



Full wwPDB EM Model Validation Report ⓘ

Apr 7, 2020 – 09:57 PM EDT

PDB ID : 6T0S
EMDB ID : EMD-10358
Title : Bat Influenza A polymerase stuttering complex using 44-mer vRNA template
with intact oligo(U) sequence
Authors : Wandzik, J.M.; Kouba, T.; Cusack, S.
Deposited on : 2019-10-03
Resolution : 3.04 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

A user guide is available at

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

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
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

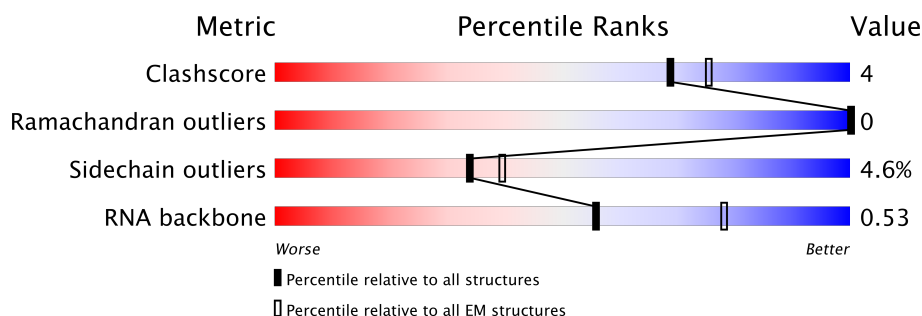
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.04 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 ≥ 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	83% 12% . .
2	B	776	82% 13% . .
3	C	809	26% 5% 69%
4	V	44	41% 30% 5% 25%
5	M	11	73% 9% 9% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14651 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	708	Total	C	N	O	S	1	0
			5780	3673	976	1094	37		

There are 26 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	134	ALA	LYS	conflict	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	743	Total	C	N	O	S	0	0
			5947	3737	1059	1112	39		

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	249	Total	C	N	O	S	0	0
			2012	1265	361	370	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

Continued on next page...

Continued from previous page...

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 vRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	33	Total	C	N	O	P	0	0
			690	309	109	239	33		

- Molecule 5 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	10	Total	C	N	O	P	0	0
			220	99	48	63	10		

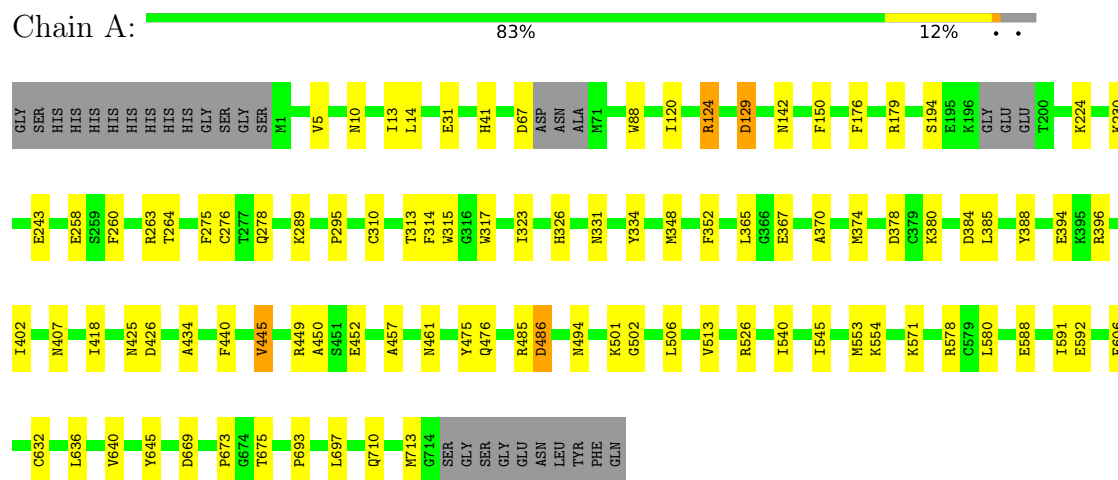
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	B	2	Total	Mg	0
			2	2	

