



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 20, 2018 – 03:29 am GMT

PDB ID : 5OSG
EMDB ID: : EMD-8343
Title : Structure of KSRP in context of Leishmania donovani 80S
Authors : Brito Querido, J.; Mancera-Martinez, E.; Vicens, Q.; Bochler, A.; Chicher, J.; Simonetti, A.; Hashem, Y.
Deposited on : 2017-08-17
Resolution : 2.90 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/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.

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) : trunk30686

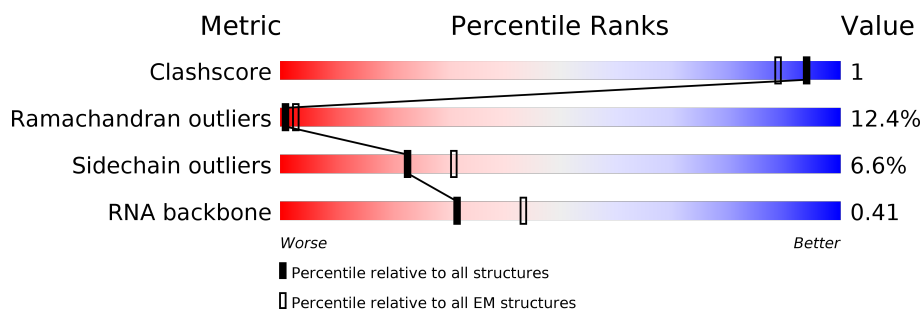
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


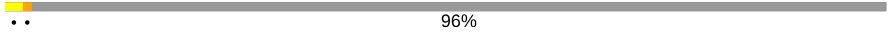

The reported resolution of this entry is 2.90 Å.

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	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531
RNA backbone	3744	458

The table below summarises the geometric issues observed across the polymeric chains. 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. 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	h	235	
2	2	2205	
3	P	249	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3465 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 RNA binding protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	h	173	Total	C	N	O	S	0	0
			1348	858	249	238	3		

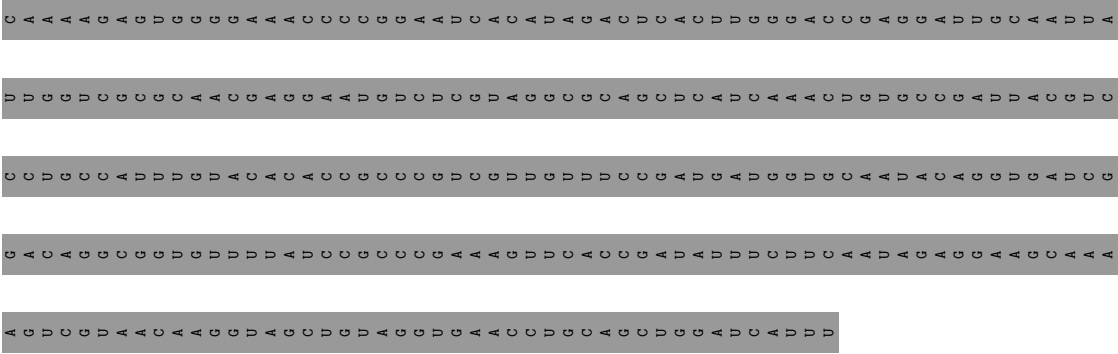
- Molecule 2 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	88	Total	C	N	O	P	0	0
			1841	832	320	607	82		

