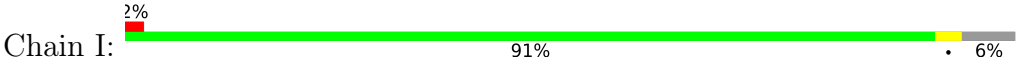


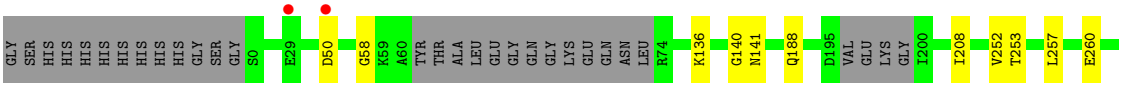


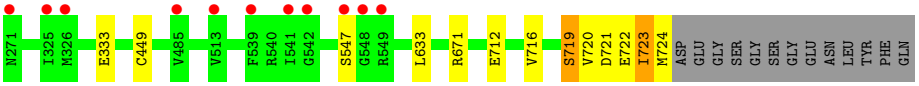


• Molecule 1: Polymerase acidic protein

Chain I:

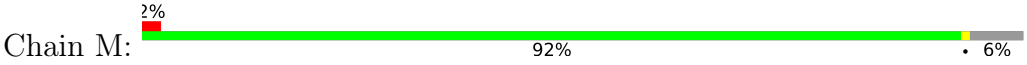


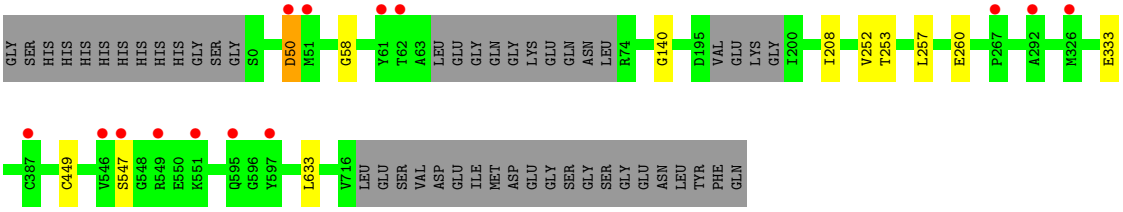




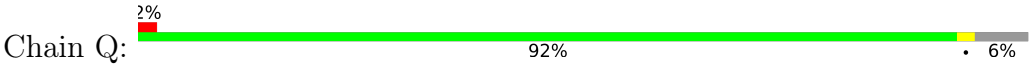
• Molecule 1: Polymerase acidic protein

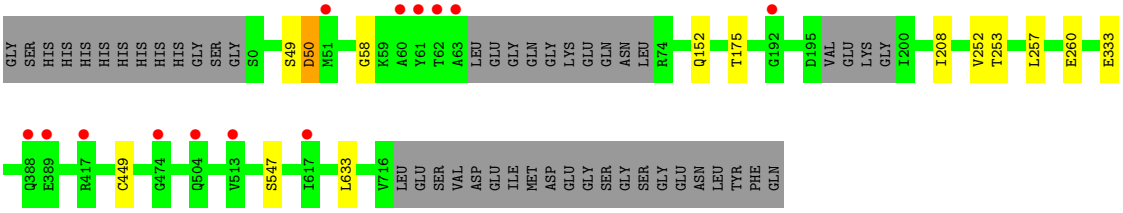
Chain M:



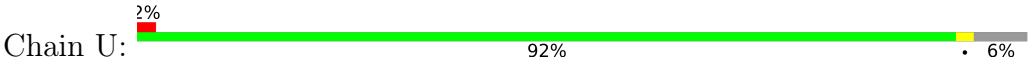


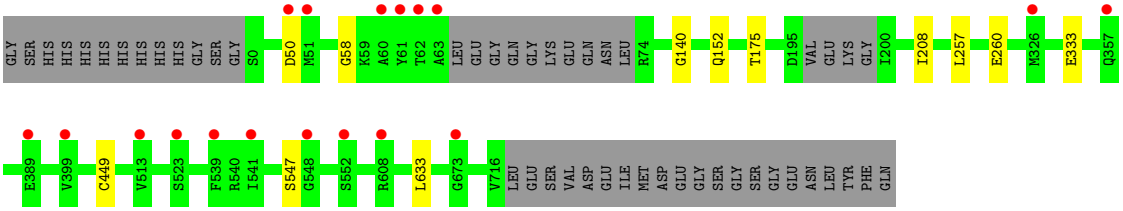
• Molecule 1: Polymerase acidic protein



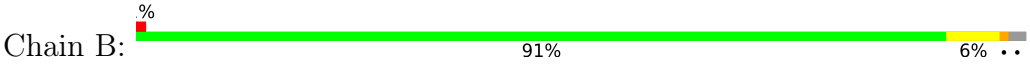


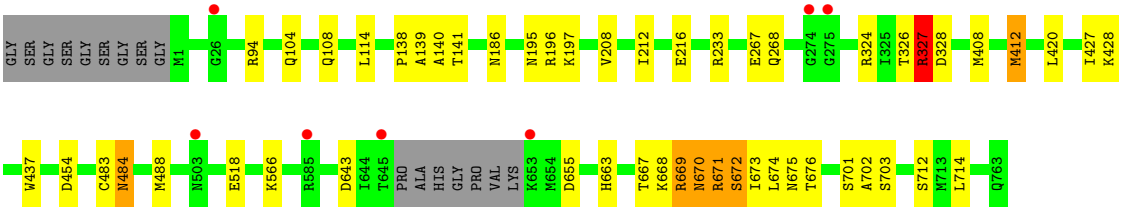
• Molecule 1: Polymerase acidic protein



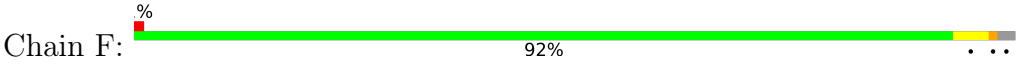


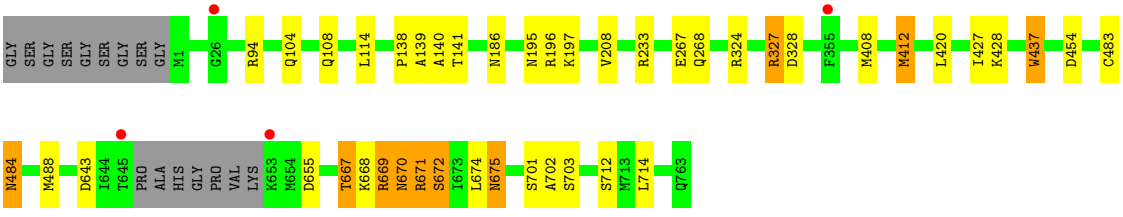
• Molecule 2: RNA-directed RNA polymerase catalytic subunit





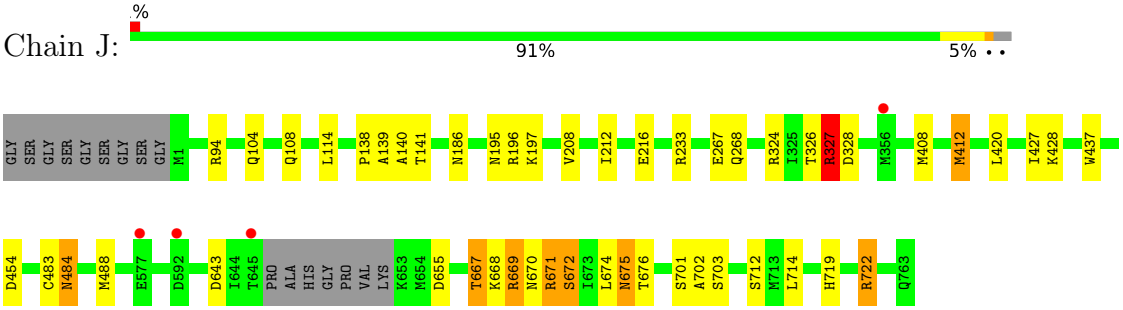
• Molecule 2: RNA-directed RNA polymerase catalytic subunit





