



# Full wwPDB EM Model Validation Report ⓘ

Apr 7, 2020 – 10:03 PM EDT

PDB ID : 6T0N  
EMDB ID : EMD-10356  
Title : Bat Influenza A polymerase pre-initiation complex  
Authors : Wandzik, J.M.; Kouba, T.; Cusack, S.  
Deposited on : 2019-10-03  
Resolution : 2.54 Å(reported)

This is a Full wwPDB EM Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.10.1

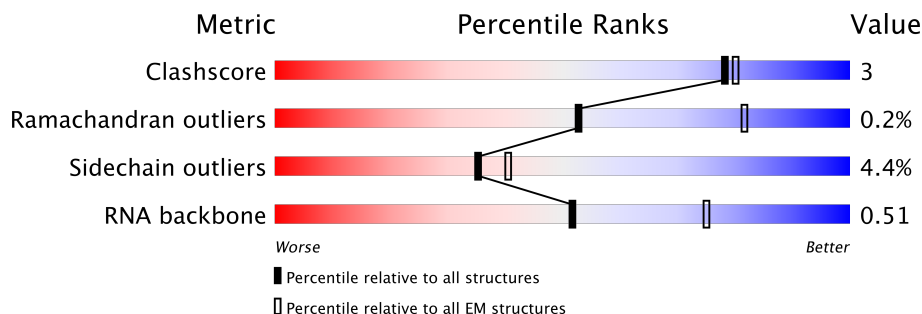
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.54 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	738	
2	B	776	
3	C	809	
4	V	14	
5	R	16	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14598 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
1	A	704	Total	C	N	O	S	0	0
			5741	3651	968	1086	36		

There are 25 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	749	Total	C	N	O	S	0	0
			5972	3756	1061	1115	40		

There are 20 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	250	Total	C	N	O	S	0	0
			2016	1267	362	371	16		

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLY	-	expression tag	UNP H6QM90
C	-7	SER	-	expression tag	UNP H6QM90
C	-6	GLY	-	expression tag	UNP H6QM90
C	-5	SER	-	expression tag	UNP H6QM90
C	-4	GLY	-	expression tag	UNP H6QM90
C	-3	SER	-	expression tag	UNP H6QM90
C	-2	GLY	-	expression tag	UNP H6QM90

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP H6QM90
C	0	GLY	-	expression tag	UNP H6QM90
C	761	GLY	-	expression tag	UNP H6QM90
C	762	TRP	-	expression tag	UNP H6QM90
C	763	SER	-	expression tag	UNP H6QM90
C	764	HIS	-	expression tag	UNP H6QM90
C	765	PRO	-	expression tag	UNP H6QM90
C	766	GLN	-	expression tag	UNP H6QM90
C	767	PHE	-	expression tag	UNP H6QM90
C	768	GLU	-	expression tag	UNP H6QM90
C	769	LYS	-	expression tag	UNP H6QM90
C	770	GLY	-	expression tag	UNP H6QM90
C	771	GLY	-	expression tag	UNP H6QM90
C	772	GLY	-	expression tag	UNP H6QM90
C	773	SER	-	expression tag	UNP H6QM90
C	774	GLY	-	expression tag	UNP H6QM90
C	775	GLY	-	expression tag	UNP H6QM90
C	776	GLY	-	expression tag	UNP H6QM90
C	777	SER	-	expression tag	UNP H6QM90
C	778	GLY	-	expression tag	UNP H6QM90
C	779	GLY	-	expression tag	UNP H6QM90
C	780	SER	-	expression tag	UNP H6QM90
C	781	ALA	-	expression tag	UNP H6QM90
C	782	TRP	-	expression tag	UNP H6QM90
C	783	SER	-	expression tag	UNP H6QM90
C	784	HIS	-	expression tag	UNP H6QM90
C	785	PRO	-	expression tag	UNP H6QM90
C	786	GLN	-	expression tag	UNP H6QM90
C	787	PHE	-	expression tag	UNP H6QM90
C	788	GLU	-	expression tag	UNP H6QM90
C	789	LYS	-	expression tag	UNP H6QM90
C	790	GLY	-	expression tag	UNP H6QM90
C	791	ARG	-	expression tag	UNP H6QM90
C	792	SER	-	expression tag	UNP H6QM90
C	793	GLY	-	expression tag	UNP H6QM90
C	794	GLY	-	expression tag	UNP H6QM90
C	795	GLU	-	expression tag	UNP H6QM90
C	796	ASN	-	expression tag	UNP H6QM90
C	797	LEU	-	expression tag	UNP H6QM90
C	798	TYR	-	expression tag	UNP H6QM90
C	799	PHE	-	expression tag	UNP H6QM90
C	800	GLN	-	expression tag	UNP H6QM90

