



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:13 am GMT

PDB ID : 1MJ1
EMDB ID: : EMD-1004
Title : FITTING THE TERNARY COMPLEX OF EF-Tu/tRNA/GTP AND RIBOSOMAL PROTEINS INTO A 13 Å CRYO-EM MAP OF THE COLI 70S RIBOSOME
Authors : Stark, H.; Rodnina, M.V.; Wieden, H.-J.; Zemlin, F.; Wintermeyer, W.; Van-heel, M.
Deposited on : 2002-08-26
Resolution : 13.00 Å (reported)
Based on PDB ID : 1B23, 1GIX, 1GIY

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

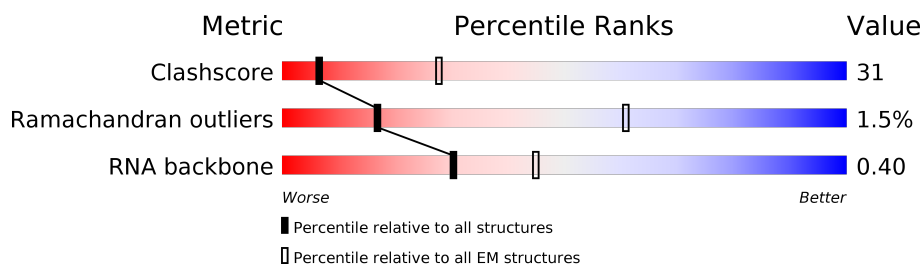
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 13.00 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	125131	1336
Ramachandran outliers	121729	1120
RNA backbone	3398	335

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	C	76	
1	D	76	
2	Q	41	
3	R	27	
4	A	405	
5	O	135	
6	P	126	
7	L	141	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5374 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 RNA chain called Phe-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	76	Total	C	N	O	P	0	0
			1652	746	294	536	76		
1	C	76	Total	C	N	O	P	0	0
			1652	746	294	536	76		

- Molecule 2 is a RNA chain called sarcin-ricin loop of 23SrRNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	Q	41	Total	P	0	41
			41	41		

- Molecule 3 is a RNA chain called helix 69 of 23S rRNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
3	R	27	Total	P	0	27
			27	27		

- Molecule 4 is a protein called Elongation Factor Tu.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	A	405	Total	C	N	O	0	0
			1620	810	405	405		

- Molecule 5 is a protein called S12 ribosomal protein.

Mol	Chain	Residues	Atoms		AltConf	Trace
5	O	124	Total	C	0	124
			124	124		

- Molecule 6 is a protein called S13 ribosomal protein.

Mol	Chain	Residues	Atoms		AltConf	Trace
6	P	125	Total 125	C 125	0	125

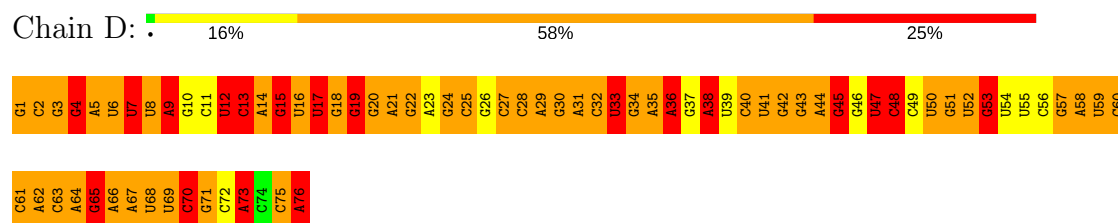
- Molecule 7 is a protein called L11 ribosomal protein.