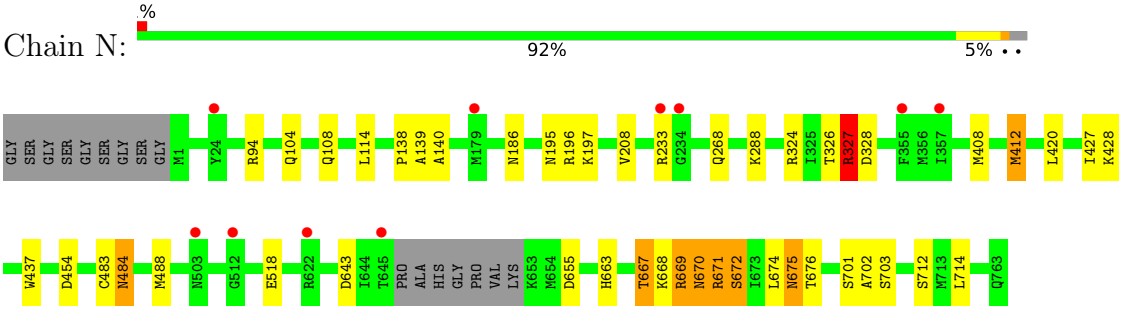
• Molecule 2: RNA-directed RNA polymerase catalytic subunit

Chain J:



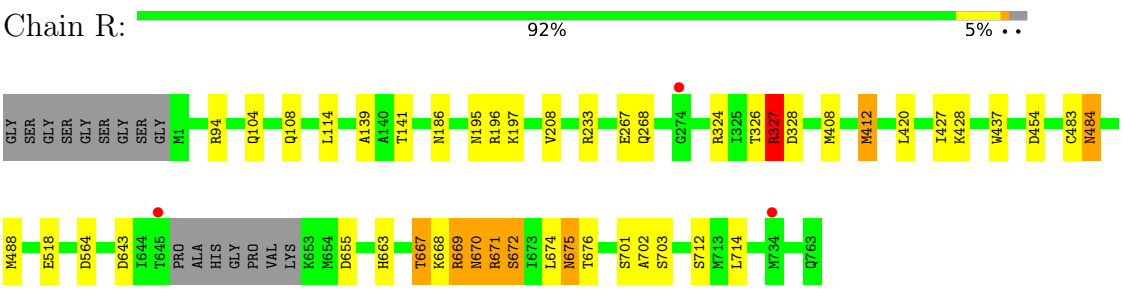
• Molecule 2: RNA-directed RNA polymerase catalytic subunit

Chain N:



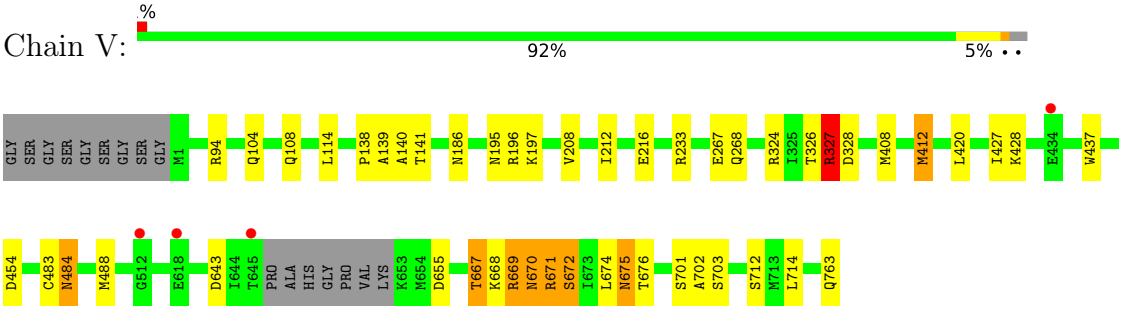
• Molecule 2: RNA-directed RNA polymerase catalytic subunit