- Molecule 4 is a RNA chain called 5' vRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	14	Total	C	N	O	P	0	0
			307	137	62	94	14		

- Molecule 5 is a RNA chain called 3' vRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	15	Total	C	N	O	P	0	0
			292	129	43	105	15		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Mg	0
			1	1	
6	V	1	Total	Mg	0
			1	1	

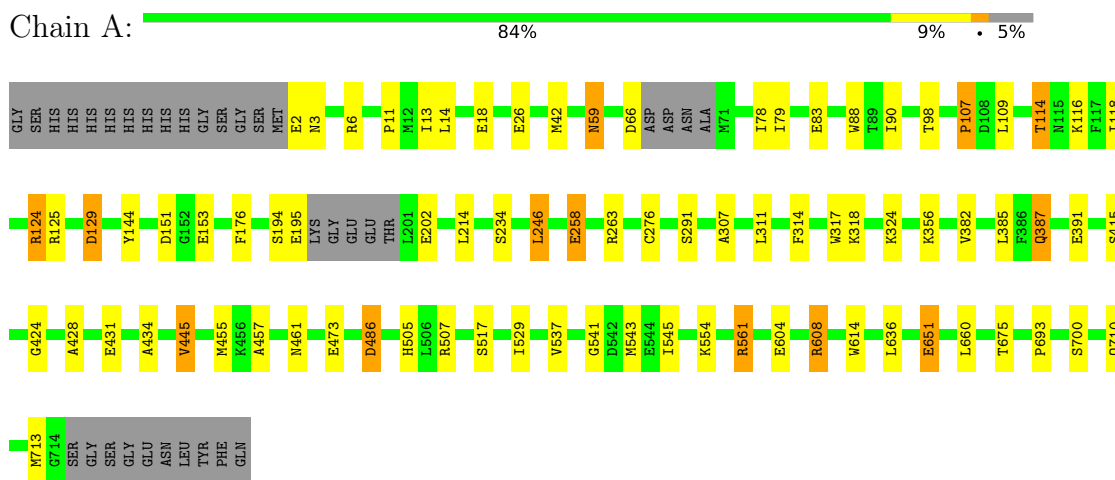
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	90	Total	O	0
			90	90	
7	B	115	Total	O	0
			115	115	
7	C	17	Total	O	0
			17	17	
7	V	37	Total	O	0
			37	37	
7	R	9	Total	O	0
			9	9	

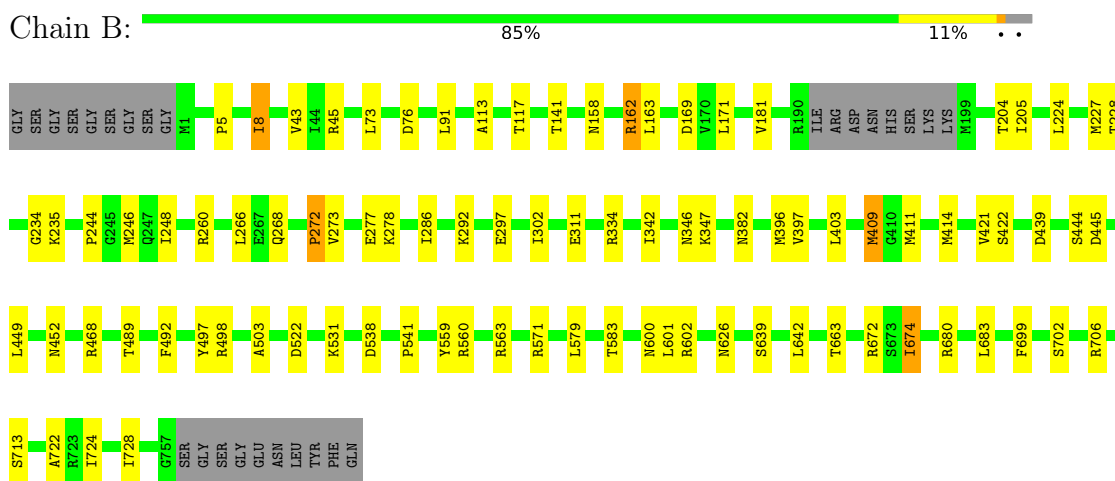
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

