



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2016 – 12:01 AM GMT

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 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

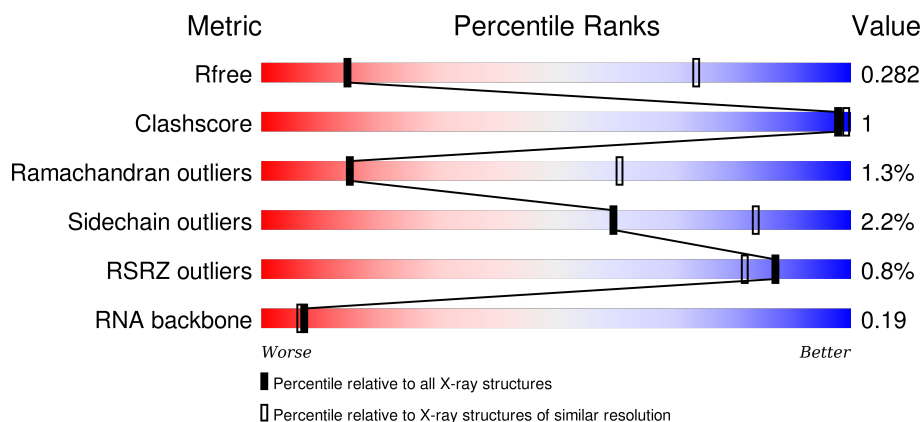
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



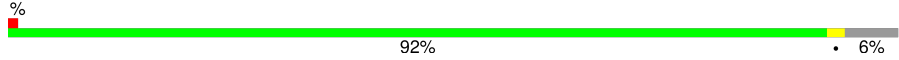
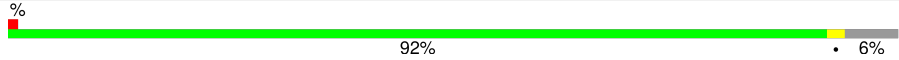
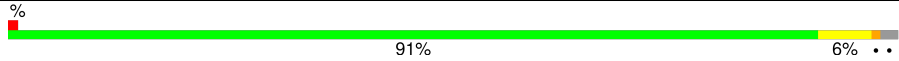
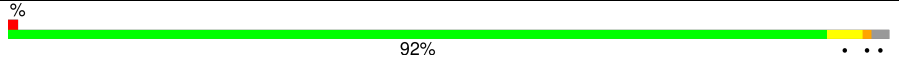
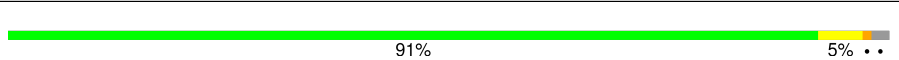
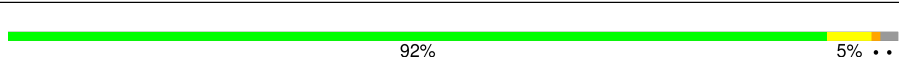
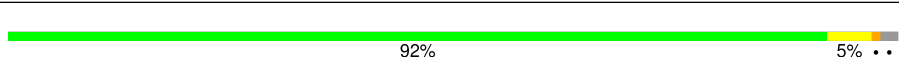
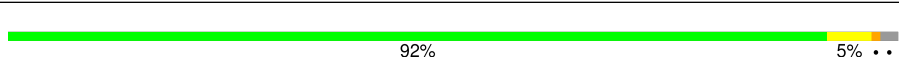
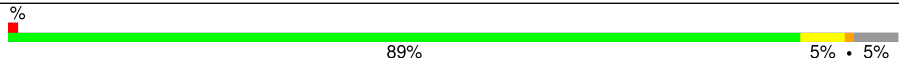
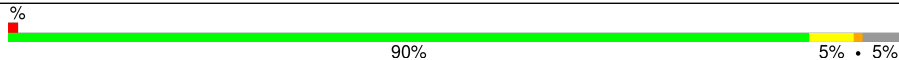


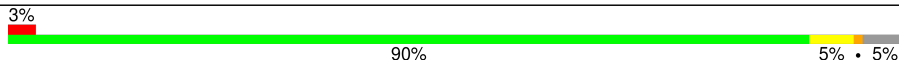
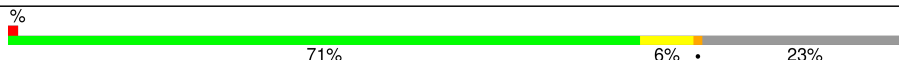


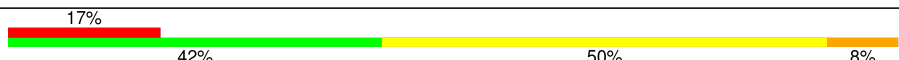


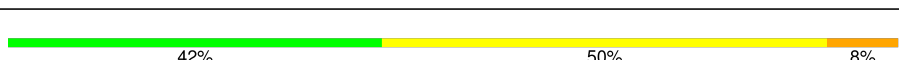
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1018 (4.60-3.60)
Clashscore	102246	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)
RSRZ outliers	91569	1022 (4.60-3.60)
RNA backbone	2183	1079 (5.04-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div style="width: 91%;"></div> <div style="width: 6%;"></div> </div>
1	E	751	<div> <div style="width: 92%;"></div> <div style="width: 6%;"></div> </div>
1	I	751	<div> <div style="width: 91%;"></div> <div style="width: 6%;"></div> </div>
1	M	751	<div> <div style="width: 92%;"></div> <div style="width: 6%;"></div> </div>

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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

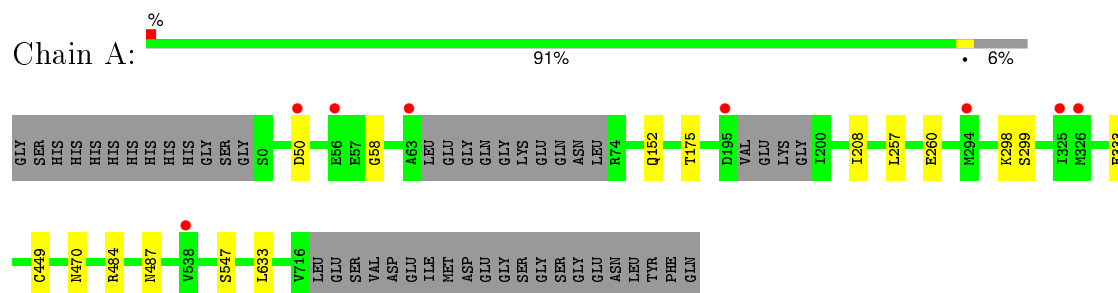
- Molecule 4 is a RNA chain called CRNA 5' END.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	12	Total 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