Mol	Chain	Residues	Atoms		AltConf	Trace
7	L	133	Total 133	C 133	0	133

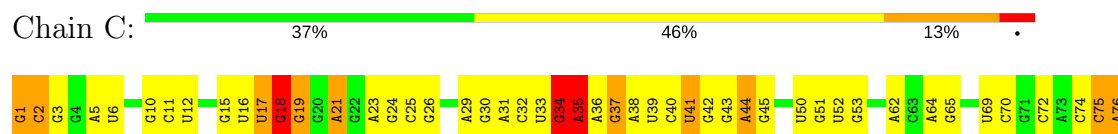
3 Residue-property plots

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: Phe-tRNA



- Molecule 1: Phe-tRNA

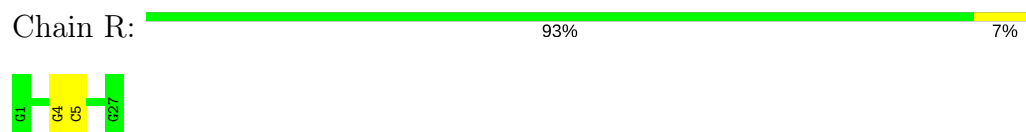


- Molecule 2: sarcin-ricin loop of 23SrRNA

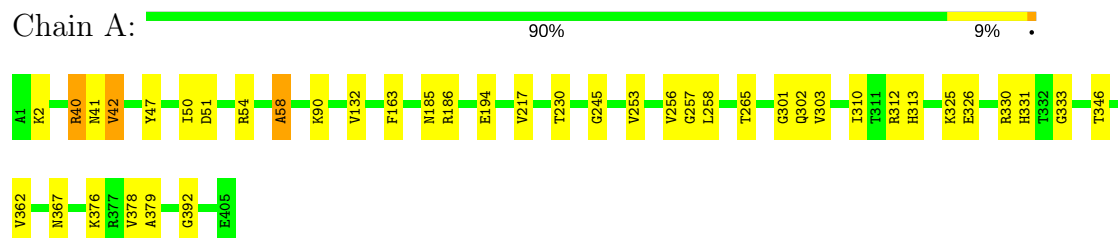


There are no outlier residues recorded for this chain.


- Molecule 3: helix 69 of 23S rRNA



- Molecule 4: Elongation Factor Tu



- Molecule 5: S12 ribosomal protein

Chain O:  89% 8%



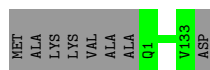
- Molecule 6: S13 ribosomal protein

Chain P:  99%



- Molecule 7: L11 ribosomal protein

Chain L:  94% 6%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	phase flip	Depositor
Microscope	FEI/PHILIPS CM20/SOPHIE	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1500	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	58500	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 5MU, OMG, H2U, YG, 2MG, 5MC, 1MA, M2G, 7MG, PSU

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	C	1.44	7/1487 (0.5%)	1.47	22/2315 (1.0%)
1	D	1.29	2/1487 (0.1%)	2.61	186/2315 (8.0%)
4	A	0.75	0/1618	1.34	8/2019 (0.4%)
All	All	1.19	9/4592 (0.2%)	1.91	216/6649 (3.2%)

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	C	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	74	C	O3'-P	-27.05	1.28	1.61
1	C	75	C	O3'-P	-25.57	1.30	1.61
1	C	44	A	O3'-P	-16.97	1.40	1.61
1	C	72	C	O3'-P	-15.88	1.42	1.61
1	C	35	A	O3'-P	8.16	1.71	1.61
1	C	1	G	OP3-P	-7.33	1.52	1.61
1	C	76	A	C2'-O2'	6.52	1.50	1.41
1	D	19	G	C2'-C1'	-5.46	1.47	1.53
1	D	47	U	C4-O4	5.15	1.27	1.23