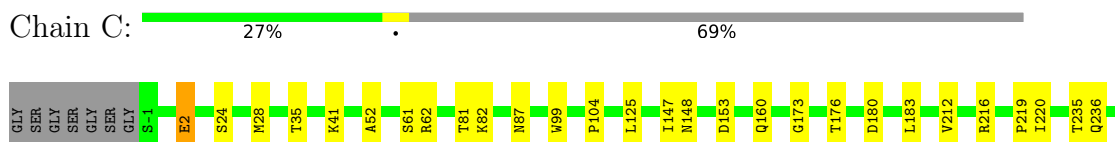
- Molecule 1: Polymerase acidic protein



- Molecule 2: RNA-directed RNA polymerase catalytic subunit



- Molecule 3: Polymerase basic protein 2







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	397731	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	32	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.32	0/5863	0.45	0/7895
2	B	0.32	0/6088	0.48	0/8216
3	C	0.30	0/2056	0.46	0/2774
4	V	0.84	1/345 (0.3%)	0.87	0/535
5	R	0.50	0/322	1.16	1/498 (0.2%)
All	All	0.34	1/14674 (0.0%)	0.51	1/19918 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	1	A	OP3-P	-11.34	1.47	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	5	C	N1-C2-O2	5.13	121.98	118.90