Chain R:



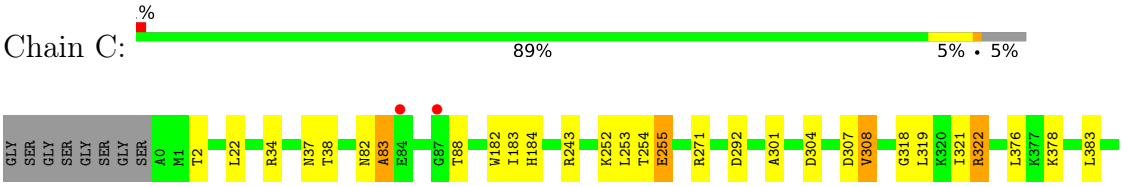
• Molecule 2: RNA-directed RNA polymerase catalytic subunit

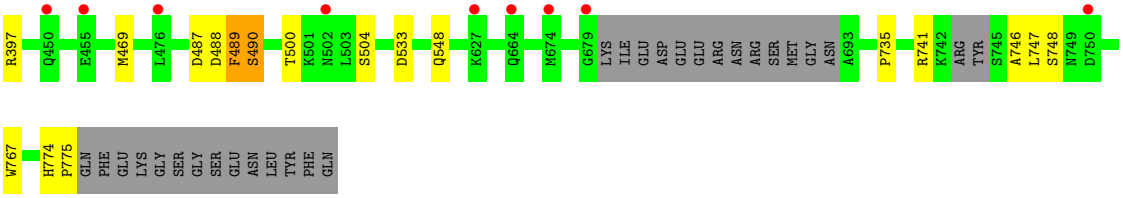
Chain V:



• Molecule 3: Polymerase basic protein 2

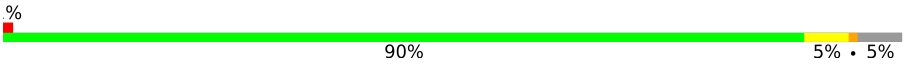
Chain C:

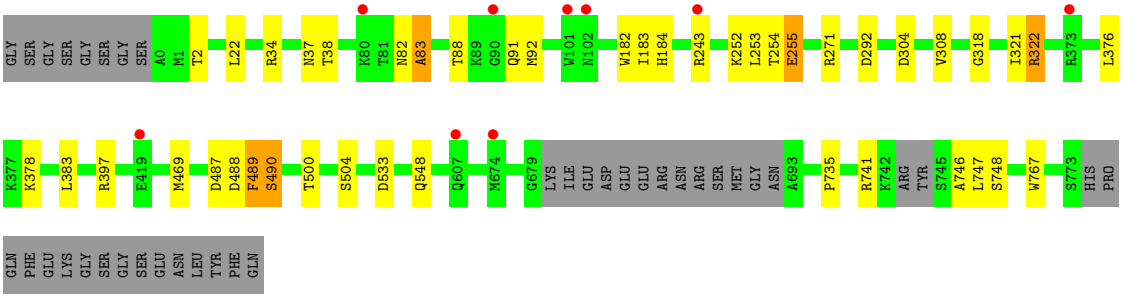




• Molecule 3: Polymerase basic protein 2

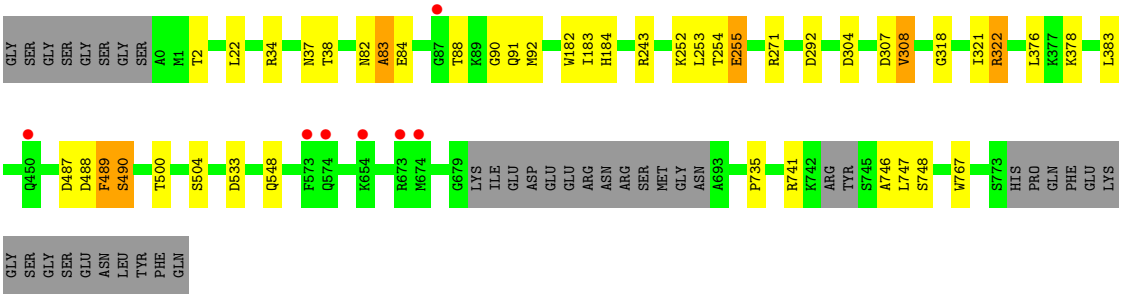
Chain G:





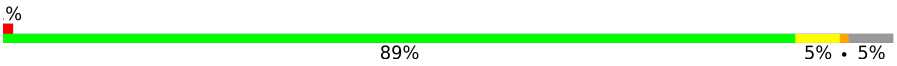
• Molecule 3: Polymerase basic protein 2

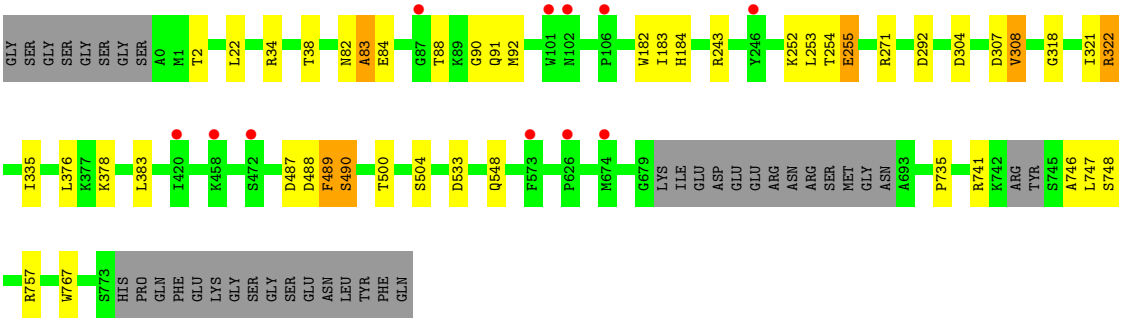
Chain K:



• Molecule 3: Polymerase basic protein 2

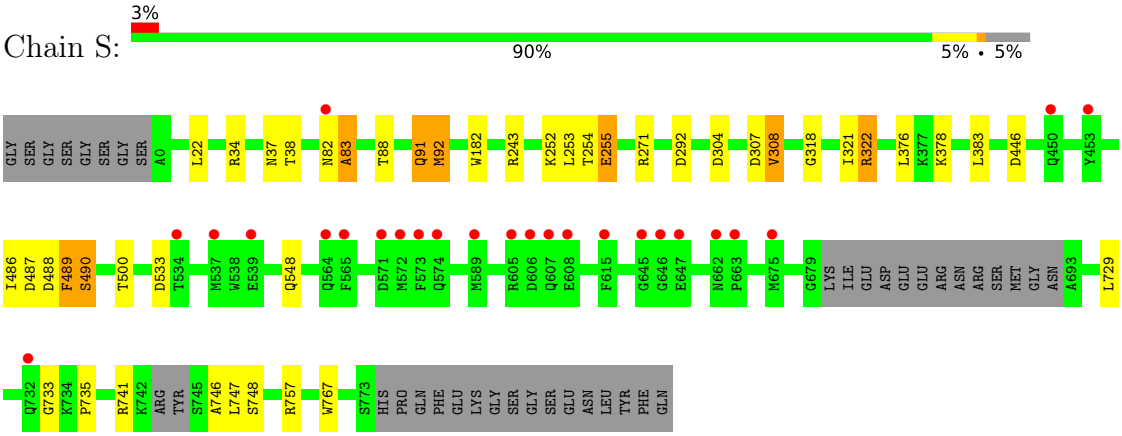
Chain O:





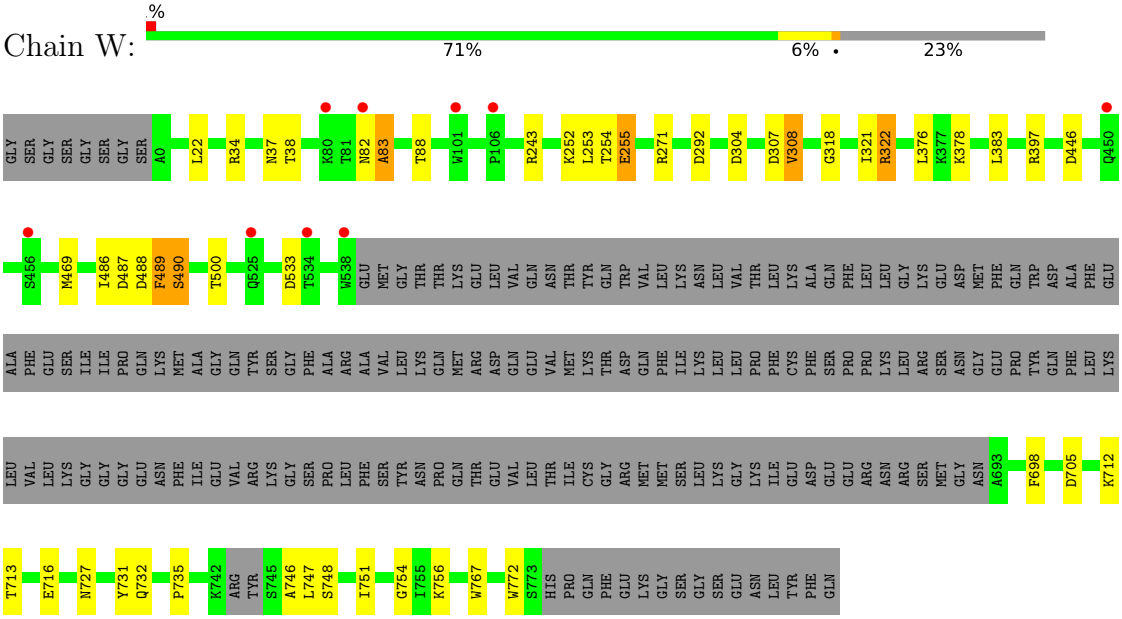
• Molecule 3: Polymerase basic protein 2

Chain S:



• Molecule 3: Polymerase basic protein 2

Chain W:

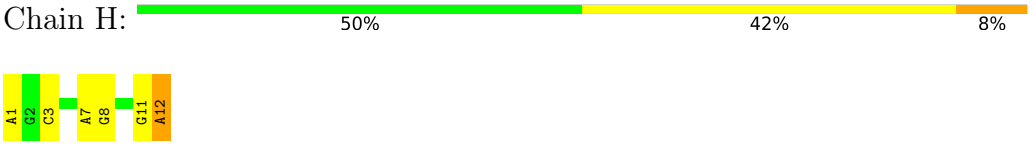


• Molecule 4: CRNA 5' END

Chain D:

• Molecule 4: CRNA 5' END

Chain H:

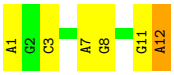


• Molecule 4: CRNA 5' END

Chain L:

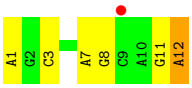
• Molecule 4: CRNA 5' END

Chain P:



• Molecule 4: CRNA 5' END

Chain T:



• Molecule 4: CRNA 5' END

Chain X:

4 Data and refinement statistics (i)

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 49.94 – 4.10	Depositor EDS
% Data completeness (in resolution range)	93.2 (49.95-4.10) 93.2 (49.94-4.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 4.14Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.257 , 0.287 0.258 , 0.283	Depositor DCC
R_{free} test set	7765 reflections (4.13%)	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)	0.25 , 100.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.24	0/5761	0.41	0/7768
1	E	0.24	0/5761	0.40	0/7768
1	I	0.24	0/5799	0.40	0/7818
1	M	0.24	0/5761	0.40	0/7768
1	Q	0.24	0/5761	0.40	0/7768
1	U	0.24	0/5761	0.40	0/7768
2	B	0.25	0/6042	0.42	0/8143
2	F	0.25	0/6042	0.42	0/8143
2	J	0.25	0/6042	0.42	0/8143
2	N	0.25	0/6042	0.42	0/8143
2	R	0.25	0/6042	0.42	0/8143
2	V	0.25	0/6042	0.42	0/8143
3	C	0.25	0/6184	0.43	0/8314
3	G	0.25	0/6165	0.43	0/8287
3	K	0.25	0/6165	0.43	0/8287
3	O	0.24	0/6165	0.43	0/8287
3	S	0.24	0/6165	0.43	0/8287
3	W	0.25	0/5003	0.44	0/6725
4	D	0.65	1/298 (0.3%)	0.69	0/462
4	H	0.64	1/298 (0.3%)	0.69	0/462
4	L	0.66	1/298 (0.3%)	0.70	0/462
4	P	0.65	1/298 (0.3%)	0.69	0/462
4	T	0.65	1/298 (0.3%)	0.71	0/462
4	X	0.65	1/298 (0.3%)	0.70	0/462
All	All	0.26	6/108491 (0.0%)	0.43	0/146475

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1	A	OP3-P	-10.70	1.48	1.61
4	T	1	A	OP3-P	-10.67	1.48	1.61
4	D	1	A	OP3-P	-10.61	1.48	1.61
4	H	1	A	OP3-P	-10.60	1.48	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	1	A	OP3-P	-10.58	1.48	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	5646	0	5621	3	1
1	E	5646	0	5621	1	0
1	I	5685	0	5661	12	1
1	M	5646	0	5621	2	0
1	Q	5646	0	5621	4	0
1	U	5646	0	5621	1	0
2	B	5927	0	5929	20	0
2	F	5927	0	5929	17	0
2	J	5927	0	5929	20	0
2	N	5927	0	5929	20	0
2	R	5927	0	5929	18	0
2	V	5927	0	5929	19	0
3	C	6078	0	6240	18	0
3	G	6061	0	6226	17	0
3	K	6061	0	6226	17	0
3	O	6061	0	6226	20	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	227	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.

The worst 5 of 227 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
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

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%)	34	71
1	E	697/751 (93%)	662 (95%)	31 (4%)	4 (1%)	25	63
1	I	702/751 (94%)	666 (95%)	31 (4%)	5 (1%)	22	60
1	M	697/751 (93%)	662 (95%)	31 (4%)	4 (1%)	25	63
1	Q	697/751 (93%)	662 (95%)	32 (5%)	3 (0%)	34	71
1	U	697/751 (93%)	662 (95%)	31 (4%)	4 (1%)	25	63
2	B	752/772 (97%)	692 (92%)	50 (7%)	10 (1%)	12	47
2	F	752/772 (97%)	693 (92%)	49 (6%)	10 (1%)	12	47
2	J	752/772 (97%)	693 (92%)	49 (6%)	10 (1%)	12	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	N	752/772 (97%)	694 (92%)	48 (6%)	10 (1%)	12 47
2	R	752/772 (97%)	693 (92%)	49 (6%)	10 (1%)	12 47
2	V	752/772 (97%)	694 (92%)	48 (6%)	10 (1%)	12 47
3	C	755/798 (95%)	681 (90%)	59 (8%)	15 (2%)	7 39
3	G	753/798 (94%)	679 (90%)	59 (8%)	15 (2%)	7 39
3	K	753/798 (94%)	677 (90%)	61 (8%)	15 (2%)	7 39
3	O	753/798 (94%)	677 (90%)	61 (8%)	15 (2%)	7 39
3	S	753/798 (94%)	678 (90%)	62 (8%)	13 (2%)	9 42
3	W	612/798 (77%)	547 (89%)	52 (8%)	13 (2%)	7 38
All	All	13078/13926 (94%)	12072 (92%)	837 (6%)	169 (1%)	12 47