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	35	A	P-O3'-C3'	27.06	152.18	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	74	C	O3'-P-O5'	24.46	150.48	104.00
1	D	18	G	P-O3'-C3'	15.21	137.96	119.70
1	C	35	A	OP1-P-O3'	14.55	137.21	105.20
1	D	21	A	O4'-C1'-N9	14.50	119.80	108.20
1	D	47	U	P-O3'-C3'	14.39	136.97	119.70
1	C	72	C	O3'-P-O5'	13.95	130.51	104.00
1	C	75	C	P-O3'-C3'	12.69	134.92	119.70
1	C	76	A	O5'-P-OP2	-12.57	94.39	105.70
1	D	3	G	O4'-C1'-N9	11.96	117.77	108.20
1	C	1	G	P-O3'-C3'	11.10	133.02	119.70
1	D	7	U	P-O3'-C3'	-10.32	107.31	119.70
1	C	74	C	OP2-P-O3'	-10.19	82.79	105.20
1	C	35	A	OP2-P-O3'	-9.66	83.94	105.20
1	D	59	U	P-O3'-C3'	9.60	131.22	119.70
1	C	34	OMG	O3'-P-O5'	9.60	122.23	104.00
1	C	44	A	OP2-P-O3'	9.56	126.24	105.20
1	C	34	OMG	OP2-P-O3'	-9.31	84.72	105.20
1	D	57	G	O4'-C1'-N9	9.23	115.59	108.20
1	C	72	C	OP1-P-O3'	-8.97	85.46	105.20
1	D	68	U	C2-N3-C4	-8.86	121.68	127.00
1	D	69	U	C2-N3-C4	-8.85	121.69	127.00
1	D	12	U	C2-N3-C4	-8.83	121.70	127.00
1	D	68	U	N3-C4-C5	8.69	119.82	114.60
1	D	60	C	O4'-C1'-N1	8.66	115.13	108.20
1	D	12	U	N3-C4-C5	8.62	119.77	114.60
1	D	65	G	O4'-C1'-N9	8.60	115.08	108.20
1	D	33	U	C2-N3-C4	-8.42	121.95	127.00
1	C	18	G	C5'-C4'-O4'	-8.41	99.00	109.10
1	D	50	U	N3-C4-C5	8.36	119.62	114.60
1	D	21	A	N9-C1'-C2'	-8.31	102.86	112.00
1	D	32	OMC	P-O3'-C3'	8.30	129.66	119.70
1	D	6	U	C2-N3-C4	-8.27	122.04	127.00
1	D	33	U	N3-C4-C5	8.26	119.55	114.60
1	D	59	U	C2-N3-C4	-8.25	122.05	127.00
1	D	8	U	P-O3'-C3'	-8.21	109.84	119.70
1	D	12	U	C5'-C4'-O4'	-8.20	120.98	125.90
1	D	3	G	N9-C1'-C2'	-8.18	103.00	112.00
1	D	7	U	C2-N3-C4	-8.17	122.10	127.00
1	C	74	C	P-O3'-C3'	-8.11	109.97	119.70
1	D	69	U	N3-C4-C5	8.10	119.46	114.60
1	D	50	U	C2-N3-C4	-8.06	122.17	127.00
1	D	41	U	N3-C4-C5	7.93	119.36	114.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	7	U	N3-C4-C5	7.92	119.35	114.60
1	D	6	U	N3-C4-C5	7.89	119.33	114.60
1	D	41	U	C2-N3-C4	-7.89	122.27	127.00
1	D	59	U	N3-C4-C5	7.85	119.31	114.60
1	C	72	C	P-O3'-C3'	-7.83	110.31	119.70
1	C	44	A	O3'-P-O5'	-7.83	89.13	104.00
1	D	8	U	N3-C4-C5	7.69	119.21	114.60
1	D	7	U	O4'-C1'-N1	7.68	114.34	108.20
1	C	75	C	O3'-P-O5'	7.60	118.43	104.00
1	D	66	A	O4'-C1'-N9	7.59	114.27	108.20
1	D	52	U	C2-N3-C4	-7.53	122.48	127.00
1	D	47	U	C2-N3-C4	-7.53	122.48	127.00
1	D	56	C	O4'-C1'-N1	7.50	114.20	108.20
1	D	52	U	N3-C4-C5	7.48	119.09	114.60
1	D	21	A	P-O3'-C3'	7.47	128.67	119.70
1	D	19	G	OP1-P-OP2	-7.46	108.41	119.60
1	D	8	U	C2-N3-C4	-7.44	122.53	127.00
1	C	75	C	O5'-P-OP1	-7.34	99.09	105.70
1	D	19	G	O4'-C1'-N9	-7.20	102.44	108.20
1	D	50	U	O4'-C1'-N1	7.17	113.93	108.20
1	D	36	A	N9-C1'-C2'	-7.15	104.13	112.00
1	D	75	C	P-O3'-C3'	7.14	128.27	119.70
1	D	61	C	P-O3'-C3'	7.10	128.22	119.70
1	D	53	G	N9-C1'-C2'	-7.05	104.25	112.00
1	D	22	G	OP1-P-OP2	-6.98	109.12	119.60
1	D	73	A	P-O3'-C3'	-6.97	111.34	119.70
1	D	73	A	N9-C1'-C2'	-6.92	104.38	112.00
1	D	69	U	P-O3'-C3'	6.91	127.99	119.70
1	D	15	G	N9-C1'-C2'	-6.82	104.50	112.00