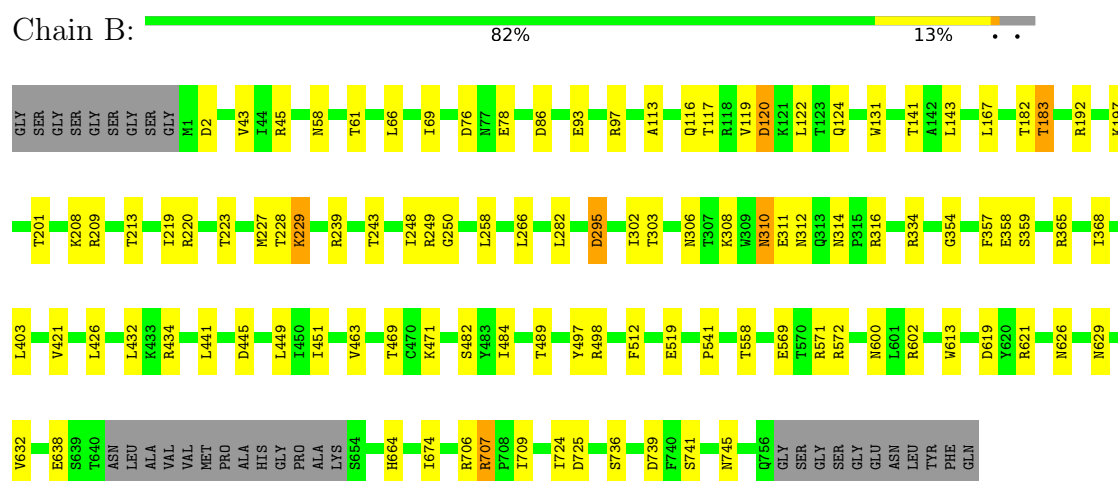
3 Residue-property plots

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.

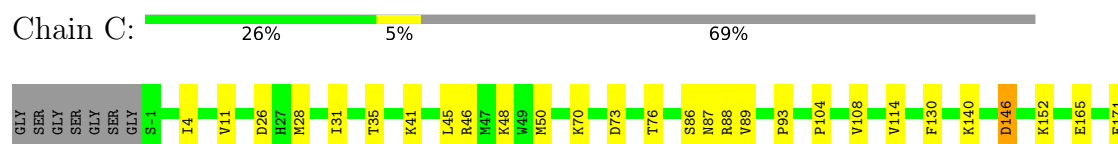
- Molecule 1: Polymerase acidic protein



- 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	61502	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 ($e^-/\text{\AA}^2$)	43	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	0.26	0/5902	0.43	0/7947
2	B	0.26	0/6061	0.45	0/8175
3	C	0.27	0/2052	0.45	0/2769
4	V	0.48	1/765 (0.1%)	0.88	0/1180
5	M	0.26	0/248	0.85	0/385
All	All	0.28	1/15028 (0.0%)	0.49	0/20456

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	1	A	OP3-P	-10.87	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	5780	0	5695	51	0
2	B	5947	0	5956	57	0
3	C	2012	0	2045	26	0
4	V	690	0	352	6	0
5	M	220	0	111	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	2	0	0	0	0
All	All	14651	0	14159	117	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 4.