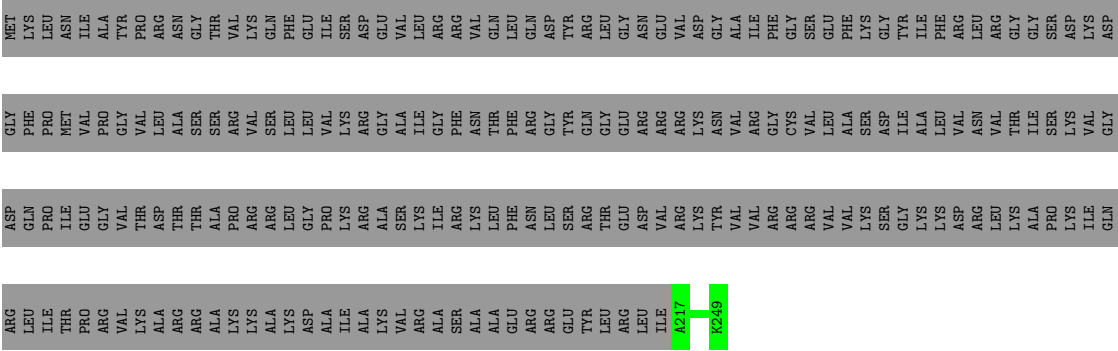
- Molecule 3 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	P	33	Total	C	N	O	0	0
			276	165	66	45		



● Molecule 3: 40S ribosomal protein S6



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	213108	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 BASE (4k x 4k)	Depositor

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	h	1.01	0/1373	1.33	7/1854 (0.4%)
2	2	1.62	1/2051 (0.0%)	2.50	235/3182 (7.4%)
3	P	1.12	0/279	0.97	0/366
All	All	1.39	1/3703 (0.0%)	2.09	242/5402 (4.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	h	0	29
2	2	0	5
All	All	0	34

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	257	A	N7-C5	-5.14	1.36	1.39