1	D	47	U	N3-C4-C5	6.81	118.69	114.60
1	D	9	A	N1-C2-N3	-6.78	125.91	129.30
1	D	76	A	N1-C2-N3	-6.77	125.92	129.30
1	D	73	A	O4'-C1'-N9	6.72	113.58	108.20
1	D	64	A	N1-C2-N3	-6.60	126.00	129.30
1	D	31	A	O4'-C1'-N9	6.57	113.46	108.20
1	D	18	G	OP1-P-OP2	-6.57	109.75	119.60
1	D	29	A	N1-C2-N3	-6.55	126.02	129.30
1	D	73	A	N1-C2-N3	-6.49	126.05	129.30
1	D	2	C	O4'-C1'-N1	6.46	113.37	108.20
1	D	60	C	OP1-P-OP2	-6.42	109.97	119.60
1	D	31	A	N1-C2-N3	-6.40	126.10	129.30
1	D	11	C	OP1-P-OP2	-6.36	110.06	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	38	A	N1-C2-N3	-6.32	126.14	129.30
1	D	66	A	N9-C1'-C2'	-6.30	105.07	112.00
1	D	17	H2U	P-O3'-C3'	6.29	127.25	119.70
1	D	18	G	C5-C6-N1	6.29	114.65	111.50
1	D	36	A	N1-C2-N3	-6.27	126.17	129.30
4	A	163	PHE	N-CA-C	-6.26	94.11	111.00
1	D	61	C	N3-C4-C5	-6.24	119.40	121.90
1	D	65	G	C5-C6-N1	6.22	114.61	111.50
1	D	57	G	OP1-P-OP2	-6.19	110.31	119.60
1	D	67	A	N1-C2-N3	-6.16	126.22	129.30
1	D	56	C	N3-C4-C5	-6.15	119.44	121.90
1	D	9	A	OP1-P-OP2	-6.14	110.38	119.60
1	D	51	G	OP1-P-OP2	-6.14	110.39	119.60
1	D	52	U	OP1-P-OP2	-6.14	110.39	119.60
1	D	5	A	O5'-P-OP2	6.14	118.07	110.70
1	D	52	U	C5-C4-O4	-6.13	122.22	125.90
1	D	50	U	C5-C4-O4	-6.11	122.23	125.90
1	D	30	G	C5-C6-N1	6.11	114.55	111.50
1	D	35	A	N1-C2-N3	-6.10	126.25	129.30
1	D	43	G	C5-C6-N1	6.09	114.55	111.50
1	D	14	A	N1-C2-N3	-6.09	126.26	129.30
1	D	15	G	O4'-C1'-N9	6.06	113.05	108.20
1	D	42	G	C5-C6-N1	6.06	114.53	111.50
1	D	29	A	P-O3'-C3'	6.03	126.93	119.70
1	D	57	G	C5-C6-N1	6.02	114.51	111.50
1	D	76	A	OP1-P-OP2	-6.02	110.57	119.60
1	D	71	G	C5-C6-N1	6.01	114.51	111.50
1	D	44	A	N1-C2-N3	-6.01	126.30	129.30
1	D	20	G	C5-C6-N1	5.99	114.50	111.50
1	D	42	G	O4'-C1'-N9	5.99	113.00	108.20
1	D	53	G	C5-C6-N1	5.99	114.50	111.50
1	D	73	A	C6-N1-C2	5.98	122.19	118.60
1	D	36	A	O4'-C1'-N9	5.93	112.94	108.20
1	D	63	C	O4'-C1'-N1	5.93	112.94	108.20
1	D	66	A	N1-C2-N3	-5.92	126.34	129.30
1	C	15	G	N9-C1'-C2'	-5.91	105.50	112.00
1	D	53	G	O4'-C1'-N9	5.90	112.92	108.20
4	A	42	VAL	N-CA-C	-5.90	95.06	111.00
1	D	5	A	N1-C2-N3	-5.89	126.36	129.30
1	D	47	U	P-O5'-C5'	-5.88	111.49	120.90
1	D	21	A	N1-C2-N3	-5.86	126.37	129.30
1	D	63	C	N3-C4-C5	-5.86	119.56	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	28	C	O5'-P-OP2	5.83	117.69	110.70
1	D	70	C	O4'-C1'-N1	5.83	112.86	108.20
1	D	9	A	C6-N1-C2	5.82	122.09	118.60
1	D	35	A	C5-C6-N1	-5.79	114.80	117.70
1	D	69	U	OP1-P-OP2	-5.78	110.94	119.60
1	D	33	U	OP1-P-OP2	-5.76	110.96	119.60
1	D	48	C	N3-C4-C5	-5.74	119.60	121.90
1	D	59	U	OP1-P-OP2	-5.74	110.99	119.60
1	D	76	A	C6-N1-C2	5.72	122.03	118.60
1	D	76	A	C5-C6-N1	-5.72	114.84	117.70
1	D	3	G	C5-C6-N1	5.70	114.35	111.50
1	D	1	G	O4'-C1'-N9	5.70	112.76	108.20
1	D	23	A	N1-C2-N3	-5.68	126.46	129.30
1	D	1	G	C5-C6-N1	5.67	114.34	111.50
1	C	74	C	N1-C1'-C2'	5.66	121.36	114.00
1	D	48	C	OP1-P-OP2	-5.66	111.11	119.60
1	D	69	U	N1-C2-N3	5.66	118.29	114.90
1	D	12	U	O5'-P-OP2	5.65	117.48	110.70