All (117) 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:88:TRP:CE2	3:C:174:ALA:HB2	2.05	0.91
2:B:354:GLY:HA3	2:B:368:ILE:O	1.78	0.83
3:C:175:ARG:HG2	3:C:175:ARG:HH11	1.46	0.80
3:C:46:ARG:O	3:C:50:MET:HB2	1.84	0.76
3:C:175:ARG:NH1	3:C:175:ARG:O	2.21	0.74
3:C:165:GLU:HG3	3:C:177:LEU:HD21	1.73	0.70
1:A:445:VAL:HG22	1:A:636:LEU:HD22	1.85	0.58
3:C:41:LYS:O	3:C:46:ARG:NH2	2.36	0.58
2:B:78:GLU:O	2:B:471:LYS:NZ	2.36	0.58
3:C:175:ARG:CG	3:C:175:ARG:HH11	2.12	0.58
2:B:489:THR:HA	2:B:497:TYR:O	2.04	0.58
2:B:119:VAL:HG12	2:B:143:LEU:HD21	1.87	0.57
2:B:302:ILE:HG12	2:B:484:ILE:HB	1.86	0.56
1:A:88:TRP:NE1	3:C:174:ALA:HB2	2.21	0.55
1:A:485:ARG:NH1	4:V:44:U:O2'	2.40	0.55
2:B:707:ARG:NH1	3:C:26:ASP:OD1	2.41	0.54
2:B:124:GLN:NE2	5:M:30:C:OP1	2.41	0.54
1:A:402:ILE:HG13	1:A:697:LEU:HD22	1.90	0.54
2:B:741:SER:O	2:B:745:ASN:ND2	2.39	0.54
1:A:425:ASN:O	2:B:602:ARG:NH1	2.41	0.54
1:A:457:ALA:O	1:A:461:ASN:ND2	2.40	0.53
2:B:308:LYS:O	2:B:312:ASN:ND2	2.42	0.53
1:A:129:ASP:OD1	1:A:129:ASP:N	2.41	0.53
3:C:114:VAL:O	3:C:209:ARG:NH1	2.42	0.53
2:B:519:GLU:OE1	2:B:664:HIS:ND1	2.42	0.52
2:B:131:TRP:O	2:B:220:ARG:NH1	2.42	0.52
2:B:167:LEU:HD21	2:B:250:GLY:HA3	1.92	0.52
2:B:558:THR:OG1	3:C:48:LYS:NZ	2.39	0.52
2:B:519:GLU:HB2	2:B:664:HIS:HB3	1.90	0.52
2:B:306:ASN:ND2	2:B:445:ASP:O	2.41	0.52
1:A:578:ARG:NH2	2:B:512:PHE:O	2.44	0.51
3:C:175:ARG:NH1	3:C:175:ARG:CG	2.73	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:HIS:NE2	1:A:120:ILE:O	2.43	0.51
1:A:124:ARG:NH2	1:A:194:SER:OG	2.44	0.51
2:B:86:ASP:N	2:B:86:ASP:OD1	2.42	0.51
1:A:449:ARG:NH1	1:A:452:GLU:OE1	2.43	0.51
2:B:295:ASP:N	2:B:295:ASP:OD1	2.42	0.51
2:B:122:LEU:HD21	2:B:250:GLY:HA2	1.94	0.50
1:A:276:CYS:HB2	1:A:693:PRO:HG3	1.93	0.49
1:A:486:ASP:OD1	1:A:486:ASP:N	2.45	0.49
2:B:182:THR:HA	2:B:209:ARG:HG2	1.95	0.49
2:B:192:ARG:NH1	2:B:197:LYS:O	2.45	0.49
3:C:235:THR:HA	3:C:242:GLN:HB3	1.94	0.49
1:A:669:ASP:OD2	2:B:498:ARG:NH1	2.42	0.49
3:C:146:ASP:OD1	3:C:146:ASP:N	2.46	0.49
2:B:310:ASN:ND2	5:M:38:A:O2'	2.44	0.48
2:B:282:LEU:HG	2:B:441:LEU:HD13	1.96	0.48
2:B:58:ASN:HD22	2:B:61:THR:H	1.61	0.48
2:B:302:ILE:HD12	2:B:449:LEU:HD23	1.95	0.48
2:B:93:GLU:OE2	2:B:97:ARG:NH1	2.46	0.47
1:A:450:ALA:HB1	1:A:640:VAL:HG21	1.95	0.47
3:C:140:LYS:HG2	3:C:221:ALA:HB2	1.96	0.47
2:B:69:ILE:HD13	2:B:316:ARG:HB2	1.96	0.47
1:A:367:GLU:OE1	1:A:475:TYR:OH	2.32	0.47
1:A:88:TRP:CD2	3:C:174:ALA:HB2	2.48	0.47
1:A:275:PHE:O	1:A:396:ARG:NH2	2.47	0.46
1:A:426:ASP:OD1	2:B:600:ASN:ND2	2.39	0.46
1:A:289:LYS:HB2	1:A:494:ASN:HB3	1.97	0.46