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	5741	0	5655	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5972	0	5983	48	0
3	C	2016	0	2048	15	0
4	V	307	0	153	0	0
5	R	292	0	149	2	0
6	B	1	0	0	0	0
6	V	1	0	0	0	0
7	A	90	0	0	1	0
7	B	115	0	0	0	0
7	C	17	0	0	0	0
7	R	9	0	0	0	0
7	V	37	0	0	0	0
All	All	14598	0	13988	88	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (88) 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:A:90:ILE:HG12	2:B:724:ILE:HG13	1.14	1.12
1:A:90:ILE:CG1	2:B:724:ILE:HG13	1.96	0.95
1:A:90:ILE:HG12	2:B:724:ILE:CG1	2.00	0.89
1:A:604:GLU:O	1:A:608:ARG:HB2	1.95	0.65
2:B:224:LEU:HD11	2:B:347:LYS:HD2	1.81	0.62
1:A:78:ILE:HA	1:A:109:LEU:HD23	1.83	0.60
2:B:409:MET:N	2:B:409:MET:SD	2.70	0.59
2:B:571:ARG:NH1	3:C:52:ALA:O	2.36	0.57
1:A:507:ARG:NH2	5:R:9:U:O2'	2.37	0.56
3:C:180:ASP:HA	3:C:183:LEU:HD12	1.88	0.55
1:A:90:ILE:HA	2:B:724:ILE:HG21	1.88	0.55
1:A:124:ARG:NH2	1:A:194:SER:O	2.40	0.54
2:B:204:THR:OG1	2:B:205:ILE:N	2.41	0.54
3:C:148:ASN:ND2	3:C:212:VAL:O	2.40	0.54
1:A:457:ALA:O	1:A:461:ASN:ND2	2.40	0.54
1:A:151:ASP:HB2	1:A:153:GLU:HG2	1.89	0.54
2:B:342:ILE:O	2:B:346:ASN:ND2	2.41	0.54
1:A:234:SER:OG	2:B:334:ARG:NH2	2.42	0.53
2:B:489:THR:HA	2:B:497:TYR:O	2.09	0.53
1:A:604:GLU:OE2	1:A:608:ARG:NH1	2.42	0.52
1:A:387:GLN:OE1	2:B:382:ASN:ND2	2.43	0.52
2:B:297:GLU:OE2	2:B:452:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:ARG:HG3	2:B:272:PRO:HG3	1.93	0.51
2:B:302:ILE:HD12	2:B:449:LEU:HD23	1.93	0.51
2:B:674:ILE:HD13	2:B:683:LEU:HD21	1.94	0.50
2:B:268:GLN:NE2	2:B:439:ASP:OD1	2.41	0.50
1:A:263:ARG:HA	1:A:710:GLN:HG2	1.93	0.50
2:B:699:PHE:HE2	2:B:722:ALA:HB2	1.77	0.50
2:B:273:VAL:HB	2:B:277:GLU:HB3	1.94	0.49
1:A:424:GLY:O	2:B:600:ASN:ND2	2.46	0.49
2:B:503:ALA:HB2	2:B:538:ASP:HB2	1.95	0.49
2:B:489:THR:HG22	2:B:498:ARG:HA	1.95	0.48
1:A:59:ASN:OD1	1:A:59:ASN:N	2.46	0.48
1:A:13:ILE:HG23	1:A:42:MET:HB3	1.96	0.48
2:B:672:ARG:NH2	3:C:82:LYS:O	2.41	0.48
2:B:158:ASN:ND2	2:B:169:ASP:OD2	2.46	0.47
1:A:314:PHE:HE1	1:A:543:MET:HB3	1.79	0.47
2:B:5:PRO:O	2:B:8:ILE:HB	2.15	0.47
2:B:713:SER:HA	3:C:24:SER:HA	1.97	0.46
2:B:266:LEU:HD13	2:B:421:VAL:HG11	1.97	0.46
3:C:2:GLU:HG3	3:C:2:GLU:H	1.43	0.46
1:A:129:ASP:OD1	1:A:129:ASP:N	2.48	0.46
1:A:258:GLU:OE1	1:A:675:THR:OG1	2.34	0.46
1:A:79:ILE:HD12	1:A:107:PRO:HG2	1.98	0.46
1:A:561:ARG:NH1	7:A:814:HOH:O	2.49	0.45
1:A:6:ARG:HA	1:A:14:LEU:HD21	1.97	0.45
1:A:445:VAL:HG22	1:A:636:LEU:HD22	1.97	0.45
3:C:219:PRO:O	3:C:236:GLN:NE2	2.45	0.45
1:A:276:CYS:HB2	1:A:693:PRO:HG3	1.99	0.45
2:B:113:ALA:O	2:B:117:THR:OG1	2.30	0.44
1:A:246:LEU:O	2:B:468:ARG:NH2	2.50	0.44
2:B:91:LEU:HB3	2:B:422:SER:HB2	1.99	0.44
1:A:486:ASP:OD1	1:A:486:ASP:N	2.50	0.44
3:C:235:THR:HA	3:C:242:GLN:HB3	2.00	0.44
1:A:88:TRP:HB3	3:C:173:GLY:HA2	1.99	0.43
2:B:45:ARG:NH2	2:B:311:GLU:OE1	2.43	0.43
2:B:162:ARG:H	2:B:162:ARG:HG2	1.68	0.43
2:B:639:SER:HA	2:B:642:LEU:HD12	1.99	0.43
2:B:626:ASN:ND2	3:C:104:PRO:O	2.49	0.43
2:B:444:SER:OG	2:B:445:ASP:N	2.50	0.43
1:A:428:ALA:HB3	1:A:431:GLU:HG3	1.99	0.43
2:B:602:ARG:HG3	3:C:125:LEU:HD21	2.01	0.43
1:A:214:LEU:HA	1:A:214:LEU:HD12	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:PRO:HG3	2:B:411:MET:SD	2.60	0.42
2:B:522:ASP:OD2	2:B:559:TYR:OH	2.27	0.42
1:A:114:THR:O	1:A:116:LYS:HG3	2.19	0.42
2:B:278:LYS:HD3	2:B:492:PHE:HE2	1.85	0.42
2:B:579:LEU:O	2:B:583:THR:OG1	2.32	0.42
1:A:307:ALA:O	1:A:311:LEU:HB2	2.20	0.42
1:A:473:GLU:OE2	1:A:505:HIS:NE2	2.41	0.42
3:C:147:ILE:HD13	3:C:216:ARG:HG3	2.02	0.42
1:A:545:ILE:HD13	1:A:554:LYS:HD2	2.02	0.41
1:A:318:LYS:HG3	1:A:541:GLY:HA2	2.01	0.41
2:B:43:VAL:HG13	2:B:403:LEU:HD13	2.03	0.41
3:C:61:SER:OG	3:C:87:ASN:O	2.37	0.41
1:A:434:ALA:HB2	2:B:541:PRO:HB2	2.01	0.41
1:A:660:LEU:HD12	1:A:660:LEU:HA	1.94	0.41
2:B:663:THR:HG21	3:C:99:TRP:CD1	2.55	0.41
1:A:324:LYS:HB3	1:A:537:VAL:HB	2.02	0.41
1:A:66:ASP:N	1:A:66:ASP:OD1	2.48	0.41
2:B:706:ARG:HH11	3:C:160:GLN:HG2	1.85	0.41
1:A:118:ILE:HD12	1:A:144:TYR:HD2	1.86	0.41
1:A:11:PRO:HA	1:A:14:LEU:HB2	2.03	0.40
1:A:651:GLU:HG3	2:B:234:GLY:H	1.85	0.40
2:B:672:ARG:NH1	5:R:9:U:OP1	2.53	0.40
1:A:382:VAL:HB	1:A:385:LEU:HB2	2.03	0.40
2:B:674:ILE:HG13	2:B:674:ILE:H	1.50	0.40
2:B:531:LYS:HE2	2:B:531:LYS:HB3	1.96	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	698/738 (95%)	663 (95%)	33 (5%)	2 (0%)	43 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	745/776 (96%)	715 (96%)	28 (4%)	2 (0%)	43	56
3	C	248/809 (31%)	236 (95%)	12 (5%)	0	100	100
All	All	1691/2323 (73%)	1614 (95%)	73 (4%)	4 (0%)	53	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	PRO
2	B	292	LYS
1	A	98	THR
2	B	272	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	630/657 (96%)	598 (95%)	32 (5%)	26	36
2	B	656/676 (97%)	631 (96%)	25 (4%)	36	50
3	C	224/706 (32%)	215 (96%)	9 (4%)	34	48
All	All	1510/2039 (74%)	1444 (96%)	66 (4%)	35	43