1	D	13	C	OP1-P-OP2	-5.64	111.14	119.60
1	D	45	G	O4'-C1'-N9	5.63	112.70	108.20
1	D	29	A	C5-C6-N1	-5.62	114.89	117.70
1	D	62	A	C5-C6-N1	-5.61	114.90	117.70
1	D	75	C	OP1-P-OP2	-5.60	111.21	119.60
1	D	30	G	OP1-P-OP2	-5.59	111.21	119.60
1	D	21	A	C5-C6-N1	-5.59	114.90	117.70
1	D	9	A	C5-C6-N1	-5.56	114.92	117.70
1	D	48	C	P-O5'-C5'	-5.56	112.01	120.90
1	D	52	U	O4'-C1'-N1	5.55	112.64	108.20
1	D	73	A	C5-C6-N1	-5.50	114.95	117.70
1	D	60	C	N3-C4-C5	-5.47	119.71	121.90
1	D	75	C	N3-C4-C5	-5.43	119.73	121.90
1	D	31	A	C6-N1-C2	5.42	121.85	118.60
1	D	25	C	N3-C4-C5	-5.42	119.73	121.90
1	D	65	G	C6-N1-C2	-5.42	121.85	125.10
1	D	38	A	OP1-P-OP2	-5.41	111.48	119.60
4	A	185	ASN	CA-C-N	-5.40	105.32	117.20
1	D	69	U	C5-C4-O4	-5.37	122.68	125.90
4	A	132	VAL	N-CA-C	-5.35	96.55	111.00
1	D	29	A	C6-N1-C2	5.35	121.81	118.60
1	D	64	A	P-O3'-C3'	-5.33	113.30	119.70
1	D	62	A	N1-C2-N3	-5.32	126.64	129.30
1	D	35	A	C6-N1-C2	5.31	121.79	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	70	C	OP1-P-OP2	-5.31	111.63	119.60
1	D	59	U	N1-C2-N3	5.29	118.07	114.90
4	A	310	ILE	N-CA-C	5.29	125.27	111.00
1	D	62	A	C6-N1-C2	5.27	121.76	118.60
1	D	68	U	OP1-P-OP2	-5.27	111.69	119.60
1	D	72	C	OP1-P-OP2	-5.27	111.70	119.60
1	D	12	U	OP1-P-OP2	-5.26	111.71	119.60
1	D	51	G	C5-C6-N1	5.23	114.11	111.50
4	A	367	ASN	N-CA-C	-5.22	96.90	111.00
1	D	38	A	C6-N1-C2	5.21	121.73	118.60
1	D	22	G	C5-C6-N1	5.20	114.10	111.50
1	D	5	A	OP1-P-OP2	-5.19	111.81	119.60
1	D	47	U	N1-C2-N3	5.18	118.01	114.90
1	D	61	C	C2-N3-C4	5.18	122.49	119.90
1	D	70	C	N3-C4-C5	-5.16	119.83	121.90
1	D	47	U	O4'-C1'-N1	5.15	112.32	108.20
1	D	67	A	O5'-C5'-C4'	-5.15	101.92	111.70
1	D	47	U	C5-C4-O4	-5.14	122.82	125.90
1	D	11	C	N3-C4-C5	-5.14	119.85	121.90
1	D	63	C	N1-C1'-C2'	-5.13	106.35	112.00
1	D	66	A	P-O5'-C5'	-5.13	112.69	120.90
1	D	12	U	N1-C2-N3	5.13	117.98	114.90
1	D	36	A	C6-N1-C2	5.13	121.68	118.60
1	D	50	U	N1-C1'-C2'	-5.13	106.36	112.00
1	D	7	U	N1-C2-N3	5.12	117.97	114.90
1	D	44	A	C5-C6-N1	-5.11	115.14	117.70
1	D	4	G	OP1-P-OP2	-5.10	111.94	119.60
1	D	22	G	C6-N1-C2	-5.10	122.04	125.10
1	D	65	G	N9-C1'-C2'	-5.10	106.39	112.00
1	D	66	A	C5-C6-N1	-5.09	115.15	117.70
1	D	24	G	C5-C6-N1	5.08	114.04	111.50
1	D	59	U	O4'-C1'-N1	5.08	112.26	108.20
1	D	36	A	C5-C6-N1	-5.06	115.17	117.70
1	D	14	A	C5-C6-N1	-5.06	115.17	117.70
1	D	19	G	C5-C6-N1	5.05	114.03	111.50
1	D	31	A	C5-C6-N1	-5.04	115.18	117.70
1	D	2	C	OP1-P-OP2	-5.04	112.04	119.60
4	A	51	ASP	N-CA-C	-5.04	97.41	111.00
1	D	56	C	C2-N3-C4	5.03	122.42	119.90
1	D	53	G	OP1-P-OP2	-5.03	112.06	119.60
1	C	21	A	C5'-C4'-C3'	5.02	124.04	116.00
4	A	185	ASN	N-CA-C	5.02	124.55	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	73	A	OP1-P-OP2	-5.01	112.08	119.60
1	D	45	G	OP1-P-OP2	-5.01	112.09	119.60
1	D	73	A	N1-C6-N6	5.01	121.61	118.60
1	D	5	A	C5-C6-N1	-5.00	115.20	117.70
1	D	62	A	OP1-P-OP2	-5.00	112.09	119.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	18	G	Sidechain
1	C	19	G	Sidechain
1	C	62	A	Sidechain