All (242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	257	A	P-O3'-C3'	15.28	138.04	119.70
2	2	257	A	N1-C6-N6	13.89	126.93	118.60
2	2	279	A	N1-C6-N6	13.53	126.72	118.60
2	2	226	G	P-O3'-C3'	12.77	135.02	119.70
2	2	229	A	N1-C6-N6	12.65	126.19	118.60
2	2	268	C	P-O3'-C3'	12.52	134.73	119.70
2	2	812	A	N1-C6-N6	12.46	126.08	118.60
2	2	275	A	N1-C6-N6	12.40	126.04	118.60
2	2	256	A	P-O3'-C3'	12.34	134.51	119.70
2	2	808	A	N1-C6-N6	12.30	125.98	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	231	A	N1-C6-N6	12.29	125.97	118.60
2	2	254	A	N1-C6-N6	12.28	125.97	118.60
2	2	261	A	N1-C6-N6	12.28	125.97	118.60
2	2	260	A	N1-C6-N6	12.27	125.96	118.60
2	2	256	A	N1-C6-N6	12.23	125.94	118.60
2	2	269	A	N1-C6-N6	12.07	125.84	118.60
2	2	281	A	N1-C6-N6	12.04	125.82	118.60
2	2	804	A	N1-C6-N6	12.00	125.80	118.60
2	2	254	A	P-O3'-C3'	11.93	134.02	119.70
2	2	255	A	N1-C6-N6	11.91	125.75	118.60
2	2	821	A	N1-C6-N6	11.85	125.71	118.60
2	2	276	G	P-O3'-C3'	11.83	133.90	119.70
2	2	200	A	N1-C6-N6	11.70	125.62	118.60
2	2	285	A	N1-C6-N6	11.70	125.62	118.60
2	2	278	A	N1-C6-N6	11.61	125.56	118.60
2	2	817	A	N1-C6-N6	11.28	125.36	118.60
2	2	276	G	N1-C6-O6	10.99	126.49	119.90
2	2	230	G	N1-C6-O6	10.90	126.44	119.90
2	2	194	U	P-O3'-C3'	10.88	132.76	119.70
2	2	196	C	P-O3'-C3'	10.73	132.57	119.70
2	2	272	G	N1-C6-O6	10.36	126.12	119.90
2	2	198	C	P-O3'-C3'	10.35	132.12	119.70
2	2	270	C	P-O3'-C3'	10.31	132.08	119.70
2	2	263	G	N1-C6-O6	10.30	126.08	119.90
2	2	228	G	N1-C6-O6	9.88	125.83	119.90
2	2	826	A	N1-C6-N6	9.49	124.29	118.60
2	2	949	G	N1-C6-O6	9.35	125.51	119.90
2	2	276	G	C5-C6-O6	-9.23	123.06	128.60
2	2	819	G	N1-C6-O6	9.23	125.44	119.90
2	2	824	C	P-O3'-C3'	9.19	130.73	119.70
2	2	230	G	C5-C6-O6	-9.13	123.12	128.60
2	2	272	G	C5-C6-O6	-9.10	123.14	128.60
2	2	823	G	N1-C6-O6	9.09	125.35	119.90
2	2	828	G	N1-C6-O6	9.01	125.30	119.90
2	2	814	G	N1-C6-O6	8.79	125.17	119.90
2	2	945	G	N1-C6-O6	8.78	125.17	119.90
2	2	273	G	N1-C6-O6	8.74	125.14	119.90
2	2	810	G	N1-C6-O6	8.73	125.14	119.90
2	2	233	G	N1-C6-O6	8.70	125.12	119.90
2	2	948	G	N1-C6-O6	8.70	125.12	119.90
2	2	803	G	N1-C6-O6	8.69	125.12	119.90
2	2	827	G	N1-C6-O6	8.68	125.11	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	226	G	N1-C6-O6	8.47	124.98	119.90
2	2	199	C	P-O3'-C3'	8.15	129.48	119.70
2	2	263	G	C5-C6-O6	-8.11	123.74	128.60
2	2	286	G	N1-C6-O6	7.96	124.68	119.90
2	2	228	G	C5-C6-O6	-7.94	123.84	128.60
2	2	256	A	O4'-C1'-N9	7.94	114.55	108.20
2	2	255	A	O4'-C1'-N9	7.77	114.41	108.20
2	2	262	U	O4'-C1'-N1	7.57	114.26	108.20
2	2	820	C	O4'-C1'-N1	7.53	114.22	108.20
2	2	280	C	O4'-C1'-N1	7.47	114.17	108.20
2	2	949	G	C5-C6-O6	-7.42	124.15	128.60
2	2	943	U	O4'-C1'-N1	7.36	114.09	108.20
2	2	822	U	O4'-C1'-N1	7.30	114.04	108.20
2	2	257	A	C4-C5-C6	7.27	120.64	117.00
2	2	819	G	C5-C6-O6	-7.26	124.24	128.60
2	2	279	A	C5-C6-N6	-7.25	117.90	123.70
2	2	282	C	O4'-C1'-N1	7.18	113.94	108.20
2	2	200	A	O4'-C1'-N9	7.17	113.94	108.20
2	2	277	U	P-O3'-C3'	7.15	128.28	119.70
2	2	827	G	C5-C6-O6	-7.09	124.34	128.60
2	2	275	A	C5-C6-N6	-7.08	118.03	123.70
2	2	232	C	O4'-C1'-N1	7.06	113.84	108.20
2	2	828	G	C5-C6-O6	-6.97	124.42	128.60
2	2	813	U	O4'-C1'-N1	6.95	113.76	108.20
2	2	825	C	O4'-C1'-N1	6.94	113.75	108.20
2	2	233	G	C5-C6-O6	-6.91	124.45	128.60
2	2	265	C	O4'-C1'-N1	6.89	113.71	108.20
2	2	271	U	O4'-C1'-N1	6.88	113.70	108.20