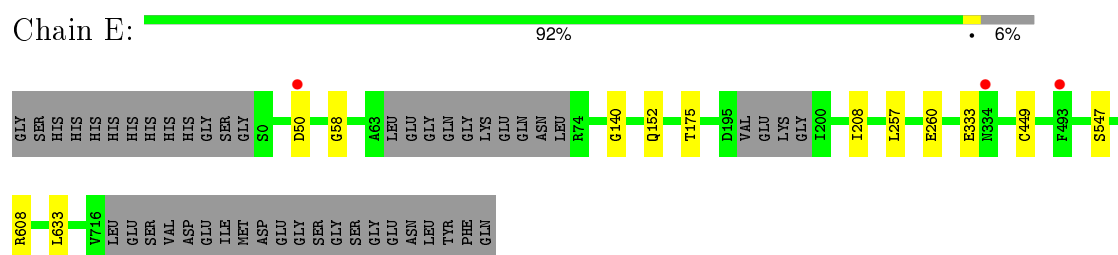
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

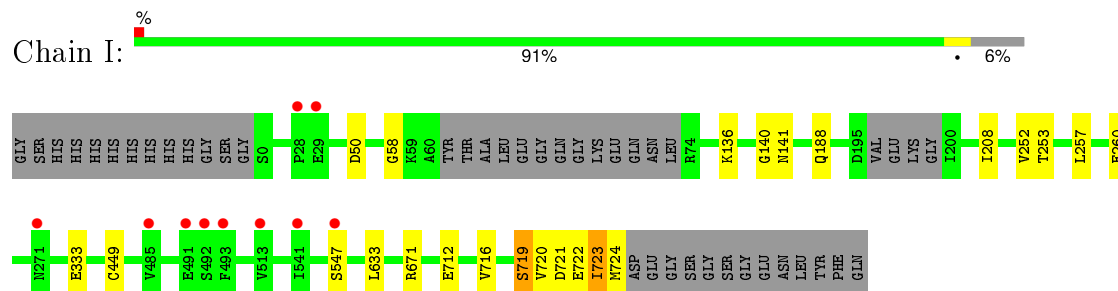
- Molecule 1: Polymerase acidic protein



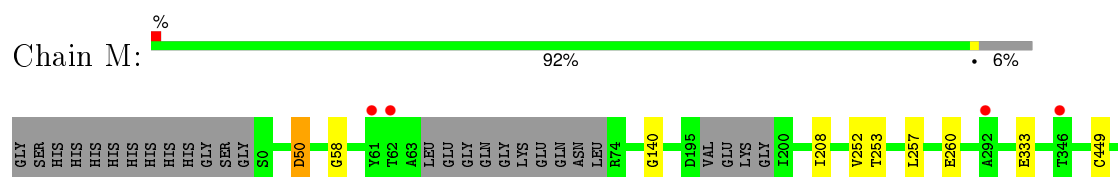
- Molecule 1: Polymerase acidic protein

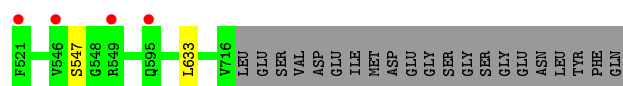


- Molecule 1: Polymerase acidic protein

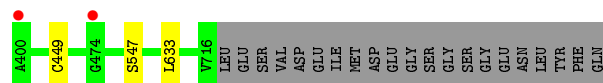
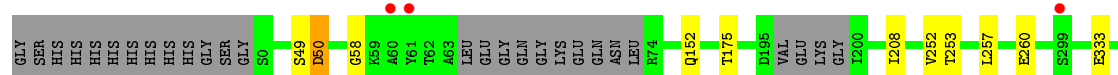
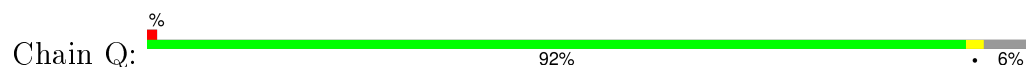


- Molecule 1: Polymerase acidic protein

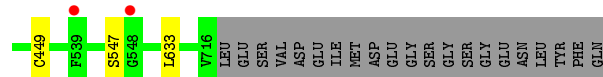
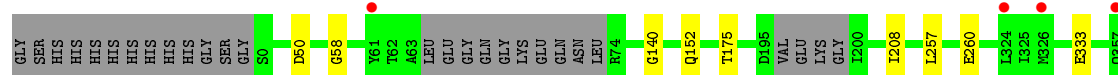
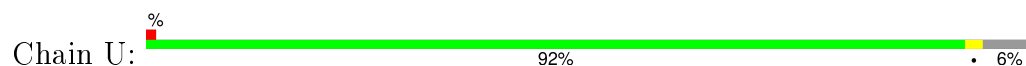




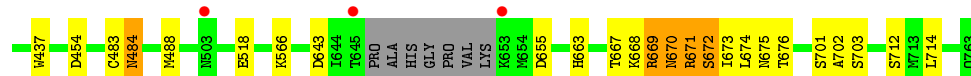
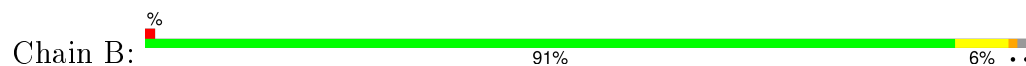
- Molecule 1: Polymerase acidic protein



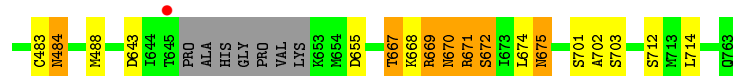
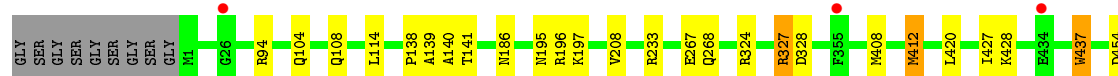
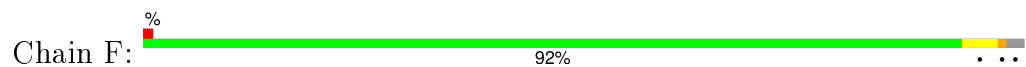
- Molecule 1: Polymerase acidic protein