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	3	ASN
1	A	18	GLU
1	A	26	GLU
1	A	59	ASN
1	A	83	GLU
1	A	114	THR
1	A	124	ARG
1	A	125	ARG
1	A	129	ASP

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Mol	Chain	Res	Type
1	A	176	PHE
1	A	195	GLU
1	A	202	GLU
1	A	246	LEU
1	A	258	GLU
1	A	291	SER
1	A	317	TRP
1	A	356	LYS
1	A	387	GLN
1	A	391	GLU
1	A	415	SER
1	A	445	VAL
1	A	455	MET
1	A	486	ASP
1	A	517	SER
1	A	529	ILE
1	A	561	ARG
1	A	608	ARG
1	A	614	TRP
1	A	651	GLU
1	A	700	SER
1	A	713	MET
2	B	8	ILE
2	B	73	LEU
2	B	76	ASP
2	B	141	THR
2	B	162	ARG
2	B	163	LEU
2	B	171	LEU
2	B	181	VAL
2	B	227	MET
2	B	228	THR
2	B	235	LYS
2	B	246	MET
2	B	248	ILE
2	B	286	ILE
2	B	396	MET
2	B	397	VAL
2	B	409	MET
2	B	414	MET
2	B	560	ARG
2	B	563	ARG

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Mol	Chain	Res	Type
2	B	601	LEU
2	B	674	ILE
2	B	680	ARG
2	B	702	SER
2	B	728	ILE
3	C	2	GLU
3	C	28	MET
3	C	35	THR
3	C	41	LYS
3	C	62	ARG
3	C	81	THR
3	C	153	ASP
3	C	176	THR
3	C	220	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	387	GLN
1	A	612	ASN
2	B	312	ASN
2	B	382	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	V	13/14 (92%)	4 (30%)	0
5	R	13/16 (81%)	1 (7%)	0
All	All	26/30 (86%)	5 (19%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	V	4	A
4	V	6	U
4	V	8	A
4	V	11	A
5	R	17	C

There are no RNA pucker outliers to report.



## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.