2	2	814	G	O4'-C1'-N9	6.87	113.69	108.20
2	2	230	G	O4'-C1'-N9	6.85	113.68	108.20
2	2	257	A	C5-C6-N6	-6.85	118.22	123.70
2	2	945	G	C5-C6-O6	-6.85	124.49	128.60
2	2	277	U	O4'-C1'-N1	6.82	113.66	108.20
2	2	826	A	C4-C5-C6	6.80	120.40	117.00
2	2	803	G	C5-C6-O6	-6.77	124.53	128.60
2	2	259	C	O4'-C1'-N1	6.77	113.62	108.20
2	2	229	A	C5-C6-N1	-6.76	114.32	117.70
2	2	814	G	C5-C6-O6	-6.72	124.57	128.60
2	2	810	G	C5-C6-O6	-6.71	124.57	128.60
2	2	816	C	O4'-C1'-N1	6.71	113.57	108.20
2	2	801	C	O4'-C1'-N1	6.70	113.56	108.20
2	2	823	G	C5-C6-O6	-6.67	124.60	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	196	C	N3-C4-N4	6.67	122.67	118.00
2	2	824	C	O4'-C1'-N1	6.66	113.53	108.20
2	2	287	C	O4'-C1'-N1	6.64	113.51	108.20
2	2	947	U	O4'-C1'-N1	6.60	113.48	108.20
2	2	812	A	C5-C6-N1	-6.60	114.40	117.70
2	2	200	A	C4-C5-C6	6.59	120.30	117.00
2	2	951	U	O4'-C1'-N1	6.57	113.46	108.20
2	2	944	U	O4'-C1'-N1	6.54	113.43	108.20
2	2	950	U	O4'-C1'-N1	6.54	113.43	108.20
2	2	273	G	C5-C6-O6	-6.53	124.68	128.60
2	2	256	A	C4-C5-C6	6.53	120.26	117.00
2	2	260	A	C5-C6-N1	-6.51	114.44	117.70
2	2	274	C	N3-C4-N4	6.50	122.55	118.00
2	2	800	C	O4'-C1'-N1	6.48	113.39	108.20
2	2	198	C	O4'-C1'-N1	6.48	113.38	108.20
2	2	808	A	C4-C5-C6	6.45	120.23	117.00
2	2	272	G	O4'-C1'-N9	6.43	113.34	108.20
2	2	226	G	C5-C6-O6	-6.41	124.76	128.60
2	2	258	C	O4'-C1'-N1	6.40	113.32	108.20
2	2	269	A	C4-C5-C6	6.40	120.20	117.00
2	2	255	A	C4-C5-C6	6.40	120.20	117.00
2	2	811	C	O4'-C1'-N1	6.39	113.31	108.20
2	2	198	C	N3-C4-N4	6.36	122.45	118.00
2	2	254	A	C4-C5-C6	6.35	120.17	117.00
2	2	199	C	O4'-C1'-N1	6.31	113.25	108.20
2	2	283	C	O4'-C1'-N1	6.30	113.24	108.20
2	2	197	U	O4'-C1'-N1	6.29	113.24	108.20
2	2	286	G	C5-C6-O6	-6.26	124.84	128.60
2	2	815	U	O4'-C1'-N1	6.26	113.20	108.20
2	2	948	G	C5-C6-O6	-6.25	124.85	128.60
1	h	170	GLN	C-N-CA	6.23	137.28	121.70
2	2	811	C	N3-C4-N4	6.23	122.36	118.00
2	2	812	A	C4-C5-C6	6.17	120.09	117.00
2	2	265	C	N3-C4-N4	6.17	122.32	118.00
2	2	270	C	O4'-C1'-N1	6.17	113.13	108.20
2	2	804	A	C4-C5-C6	6.11	120.06	117.00
2	2	275	A	O4'-C1'-N9	6.07	113.06	108.20
2	2	267	U	O4'-C1'-N1	6.07	113.06	108.20
2	2	264	C	N3-C4-C5	-6.06	119.48	121.90
2	2	275	A	C4-C5-C6	6.06	120.03	117.00
2	2	261	A	C4-C5-C6	6.05	120.03	117.00
2	2	281	A	C4-C5-C6	6.02	120.01	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	231	A	C4-C5-C6	6.01	120.01	117.00
2	2	809	C	O4'-C1'-N1	6.00	113.00	108.20
2	2	821	A	C4-C5-C6	6.00	120.00	117.00
2	2	802	U	O4'-C1'-N1	6.00	113.00	108.20
2	2	946	U	O4'-C1'-N1	5.97	112.97	108.20
2	2	260	A	C4-C5-C6	5.96	119.98	117.00
2	2	231	A	C5-C6-N1	-5.94	114.73	117.70
2	2	279	A	C4-C5-C6	5.93	119.97	117.00
2	2	195	U	O4'-C1'-N1	5.92	112.93	108.20
2	2	803	G	O4'-C1'-N9	5.89	112.92	108.20
2	2	256	A	C5-C6-N1	-5.85	114.77	117.70
2	2	254	A	C5-C6-N6	-5.83	119.04	123.70
2	2	261	A	C5-C6-N6	-5.82	119.05	123.70
2	2	285	A	C5-C6-N6	-5.82	119.05	123.70
2	2	259	C	N3-C4-N4	5.80	122.06	118.00
2	2	808	A	C5-C6-N6	-5.79	119.07	123.70
2	2	264	C	N3-C4-N4	5.79	122.05	118.00
2	2	198	C	C2'-C3'-O3'	5.76	122.92	113.70
2	2	280	C	N3-C4-C5	-5.76	119.60	121.90
2	2	820	C	N3-C4-N4	5.76	122.03	118.00
2	2	278	A	O4'-C1'-N9	5.76	112.81	108.20
2	2	278	A	C4-C5-C6	5.76	119.88	117.00
2	2	257	A	C5-C6-N1	-5.73	114.83	117.70
2	2	949	G	O4'-C1'-N9	5.70	112.76	108.20
2	2	258	C	N3-C4-C5	-5.70	119.62	121.90