- Molecule 2: RNA-directed RNA polymerase catalytic subunit

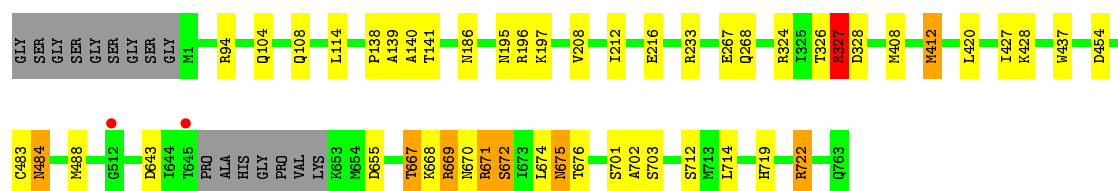


- Molecule 2: RNA-directed RNA polymerase catalytic subunit



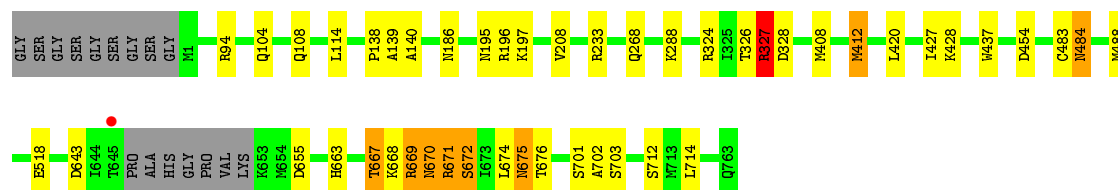
- Molecule 2: RNA-directed RNA polymerase catalytic subunit





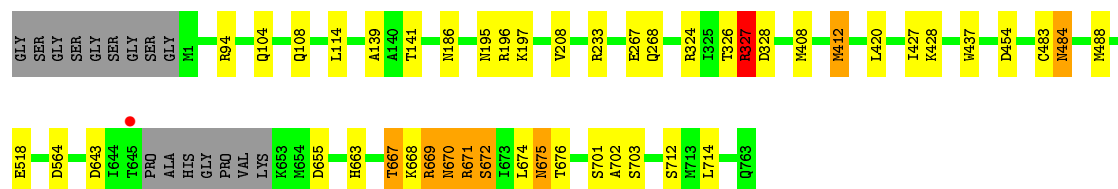
- Molecule 2: RNA-directed RNA polymerase catalytic subunit

Chain N: 92% 5% ..



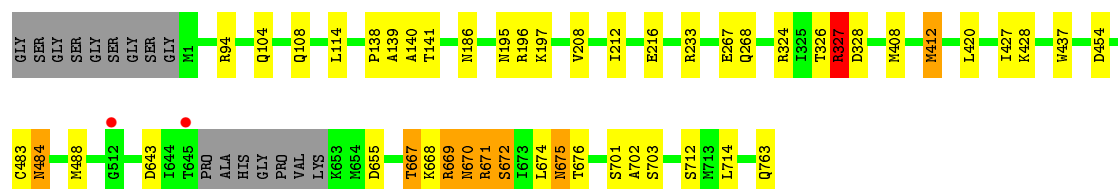
- Molecule 2: RNA-directed RNA polymerase catalytic subunit

Chain R: 92% 5% ..



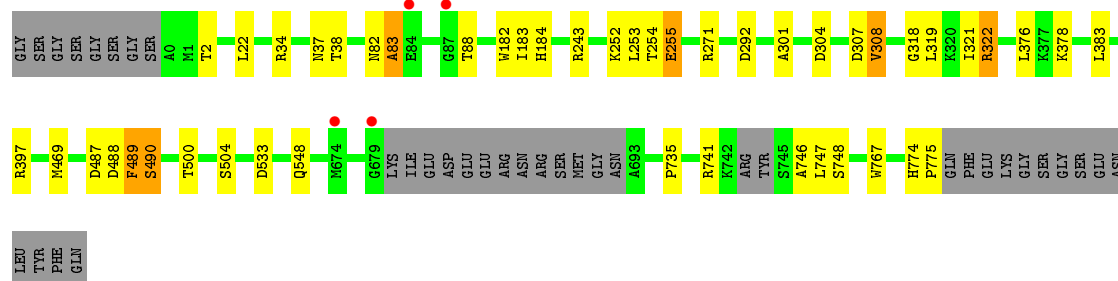
- Molecule 2: RNA-directed RNA polymerase catalytic subunit

Chain V: 92% 5% ..