2:B:426:LEU:HD22	2:B:469:THR:HG21	1.96	0.46
1:A:365:LEU:HD13	1:A:502:GLY:HA2	1.97	0.46
1:A:230:LYS:HG2	2:B:334:ARG:HH21	1.81	0.46
1:A:370:ALA:HB2	4:V:10:A:H3'	1.98	0.46
1:A:588:GLU:O	1:A:592:GLU:N	2.48	0.46
2:B:569:GLU:OE1	4:V:42:G:N2	2.49	0.46
2:B:239:ARG:NH2	5:M:38:A:N7	2.63	0.46
1:A:317:TRP:HZ3	1:A:540:ILE:HD12	1.82	0.45
2:B:302:ILE:HD11	2:B:463:VAL:HG22	1.97	0.45
1:A:571:LYS:HB2	3:C:45:LEU:HD13	1.97	0.45
1:A:407:ASN:HD21	2:B:2:ASP:HA	1.81	0.45
2:B:626:ASN:ND2	3:C:104:PRO:O	2.50	0.45
2:B:706:ARG:HD3	2:B:706:ARG:HA	1.80	0.45
3:C:70:LYS:NZ	3:C:76:THR:OG1	2.46	0.45
1:A:545:ILE:HG13	1:A:554:LYS:HD3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:ASP:N	2:B:76:ASP:OD1	2.48	0.45
1:A:10:ASN:HB2	1:A:13:ILE:HG12	1.99	0.45
2:B:266:LEU:HD13	2:B:421:VAL:HG11	1.98	0.45
2:B:229:LYS:NZ	4:V:18:U:O4	2.41	0.45
1:A:278:GLN:OE1	1:A:645:TYR:OH	2.32	0.44
2:B:45:ARG:NH1	2:B:311:GLU:OE2	2.50	0.44
3:C:46:ARG:O	3:C:50:MET:CB	2.62	0.44
1:A:501:LYS:HB3	1:A:501:LYS:HE3	1.87	0.44
3:C:28:MET:HA	3:C:31:ILE:HG12	1.98	0.44
2:B:219:ILE:O	2:B:223:THR:OG1	2.29	0.44
1:A:378:ASP:OD1	1:A:378:ASP:N	2.50	0.43
2:B:113:ALA:O	2:B:117:THR:OG1	2.27	0.43
2:B:357:PHE:O	2:B:365:ARG:HA	2.18	0.43
1:A:331:ASN:HA	1:A:334:TYR:HD2	1.83	0.43
1:A:388:TYR:HE1	2:B:358:GLU:HB2	1.84	0.43
1:A:418:ILE:HD13	1:A:580:LEU:HD11	2.00	0.43
2:B:736:SER:OG	2:B:739:ASP:OD1	2.36	0.43
1:A:88:TRP:CE2	3:C:174:ALA:CB	2.91	0.43
2:B:183:THR:N	2:B:208:LYS:O	2.51	0.43
3:C:86:SER:OG	3:C:87:ASN:N	2.51	0.43
1:A:380:LYS:HB2	1:A:380:LYS:HE3	1.92	0.43
2:B:43:VAL:HG22	2:B:403:LEU:HD13	2.01	0.42
2:B:303:THR:O	2:B:482:SER:HA	2.19	0.42
1:A:310:CYS:O	1:A:313:THR:OG1	2.35	0.42
1:A:326:HIS:N	1:A:331:ASN:OD1	2.46	0.42
1:A:142:ASN:OD1	1:A:142:ASN:N	2.44	0.42
1:A:323:ILE:HA	1:A:323:ILE:HD13	1.94	0.42
1:A:591:ILE:HG12	1:A:606:PHE:HD2	1.85	0.42
3:C:175:ARG:C	3:C:175:ARG:NH1	2.73	0.42
1:A:314:PHE:O	1:A:317:TRP:NE1	2.52	0.42
1:A:260:PHE:HB3	1:A:673:PRO:HG2	2.01	0.42
1:A:67:ASP:N	1:A:67:ASP:OD1	2.53	0.42
1:A:263:ARG:HA	1:A:710:GLN:HG2	2.00	0.41
2:B:432:LEU:HB3	2:B:434:ARG:HD2	2.03	0.41
2:B:613:TRP:O	2:B:621:ARG:NH2	2.53	0.41
2:B:572:ARG:HD2	3:C:93:PRO:HB2	2.02	0.41
1:A:150:PHE:HB3	1:A:179:ARG:HG3	2.03	0.41
1:A:434:ALA:HB2	2:B:541:PRO:HB2	2.02	0.41
1:A:385:LEU:HD23	2:B:359:SER:HB2	2.03	0.40
2:B:120:ASP:OD1	2:B:707:ARG:NH2	2.53	0.40
2:B:724:ILE:HD12	2:B:724:ILE:HA	1.97	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:24:C:H2'	4:V:25:G:C8	2.56	0.40
3:C:130:PHE:HE1	3:C:234:LEU:HD21	1.86	0.40
1:A:476:GLN:NE2	4:V:41:U:O4	2.55	0.40