1	h	61	ASN	N-CA-CB	5.68	120.83	110.60
2	2	258	C	N3-C4-N4	5.68	121.98	118.00
2	2	285	A	C4-C5-C6	5.68	119.84	117.00
2	2	826	A	C5-C6-N1	-5.67	114.87	117.70
2	2	268	C	N3-C4-N4	5.66	121.96	118.00
2	2	281	A	C5-C6-N6	-5.64	119.19	123.70
2	2	283	C	N3-C4-N4	5.64	121.95	118.00
2	2	804	A	C5-C6-N6	-5.64	119.19	123.70
2	2	269	A	C5-C6-N6	-5.63	119.19	123.70
2	2	824	C	N3-C4-N4	5.63	121.94	118.00
2	2	255	A	C5-C6-N1	-5.62	114.89	117.70
2	2	198	C	N3-C4-C5	-5.61	119.66	121.90
2	2	816	C	N3-C4-C5	-5.60	119.66	121.90
2	2	801	C	N3-C4-C5	-5.58	119.67	121.90
2	2	278	A	C5-C6-N6	-5.58	119.24	123.70
2	2	268	C	N3-C4-C5	-5.57	119.67	121.90
2	2	270	C	N3-C4-C5	-5.56	119.67	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	817	A	C4-C5-C6	5.56	119.78	117.00
2	2	821	A	C5-C6-N6	-5.55	119.26	123.70
2	2	229	A	C4-C5-C6	5.55	119.77	117.00
2	2	809	C	N3-C4-N4	5.55	121.88	118.00
2	2	824	C	N3-C4-C5	-5.53	119.69	121.90
2	2	256	A	C5-C6-N6	-5.52	119.28	123.70
2	2	266	U	O4'-C1'-N1	5.51	112.61	108.20
2	2	284	C	N3-C4-N4	5.51	121.86	118.00
2	2	231	A	C5-C6-N6	-5.50	119.30	123.70
2	2	808	A	C5-C6-N1	-5.49	114.95	117.70
1	h	133	GLU	C-N-CA	5.49	135.43	121.70
2	2	232	C	N3-C4-N4	5.49	121.84	118.00
2	2	200	A	C5-C6-N1	-5.48	114.96	117.70
2	2	811	C	N3-C4-C5	-5.48	119.71	121.90
2	2	816	C	N3-C4-N4	5.48	121.83	118.00
2	2	270	C	N3-C4-N4	5.48	121.83	118.00
2	2	269	A	C5-C6-N1	-5.47	114.97	117.70
2	2	825	C	N3-C4-C5	-5.46	119.72	121.90
2	2	287	C	N3-C4-N4	5.45	121.82	118.00
2	2	800	C	N3-C4-N4	5.45	121.81	118.00
2	2	259	C	N3-C4-C5	-5.45	119.72	121.90
2	2	264	C	O4'-C1'-N1	5.45	112.56	108.20
2	2	254	A	C5-C6-N1	-5.44	114.98	117.70
2	2	800	C	N3-C4-C5	-5.43	119.73	121.90
1	h	205	SER	C-N-CA	5.43	135.28	121.70
2	2	231	A	O4'-C1'-N9	5.43	112.54	108.20
2	2	261	A	C5-C6-N1	-5.43	114.99	117.70
2	2	255	A	C5-C6-N6	-5.42	119.36	123.70
2	2	281	A	C5-C6-N1	-5.42	114.99	117.70
2	2	945	G	O4'-C1'-N9	5.40	112.52	108.20
2	2	817	A	C5-C6-N1	-5.39	115.00	117.70
2	2	199	C	N3-C4-C5	-5.38	119.75	121.90
2	2	804	A	C5-C6-N1	-5.38	115.01	117.70
2	2	283	C	N3-C4-C5	-5.37	119.75	121.90
2	2	284	C	O4'-C1'-N1	5.36	112.49	108.20
2	2	274	C	N3-C4-C5	-5.35	119.76	121.90
2	2	200	A	C5-C6-N6	-5.35	119.42	123.70
2	2	810	G	O4'-C1'-N9	5.34	112.47	108.20
2	2	821	A	C5-C6-N1	-5.34	115.03	117.70
2	2	820	C	N3-C4-C5	-5.32	119.77	121.90
2	2	801	C	N3-C4-N4	5.32	121.72	118.00
2	2	280	C	N3-C4-N4	5.29	121.70	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	229	A	C5-C6-N6	-5.29	119.47	123.70
2	2	232	C	N3-C4-C5	-5.27	119.79	121.90
2	2	284	C	N3-C4-C5	-5.27	119.79	121.90
2	2	282	C	N3-C4-N4	5.26	121.68	118.00
2	2	194	U	O4'-C1'-N1	5.24	112.39	108.20
2	2	812	A	C5-C6-N6	-5.23	119.51	123.70
2	2	287	C	N3-C4-C5	-5.20	119.82	121.90
2	2	268	C	O4'-C1'-N1	5.20	112.36	108.20
2	2	274	C	O4'-C1'-N1	5.20	112.36	108.20
1	h	206	ALA	N-CA-CB	5.20	117.38	110.10
2	2	257	A	O4'-C1'-N9	5.19	112.35	108.20
2	2	809	C	N3-C4-C5	-5.16	119.83	121.90
2	2	260	A	C5-C6-N6	-5.13	119.59	123.70
2	2	817	A	C5-C6-N6	-5.09	119.63	123.70
1	h	179	SER	N-CA-CB	5.08	118.12	110.50
2	2	261	A	O4'-C1'-N9	5.08	112.26	108.20
2	2	812	A	O4'-C1'-N9	5.05	112.24	108.20
2	2	285	A	O4'-C1'-N9	5.03	112.23	108.20
2	2	825	C	N3-C4-N4	5.03	121.52	118.00
2	2	278	A	C5-C6-N1	-5.03	115.19	117.70
1	h	100	ALA	N-CA-CB	5.01	117.12	110.10
2	2	825	C	C6-N1-C2	-5.01	118.30	120.30