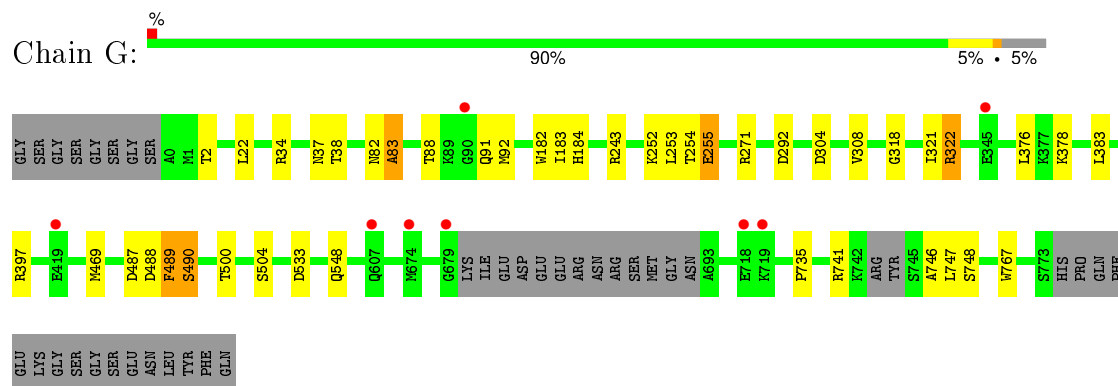


- Molecule 3: Polymerase basic protein 2

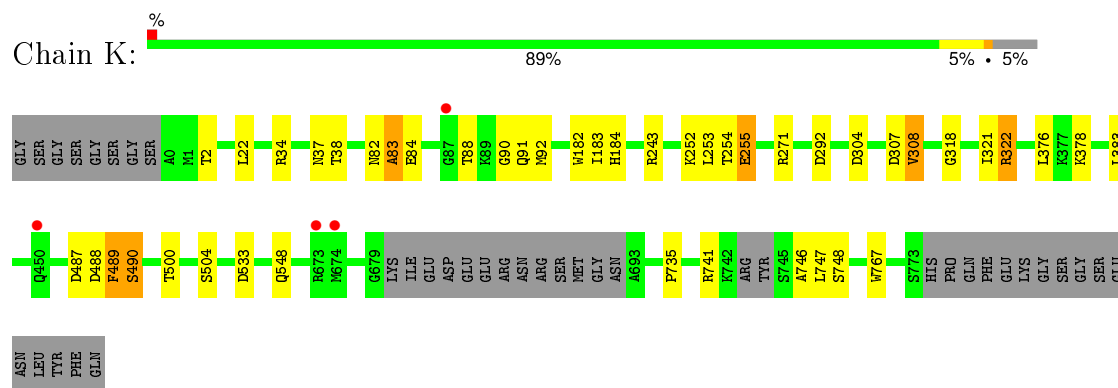
Chain C: 89% 5% • 5%



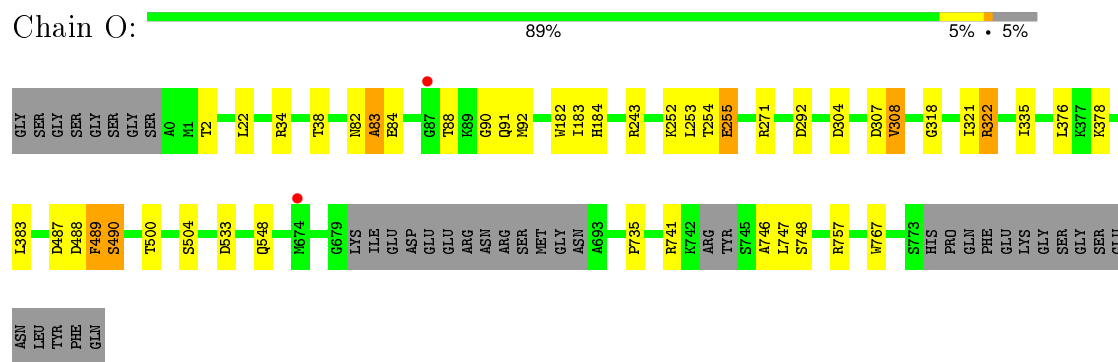
- Molecule 3: Polymerase basic protein 2



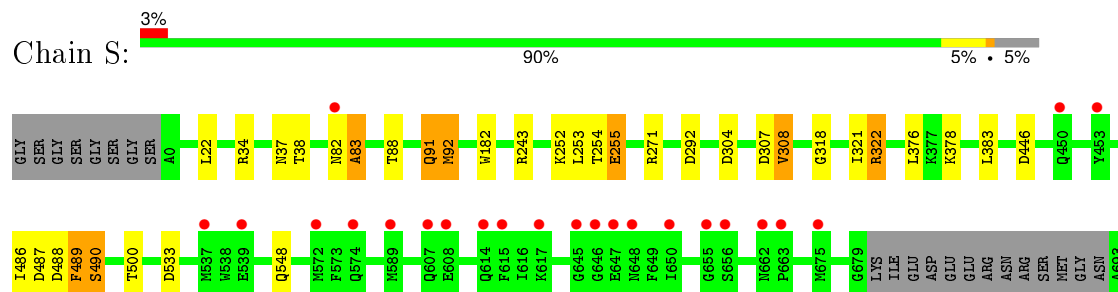
- Molecule 3: Polymerase basic protein 2



- Molecule 3: Polymerase basic protein 2

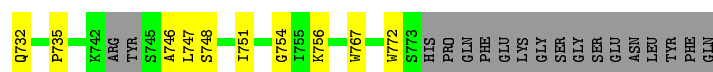
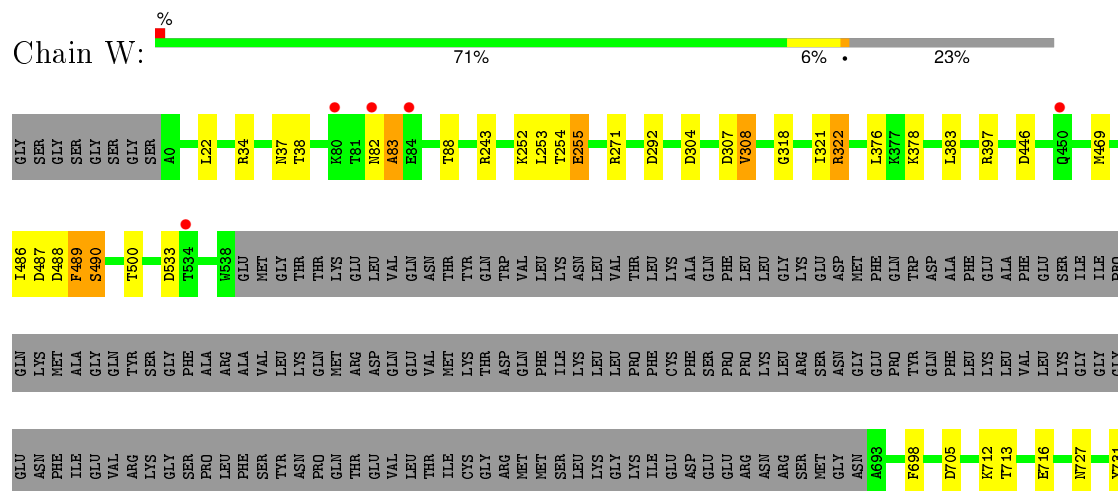


- Molecule 3: Polymerase basic protein 2





• Molecule 3: Polymerase basic protein 2



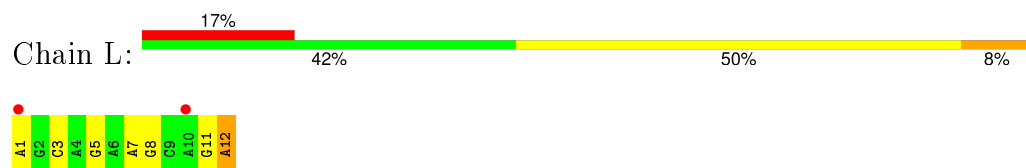
• Molecule 4: CRNA 5' END



• Molecule 4: CRNA 5' END



• Molecule 4: CRNA 5' END

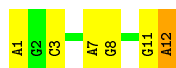


• Molecule 4: CRNA 5' END



• Molecule 4: CRNA 5' END

Chain T:  50% 42% 8%



- Molecule 4: CRNA 5' END

Chain X:  42% 50% 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 49.94 – 4.10	Depositor EDS
% Data completeness (in resolution range)	93.2 (49.95-4.10) 74.2 (49.94-4.10)	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 (4.13%)	DCC
Wilson B-factor (Å ²)	154.8	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 112.1	EDS
Estimated twinning fraction	0.040 for -h,h+k+l,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 188134 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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

All (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
4	X	1	A	OP3-P	-10.57	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 ⓘ

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.