5 of 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

5.3.2 Protein sidechains (i)

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%)	618 (99%)	7 (1%)	73 84
1	E	625/664 (94%)	618 (99%)	7 (1%)	73 84
1	I	631/664 (95%)	623 (99%)	8 (1%)	69 81
1	M	625/664 (94%)	619 (99%)	6 (1%)	76 85
1	Q	625/664 (94%)	619 (99%)	6 (1%)	76 85
1	U	625/664 (94%)	619 (99%)	6 (1%)	76 85
2	B	647/657 (98%)	626 (97%)	21 (3%)	39 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	647/657 (98%)	625 (97%)	22 (3%)	37	61
2	J	647/657 (98%)	624 (96%)	23 (4%)	35	60
2	N	647/657 (98%)	626 (97%)	21 (3%)	39	62
2	R	647/657 (98%)	625 (97%)	22 (3%)	37	61
2	V	647/657 (98%)	625 (97%)	22 (3%)	37	61
3	C	664/694 (96%)	652 (98%)	12 (2%)	59	77
3	G	662/694 (95%)	649 (98%)	13 (2%)	55	73
3	K	662/694 (95%)	650 (98%)	12 (2%)	59	77
3	O	662/694 (95%)	650 (98%)	12 (2%)	59	77
3	S	662/694 (95%)	648 (98%)	14 (2%)	53	72
3	W	538/694 (78%)	521 (97%)	17 (3%)	39	62
All	All	11488/12090 (95%)	11237 (98%)	251 (2%)	52	71

5 of 251 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	327	ARG
3	S	88	THR
2	R	484	ASN
3	O	767	TRP
3	W	243	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

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%)

5 of 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

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.07	13 (1%) 68 59	108, 190, 258, 348	0
1	E	703/751 (93%)	-0.02	8 (1%) 80 72	115, 214, 280, 335	0
1	I	708/751 (94%)	-0.10	13 (1%) 68 59	103, 198, 269, 354	0
1	M	703/751 (93%)	0.00	14 (1%) 65 56	111, 222, 292, 352	0
1	Q	703/751 (93%)	-0.05	13 (1%) 68 59	105, 211, 278, 388	0
1	U	703/751 (93%)	0.00	18 (2%) 56 45	111, 213, 276, 338	0
2	B	756/772 (97%)	-0.19	7 (0%) 84 77	103, 163, 216, 276	0
2	F	756/772 (97%)	-0.15	4 (0%) 91 85	110, 182, 241, 298	0
2	J	756/772 (97%)	-0.22	4 (0%) 91 85	88, 157, 228, 301	0
2	N	756/772 (97%)	-0.12	10 (1%) 77 68	91, 181, 247, 297	0
2	R	756/772 (97%)	-0.19	3 (0%) 92 87	100, 170, 231, 306	0
2	V	756/772 (97%)	-0.18	4 (0%) 91 85	100, 172, 239, 302	0
3	C	761/798 (95%)	-0.05	11 (1%) 75 65	97, 192, 261, 362	0
3	G	759/798 (95%)	-0.05	9 (1%) 79 70	116, 203, 265, 391	0
3	K	759/798 (95%)	-0.13	7 (0%) 84 77	106, 176, 256, 336	0
3	O	759/798 (95%)	-0.09	11 (1%) 75 65	121, 188, 258, 353	0
3	S	759/798 (95%)	0.01	25 (3%) 46 37	104, 192, 296, 382	0
3	W	618/798 (77%)	-0.14	9 (1%) 73 63	114, 188, 261, 361	0
4	D	12/12 (100%)	0.37	0 100 100	163, 174, 202, 224	0
4	H	12/12 (100%)	0.42	0 100 100	177, 206, 218, 219	0
4	L	12/12 (100%)	1.08	2 (16%) 1 2	151, 190, 224, 232	0
4	P	12/12 (100%)	0.97	0 100 100	175, 208, 246, 251	0
4	T	12/12 (100%)	0.93	1 (8%) 11 10	187, 211, 225, 235	0
4	X	12/12 (100%)	0.92	1 (8%) 11 10	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%)	-0.09	187 (1%)	75	65	88, 188, 266, 391	0

The worst 5 of 187 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	63	ALA	8.8
1	Q	61	TYR	8.5
2	N	645	THR	7.6
2	J	645	THR	7.4
1	U	61	TYR	6.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.