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	229	A	Sidechain
2	2	230	G	Sidechain
2	2	277	U	Sidechain
2	2	812	A	Sidechain
2	2	823	G	Sidechain
1	h	110	GLU	Peptide
1	h	112	GLU	Peptide
1	h	117	THR	Peptide
1	h	118	VAL	Peptide
1	h	123	ALA	Peptide
1	h	124	LYS	Peptide
1	h	125	ALA	Peptide
1	h	133	GLU	Peptide
1	h	141	SER	Peptide
1	h	161	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	h	176	TYR	Sidechain,Peptide
1	h	189	GLU	Peptide
1	h	192	GLY	Peptide
1	h	207	ARG	Peptide
1	h	56	GLY	Peptide
1	h	61	ASN	Peptide
1	h	62	TRP	Peptide
1	h	64	THR	Peptide
1	h	66	SER	Peptide
1	h	76	ALA	Peptide
1	h	78	GLY	Peptide
1	h	79	LYS	Peptide
1	h	80	VAL	Peptide
1	h	81	VAL	Peptide
1	h	83	VAL	Peptide
1	h	89	ARG	Peptide
1	h	91	ALA	Mainchain,Peptide

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	h	1348	0	1386	0	0
2	2	1841	0	956	2	0
3	P	276	0	288	0	0
All	All	3465	0	2630	2	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 1.