All (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
3:G:397:ARG:HE	3:G:469:MET:HG3	1.61	0.66
1:I:723:ILE:HG13	1:I:724:MET:H	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
3:G:487:ASP:OD1	3:G:488:ASP:N	2.41	0.52
2:J:714:LEU:HB2	3:K:22:LEU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:667:THR:HG22	2:R:668:LYS:H	1.73	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: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
3:K:489:PHE:O	3:K:490:SER:OG	2.29	0.51
1:I:712:GLU:O	1:I:716:VAL:HG23	2.11	0.50
2:N:288:LYS:HZ2	3:O:335:ILE:HD12	1.75	0.50
3:G:489:PHE:O	3:G:490:SER:OG	2.28	0.50
2:R:714:LEU:HB2	3:S:22:LEU:HB3	1.92	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
3:C:376:LEU:HD11	3:C:383:LEU:HD11	1.92	0.50
2:F:671:ARG:O	2:F:672:SER:CB	2.60	0.50
3:C:489:PHE:O	3:C:490:SER:OG	2.29	0.50
2:V:671:ARG:O	2:V:672:SER:CB	2.60	0.50
3:O:489:PHE:O	3:O:490:SER:OG	2.30	0.49
2:J:671:ARG:O	2:J:672:SER:CB	2.60	0.49
3:W:376:LEU:HD11	3:W:383:LEU:HD11	1.94	0.49
3:O:376:LEU:HD11	3:O:383:LEU:HD11	1.94	0.49
2:V:714:LEU:HB2	3:W:22:LEU:HB3	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:R:671:ARG:O	2:R:672:SER:CB	2.60	0.49
2:N:671:ARG:O	2:N: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:J:668:LYS:HE2	3:K:92:MET:SD	2.56	0.46
2:F:668:LYS:O	2:F:669:ARG:CB	2.63	0.46
3:K:91:GLN:O	3:K:92:MET:HG3	2.15	0.46
3:C:746:ALA:O	3:C:748:SER:N	2.49	0.46
2:V:141:THR:HG21	3:W:37:ASN:O	2.16	0.46
3:S:253:LEU:O	3:S:255:GLU:N	2.48	0.46
3:C:253:LEU:O	3:C:255:GLU:N	2.48	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:S:307:ASP:OD1	3:S:308:VAL:N	2.46	0.46
3:O:307:ASP:OD1	3:O:308:VAL:N	2.48	0.46
3:G:253:LEU:O	3:G:255:GLU:N	2.48	0.46
1:I:716:VAL:O	1:I:719:SER:OG	2.28	0.45
2:B:674:LEU:C	2:B:676:THR:H	2.19	0.45
3:O:253:LEU:O	3:O:255:GLU:N	2.49	0.45
2:R:195:ASN:O	2:R:197:LYS:N	2.49	0.45
3:W:307:ASP:OD1	3:W:308:VAL:N	2.47	0.45
3:G:746:ALA:O	3:G:748:SER:N	2.50	0.45
2:J:722:ARG:NH1	2:V:763:GLN:O	2.49	0.45
2:F:195:ASN:O	2:F:197:LYS:N	2.49	0.45
3:G:376:LEU:CD1	3:G:383:LEU:HD11	2.47	0.45
1:M:50:ASP:O	3:O:757:ARG:NH1	2.50	0.45
3:K:321:ILE:O	3:K:322:ARG:HB2	2.17	0.45
2:B:195:ASN:O	2:B:197:LYS:N	2.50	0.45
2:N:195:ASN:O	2:N:197:LYS:N	2.49	0.45
3:O:321:ILE:O	3:O:322:ARG:HB2	2.17	0.45
3:K:253:LEU:O	3:K:255:GLU:N	2.49	0.45
2:B:673:ILE:O	2:B:674:LEU:HB2	2.16	0.44
2:B:483:CYS:SG	2:B:484:ASN:N	2.91	0.44
2:N:483:CYS:SG	2:N:484:ASN:N	2.91	0.44
3:C:376:LEU:CD1	3:C:383:LEU:HD11	2.47	0.44
3:S:376:LEU:CD1	3:S:383:LEU:HD11	2.47	0.44
3:S:321:ILE:O	3:S:322:ARG:CB	2.65	0.44
2:V:483:CYS:SG	2:V:484:ASN:N	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:V:674:LEU:HD11	4:X:12:A:O2'	2.17	0.44
3:W:376:LEU:CD1	3:W:383:LEU:HD11	2.48	0.44
3:K:321:ILE:O	3:K:322:ARG:CB	2.65	0.44
2:J:195:ASN:O	2:J:197:LYS:N	2.51	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: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
3:S:182:TRP:CZ3	3:S:729:LEU:HG	2.53	0.44
3:S:182:TRP:HB2	3:S:733:GLY:HA2	1.99	0.43
3:G:321:ILE:O	3:G:322:ARG:CB	2.65	0.43
3:S:321:ILE:O	3:S:322:ARG:HB2	2.18	0.43
2:N:454:ASP:OD1	2:N:454:ASP:N	2.51	0.43
3:W:489:PHE:O	3:W:490:SER:OG	2.30	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
2:F:454:ASP:OD1	2:F:454:ASP:N	2.52	0.43
3:O:376:LEU:CD1	3:O:383:LEU:HD11	2.48	0.43
2:B:673:ILE:HG22	2:B:674:LEU:HG	2.01	0.43
2:B:670:ASN:O	2:B:672:SER:N	2.51	0.43
2:J:483:CYS:SG	2:J:484:ASN:N	2.92	0.43
3:O:321:ILE:O	3:O:322:ARG:CB	2.65	0.43
3:C:321:ILE:O	3:C:322:ARG:HB2	2.19	0.43
2:R:454:ASP:N	2:R:454:ASP:OD1	2.51	0.43
3:G:321:ILE:O	3:G:322:ARG:HB2	2.18	0.43
1:Q:152:GLN:OE1	1:Q:175:THR:OG1	2.36	0.43
2:J:454:ASP:N	2:J:454:ASP:OD1	2.51	0.43
3:C:307:ASP:OD1	3:C:308:VAL:N	2.50	0.42
1:M:252:VAL:O	1:M:253:THR:OG1	2.34	0.42
2:V:670:ASN:O	2:V:672:SER:N	2.52	0.42
2:F:483:CYS:SG	2:F:484:ASN:N	2.91	0.42
3:S:91:GLN:C	3:S:92:MET:HG3	2.39	0.42
2:R:141:THR:HG21	3:S:37:ASN:O	2.19	0.42
2:J:719:HIS:HA	2:J:722:ARG:HD2	2.01	0.42
1:A:152:GLN:OE1	1:A:175:THR:OG1	2.36	0.42
2:J:674:LEU:O	2:J:676:THR:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:141:THR:HG21	3:K:37:ASN:O	2.20	0.42
2:R:427:ILE:O	2:R:428:LYS:HB2	2.20	0.42
3:C:82:ASN:O	3:C:83:ALA:C	2.58	0.42
2:N:668:LYS:HE2	3:O:92:MET:SD	2.60	0.42
2:J:427:ILE:O	2:J:428:LYS:HB2	2.20	0.42
2:B:454:ASP:OD1	2:B:454:ASP:N	2.52	0.42
1:Q:252:VAL:O	1:Q:253:THR:OG1	2.35	0.42
2:B:518:GLU:OE1	2:B:663:HIS:ND1	2.52	0.42
2:F:674:LEU:O	2:F:675:ASN:C	2.58	0.42
1:A:299:SER:HB2	2:B:566:LYS:C	2.40	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
2:N:674:LEU:O	2:N:675:ASN:C	2.58	0.42
3:O:82:ASN:O	3:O:83:ALA:C	2.59	0.42
2:R:674:LEU:O	2:R:675:ASN:C	2.58	0.41
1:A:298:LYS:N	1:A:484:ARG:HH22	2.17	0.41
3:W:751:ILE:O	3:W:754:GLY:N	2.52	0.41
3:O:307:ASP:CG	3:O:308:VAL:N	2.74	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:J:674:LEU:O	2:J:675:ASN:C	2.58	0.41
2:R:674:LEU:HD11	4:T:12:A:O2'	2.20	0.41
1:I:252:VAL:O	1:I:253:THR:OG1	2.35	0.41
3:G:82:ASN:O	3:G:83:ALA:C	2.58	0.41
3:C:301:ALA:HB2	3:C:319:LEU:HD13	2.03	0.41
2:V:674:LEU:O	2:V:675:ASN:C	2.59	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
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
3:S:82:ASN:O	3:S:83:ALA:C	2.59	0.41
2:N:427:ILE:O	2:N:428:LYS:HB2	2.20	0.41
2:N:674:LEU:HD11	4:P:12:A:O2'	2.21	0.41
3:W:82:ASN:O	3:W:83:ALA:C	2.59	0.41
2:R:326:THR:O	2:R:327:ARG:C	2.59	0.41
2:F:427:ILE:O	2:F:428:LYS:HB2	2.20	0.41
2:B:212:ILE:HG23	2:B:216:GLU:HB2	2.03	0.41
2:N:138:PRO:O	2:N:140:ALA:N	2.54	0.41
1:Q:50:ASP:O	3:S:757:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:212:ILE:HG23	2:V:216:GLU:HB2	2.03	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:518:GLU:OE1	2:R:663:HIS:ND1	2.53	0.41
2:N:518:GLU:OE1	2:N:663:HIS:ND1	2.54	0.41
2:R:483:CYS:SG	2:R:484:ASN:N	2.93	0.41
2:J:326:THR:O	2:J:327:ARG:C	2.60	0.41
2:V:138:PRO:O	2:V:140:ALA:N	2.54	0.41
2:F:670:ASN:O	2:F:672:SER:N	2.53	0.40
3:S:486:ILE:HG22	3:S:487:ASP:N	2.36	0.40
1:Q:49:SER:O	1:Q:50:ASP:C	2.60	0.40
2:B:326:THR:O	2:B:327:ARG:C	2.60	0.40
3:S:307:ASP:CG	3:S:308:VAL:N	2.74	0.40
2:J:138:PRO:O	2:J:140:ALA:N	2.54	0.40
3:K:82:ASN:O	3:K:83:ALA:C	2.58	0.40
2:N:326:THR:O	2:N:327:ARG:C	2.59	0.40
2:J:212:ILE:HG23	2:J:216:GLU:HB2	2.03	0.40
1:U:152:GLN:OE1	1:U:175:THR:OG1	2.39	0.40
2:V:326:THR:O	2:V:327:ARG:C	2.60	0.40
3:G:397:ARG:HG2	3:G:469:MET:HG3	2.04	0.40
3:W:307:ASP:CG	3:W:308:VAL:N	2.75	0.40
3:K:307:ASP:CG	3:K:308:VAL:N	2.75	0.40
3:K:84:GLU:HA	3:K:90:GLY:O	2.21	0.40
2:F:437:TRP:CD1	2:F:437:TRP:C	2.95	0.40
2:R:564:ASP:OD1	2:R:564:ASP:N	2.54	0.40
3:W:486:ILE:HG22	3:W:487:ASP:N	2.36	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%)	39	79
1	E	697/751 (93%)	662 (95%)	31 (4%)	4 (1%)	30	73
1	I	702/751 (94%)	666 (95%)	31 (4%)	5 (1%)	26	71
1	M	697/751 (93%)	662 (95%)	31 (4%)	4 (1%)	30	73
1	Q	697/751 (93%)	662 (95%)	32 (5%)	3 (0%)	39	79
1	U	697/751 (93%)	662 (95%)	31 (4%)	4 (1%)	30	73
2	B	752/772 (97%)	692 (92%)	50 (7%)	10 (1%)	15	61
2	F	752/772 (97%)	693 (92%)	49 (6%)	10 (1%)	15	61
2	J	752/772 (97%)	693 (92%)	49 (6%)	10 (1%)	15	61
2	N	752/772 (97%)	694 (92%)	48 (6%)	10 (1%)	15	61
2	R	752/772 (97%)	693 (92%)	49 (6%)	10 (1%)	15	61
2	V	752/772 (97%)	694 (92%)	48 (6%)	10 (1%)	15	61
3	C	755/798 (95%)	681 (90%)	59 (8%)	15 (2%)	9	54
3	G	753/798 (94%)	679 (90%)	59 (8%)	15 (2%)	9	54
3	K	753/798 (94%)	677 (90%)	61 (8%)	15 (2%)	9	54
3	O	753/798 (94%)	677 (90%)	61 (8%)	15 (2%)	9	54
3	S	753/798 (94%)	678 (90%)	62 (8%)	13 (2%)	11	56
3	W	612/798 (77%)	547 (89%)	52 (8%)	13 (2%)	9	52
All	All	13078/13926 (94%)	12072 (92%)	837 (6%)	169 (1%)	15	61