There are no symmetry-related clashes.

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 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	703/738 (95%)	685 (97%)	18 (3%)	0	100	100
2	B	739/776 (95%)	718 (97%)	21 (3%)	0	100	100
3	C	247/809 (30%)	239 (97%)	8 (3%)	0	100	100
All	All	1689/2323 (73%)	1642 (97%)	47 (3%)	0	100	100

There are no Ramachandran outliers to report.

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 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	634/656 (97%)	607 (96%)	27 (4%)	32	68
2	B	655/676 (97%)	628 (96%)	27 (4%)	33	70
3	C	224/706 (32%)	209 (93%)	15 (7%)	18	50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1513/2038 (74%)	1444 (95%)	69 (5%)	34 66

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	14	LEU
1	A	31	GLU
1	A	124	ARG
1	A	129	ASP
1	A	176	PHE
1	A	224	LYS
1	A	243	GLU
1	A	258	GLU
1	A	264	THR
1	A	295	PRO
1	A	315	TRP
1	A	348	MET
1	A	352	PHE
1	A	374	MET
1	A	384	ASP
1	A	394	GLU
1	A	440	PHE
1	A	445	VAL
1	A	486	ASP
1	A	506	LEU
1	A	513	VAL
1	A	526	ARG
1	A	553	MET
1	A	632	CYS
1	A	675	THR
1	A	713	MET
2	B	66	LEU
2	B	116	GLN
2	B	120	ASP
2	B	141	THR
2	B	183	THR
2	B	201	THR
2	B	213	THR
2	B	227	MET
2	B	228	THR
2	B	229	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	243	THR
2	B	248	ILE
2	B	249	ARG
2	B	258	LEU
2	B	295	ASP
2	B	310	ASN
2	B	314	ASN
2	B	451	ILE
2	B	571	ARG
2	B	619	ASP
2	B	629	ASN
2	B	632	VAL
2	B	638	GLU
2	B	674	ILE
2	B	707	ARG
2	B	709	ILE
2	B	725	ASP
3	C	4	ILE
3	C	11	VAL
3	C	35	THR
3	C	73	ASP
3	C	88	ARG
3	C	89	VAL
3	C	108	VAL
3	C	146	ASP
3	C	152	LYS
3	C	171	GLU
3	C	176	THR
3	C	177	LEU
3	C	196	CYS
3	C	213	ARG
3	C	217	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
2	B	382	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	V	30/44 (68%)	9 (30%)	0
5	M	9/11 (81%)	1 (11%)	0
All	All	39/55 (70%)	10 (25%)	0

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	V	7	A
4	V	11	A
4	V	13	A
4	V	18	U
4	V	19	U
4	V	28	U
4	V	29	C
4	V	40	C
4	V	44	U
5	M	38	A

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.