All (2) 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)
2:2:812:A:N1	2:2:823:G:N1	2.52	0.58
2:2:812:A:C2	2:2:823:G:C2	2.98	0.51

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	h	171/235 (73%)	114 (67%)	32 (19%)	25 (15%)	0	0
3	P	31/249 (12%)	30 (97%)	1 (3%)	0	100	100
All	All	202/484 (42%)	144 (71%)	33 (16%)	25 (12%)	1	1

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	h	61	ASN
1	h	77	ALA
1	h	80	VAL
1	h	108	PHE
1	h	111	LYS
1	h	118	VAL
1	h	158	ALA
1	h	169	ARG
1	h	179	SER
1	h	210	GLU
1	h	100	ALA
1	h	122	PRO
1	h	123	ALA
1	h	178	ASP
1	h	181	ALA
1	h	133	GLU
1	h	134	ASN
1	h	170	GLN
1	h	197	GLY
1	h	79	LYS
1	h	154	MET
1	h	99	ALA

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Mol	Chain	Res	Type
1	h	206	ALA
1	h	105	ILE
1	h	180	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	h	140/179 (78%)	129 (92%)	11 (8%)	13	37
3	P	27/208 (13%)	27 (100%)	0	100	100
All	All	167/387 (43%)	156 (93%)	11 (7%)	23	47

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	h	79	LYS
1	h	85	LEU
1	h	95	PHE
1	h	118	VAL
1	h	124	LYS
1	h	133	GLU
1	h	165	LEU
1	h	167	MET
1	h	177	LEU
1	h	204	LEU
1	h	208	SER

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
2	2	85/2205 (3%)	29 (34%)	12 (14%)

All (29) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	195	U
2	2	197	U
2	2	198	C
2	2	199	C
2	2	200	A
2	2	227	U
2	2	228	G
2	2	230	G
2	2	255	A
2	2	256	A
2	2	257	A
2	2	258	C
2	2	269	A
2	2	270	C
2	2	271	U
2	2	275	A
2	2	277	U
2	2	278	A
2	2	280	C
2	2	281	A
2	2	799	U
2	2	819	G
2	2	820	C
2	2	821	A
2	2	822	U
2	2	824	C
2	2	825	C
2	2	826	A
2	2	945	G

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	194	U
2	2	196	C
2	2	198	C
2	2	226	G
2	2	254	A
2	2	256	A
2	2	257	A
2	2	268	C
2	2	270	C

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Mol	Chain	Res	Type
2	2	274	C
2	2	276	G
2	2	824	C

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](#)

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.