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 [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%)	80	90
1	E	625/664 (94%)	618 (99%)	7 (1%)	80	90
1	I	631/664 (95%)	623 (99%)	8 (1%)	76	89
1	M	625/664 (94%)	619 (99%)	6 (1%)	82	91
1	Q	625/664 (94%)	619 (99%)	6 (1%)	82	91
1	U	625/664 (94%)	619 (99%)	6 (1%)	82	91
2	B	647/657 (98%)	626 (97%)	21 (3%)	46	78
2	F	647/657 (98%)	625 (97%)	22 (3%)	44	77
2	J	647/657 (98%)	624 (96%)	23 (4%)	42	76
2	N	647/657 (98%)	626 (97%)	21 (3%)	46	78
2	R	647/657 (98%)	625 (97%)	22 (3%)	44	77
2	V	647/657 (98%)	625 (97%)	22 (3%)	44	77
3	C	664/694 (96%)	652 (98%)	12 (2%)	66	87
3	G	662/694 (95%)	649 (98%)	13 (2%)	63	86
3	K	662/694 (95%)	650 (98%)	12 (2%)	66	87
3	O	662/694 (95%)	650 (98%)	12 (2%)	66	87
3	S	662/694 (95%)	648 (98%)	14 (2%)	61	85
3	W	538/694 (78%)	521 (97%)	17 (3%)	46	78
All	All	11488/12090 (95%)	11237 (98%)	251 (2%)	60	84

All (251) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	ILE
1	A	257	LEU
1	A	260	GLU
1	A	333	GLU
1	A	449	CYS
1	A	470	ASN
1	A	633	LEU
1	E	208	ILE
1	E	257	LEU
1	E	260	GLU
1	E	333	GLU
1	E	449	CYS
1	E	608	ARG
1	E	633	LEU

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Mol	Chain	Res	Type
1	I	188	GLN
1	I	208	ILE
1	I	257	LEU
1	I	260	GLU
1	I	333	GLU
1	I	449	CYS
1	I	633	LEU
1	I	719	SER
1	M	208	ILE
1	M	257	LEU
1	M	260	GLU
1	M	333	GLU
1	M	449	CYS
1	M	633	LEU
1	Q	208	ILE
1	Q	257	LEU
1	Q	260	GLU
1	Q	333	GLU
1	Q	449	CYS
1	Q	633	LEU
1	U	208	ILE
1	U	257	LEU
1	U	260	GLU
1	U	333	GLU
1	U	449	CYS
1	U	633	LEU
2	B	94	ARG
2	B	104	GLN
2	B	108	GLN
2	B	114	LEU
2	B	186	ASN
2	B	208	VAL
2	B	233	ARG
2	B	267	GLU
2	B	268	GLN
2	B	324	ARG
2	B	327	ARG
2	B	328	ASP
2	B	408	MET
2	B	412	MET
2	B	420	LEU
2	B	437	TRP

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Mol	Chain	Res	Type
2	B	484	ASN
2	B	488	MET
2	B	643	ASP
2	B	655	ASP
2	B	712	SER
2	F	94	ARG
2	F	104	GLN
2	F	108	GLN
2	F	114	LEU
2	F	186	ASN
2	F	208	VAL
2	F	233	ARG
2	F	267	GLU
2	F	268	GLN
2	F	324	ARG
2	F	327	ARG
2	F	328	ASP
2	F	408	MET
2	F	412	MET
2	F	420	LEU
2	F	437	TRP
2	F	484	ASN
2	F	488	MET
2	F	643	ASP
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	186	ASN
2	J	208	VAL
2	J	233	ARG
2	J	267	GLU
2	J	268	GLN
2	J	324	ARG
2	J	327	ARG
2	J	328	ASP
2	J	408	MET
2	J	412	MET
2	J	420	LEU

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Mol	Chain	Res	Type
2	J	437	TRP
2	J	484	ASN
2	J	488	MET
2	J	643	ASP
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	186	ASN
2	N	208	VAL
2	N	233	ARG
2	N	268	GLN
2	N	324	ARG
2	N	327	ARG
2	N	328	ASP
2	N	408	MET
2	N	412	MET
2	N	420	LEU
2	N	437	TRP
2	N	484	ASN
2	N	488	MET
2	N	643	ASP
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	186	ASN
2	R	208	VAL
2	R	233	ARG
2	R	267	GLU
2	R	268	GLN
2	R	324	ARG
2	R	327	ARG
2	R	328	ASP
2	R	408	MET

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Mol	Chain	Res	Type
2	R	412	MET
2	R	420	LEU
2	R	437	TRP
2	R	484	ASN
2	R	488	MET
2	R	643	ASP
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	186	ASN
2	V	208	VAL
2	V	233	ARG
2	V	267	GLU
2	V	268	GLN
2	V	324	ARG
2	V	327	ARG
2	V	328	ASP
2	V	408	MET
2	V	412	MET
2	V	420	LEU
2	V	437	TRP
2	V	484	ASN
2	V	488	MET
2	V	643	ASP
2	V	655	ASP
2	V	667	THR
2	V	712	SER
3	C	34	ARG
3	C	88	THR
3	C	243	ARG
3	C	255	GLU
3	C	271	ARG
3	C	304	ASP
3	C	378	LYS
3	C	500	THR
3	C	504	SER
3	C	533	ASP
3	C	548	GLN

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Mol	Chain	Res	Type
3	C	767	TRP
3	G	34	ARG
3	G	88	THR
3	G	91	GLN
3	G	243	ARG
3	G	255	GLU
3	G	271	ARG
3	G	304	ASP
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	34	ARG
3	K	88	THR
3	K	243	ARG
3	K	255	GLU
3	K	271	ARG
3	K	304	ASP
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	34	ARG
3	O	88	THR
3	O	243	ARG
3	O	255	GLU
3	O	271	ARG
3	O	304	ASP
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	34	ARG
3	S	88	THR
3	S	91	GLN
3	S	92	MET

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Mol	Chain	Res	Type
3	S	243	ARG
3	S	255	GLU
3	S	271	ARG
3	S	304	ASP
3	S	378	LYS
3	S	446	ASP
3	S	500	THR
3	S	533	ASP
3	S	548	GLN
3	S	767	TRP
3	W	34	ARG
3	W	88	THR
3	W	243	ARG
3	W	255	GLU
3	W	271	ARG
3	W	304	ASP
3	W	378	LYS
3	W	446	ASP
3	W	500	THR
3	W	533	ASP
3	W	698	PHE
3	W	705	ASP
3	W	713	THR
3	W	727	ASN
3	W	731	TYR
3	W	756	LYS
3	W	767	TRP

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

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
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 ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	703/751 (93%)	-0.23	8 (1%) 82 75	108, 190, 258, 348	0
1	E	703/751 (93%)	-0.22	3 (0%) 93 90	115, 214, 280, 335	0
1	I	708/751 (94%)	-0.19	10 (1%) 78 69	103, 198, 269, 354	0
1	M	703/751 (93%)	-0.13	8 (1%) 82 75	111, 222, 292, 352	0
1	Q	703/751 (93%)	-0.21	5 (0%) 89 84	105, 211, 278, 388	0
1	U	703/751 (93%)	-0.17	6 (0%) 85 79	111, 213, 276, 338	0
2	B	756/772 (97%)	-0.31	6 (0%) 87 82	103, 163, 216, 276	0
2	F	756/772 (97%)	-0.34	4 (0%) 91 88	110, 182, 241, 298	0
2	J	756/772 (97%)	-0.34	2 (0%) 94 92	88, 157, 228, 301	0
2	N	756/772 (97%)	-0.28	1 (0%) 95 95	91, 181, 247, 297	0
2	R	756/772 (97%)	-0.33	1 (0%) 95 95	100, 170, 231, 306	0
2	V	756/772 (97%)	-0.33	2 (0%) 94 92	100, 172, 239, 302	0
3	C	761/798 (95%)	-0.26	4 (0%) 91 88	97, 192, 261, 362	0
3	G	759/798 (95%)	-0.25	8 (1%) 82 75	116, 203, 265, 391	0
3	K	759/798 (95%)	-0.31	4 (0%) 91 88	106, 176, 256, 336	0
3	O	759/798 (95%)	-0.27	2 (0%) 94 92	121, 188, 258, 353	0
3	S	759/798 (95%)	-0.12	23 (3%) 54 41	104, 192, 296, 382	0
3	W	618/798 (77%)	-0.26	5 (0%) 87 82	114, 188, 261, 361	0
4	D	12/12 (100%)	0.03	0 100 100	163, 174, 202, 224	0
4	H	12/12 (100%)	0.20	0 100 100	177, 206, 218, 219	0
4	L	12/12 (100%)	0.88	2 (16%) 2 3	151, 190, 224, 232	0
4	P	12/12 (100%)	0.39	0 100 100	175, 208, 246, 251	0
4	T	12/12 (100%)	0.35	0 100 100	187, 211, 225, 235	0
4	X	12/12 (100%)	0.54	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%)	-0.25	104 (0%) 87 82	88, 188, 266, 391	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	61	TYR	5.6
2	J	645	THR	5.5
3	S	647	GLU	5.2
3	S	646	GLY	5.1
3	O	87	GLY	4.8
1	M	61	TYR	4.7
3	C	679	GLY	4.6
2	V	645	THR	4.4
2	R	645	THR	4.3
1	I	29	GLU	4.1
1	A	50	ASP	4.0
3	S	645	GLY	3.9
3	C	87	GLY	3.8
1	E	50	ASP	3.8
3	S	607	GLN	3.7
1	U	61	TYR	3.7
2	B	645	THR	3.7
3	G	90	GLY	3.6
1	A	325	ILE	3.6
1	Q	60	ALA	3.6
3	W	82	ASN	3.5
1	A	56	GLU	3.5
1	A	63	ALA	3.4
3	C	84	GLU	3.4
2	N	645	THR	3.3
3	G	419	GLU	3.3
3	S	82	ASN	3.3
3	K	674	MET	3.2
1	I	547	SER	3.2
3	S	539	GLU	3.1
3	C	674	MET	3.1
1	U	357	GLN	3.0
1	U	548	GLY	3.0
1	Q	400	ALA	3.0
1	I	541	ILE	2.9
3	S	617	LYS	2.8
1	A	326	MET	2.8

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Mol	Chain	Res	Type	RSRZ
4	L	1	A	2.8
3	K	450	GLN	2.8
1	M	292	ALA	2.7
2	F	645	THR	2.7
3	G	607	GLN	2.6
3	S	608	GLU	2.6
3	S	675	MET	2.6
3	S	589	MET	2.6
1	M	62	THR	2.6
1	I	271	ASN	2.5
2	B	503	ASN	2.5
4	L	10	A	2.5
3	S	662	ASN	2.5
3	S	615	PHE	2.5
1	I	485	VAL	2.5
1	I	513	VAL	2.5
1	I	492	SER	2.5
1	Q	299	SER	2.5
1	I	28	PRO	2.5
1	A	294	MET	2.5
2	B	275	GLY	2.4
3	K	673	ARG	2.4
3	G	718	GLU	2.4
2	F	355	PHE	2.4
3	K	87	GLY	2.4
3	W	80	LYS	2.4
1	E	493	PHE	2.4
1	U	326	MET	2.4
2	B	274	GLY	2.4
2	F	434	GLU	2.4
1	A	538	VAL	2.4
3	O	674	MET	2.3
1	I	493	PHE	2.3
3	S	648	ASN	2.3
3	S	614	GLN	2.3
1	M	549	ARG	2.3
3	S	572	MET	2.3
2	V	512	GLY	2.3
3	S	655	GLY	2.3
1	M	546	VAL	2.3
3	S	650	ILE	2.3
3	G	345	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	S	656	SER	2.2
3	G	719	LYS	2.2
2	F	26	GLY	2.2
3	S	453	TYR	2.2
1	U	324	LEU	2.2
3	S	450	GLN	2.1
3	S	537	MET	2.1
3	W	450	GLN	2.1
1	I	491	GLU	2.1
1	E	334	ASN	2.1
3	S	663	PRO	2.1
1	A	195	ASP	2.1
3	W	84	GLU	2.1
3	W	534	THR	2.1
1	M	595	GLN	2.1
1	U	539	PHE	2.1
3	G	674	MET	2.1
3	G	679	GLY	2.1
2	J	512	GLY	2.1
1	M	346	THR	2.0
1	M	521	PHE	2.0
2	B	653	LYS	2.0
3	S	574	GLN	2.0
1	Q	474	GLY	2.0
2	B	26	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.