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	C	1652	0	862	52	0
1	D	1652	0	859	149	0
2	Q	41	0	0	0	0
3	R	27	0	0	2	0
4	A	1620	0	481	53	0
5	O	124	0	0	5	0
6	P	125	0	0	0	0
7	L	133	0	0	0	0
All	All	5374	0	2202	232	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 31.

All (232) 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)
4:A:258:LEU:O	4:A:376:LYS:CA	1.70	1.39

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:G:N2	1:C:2:C:H41	1.22	1.38
1:C:1:G:N2	1:C:2:C:N4	1.77	1.31
1:D:50:U:O2'	4:A:331:HIS:N	1.71	1.22
1:D:12:U:O2'	5:O:48:LEU:CA	1.92	1.18
1:C:25:C:O3'	1:C:26:M2G:P	2.12	1.07
4:A:258:LEU:O	4:A:376:LYS:C	1.79	1.06
1:D:37:YG:N20	1:D:37:YG:H101	1.76	0.99
1:D:1:G:H2'	1:D:2:C:H6	1.27	0.98
1:C:41:U:H5'	1:C:41:U:H6	1.34	0.91
1:C:33:U:C2	1:C:35:A:H5'	2.06	0.91
1:C:1:G:H22	1:C:2:C:N4	1.65	0.90
1:D:1:G:H2'	1:D:2:C:C6	2.08	0.89
1:D:3:G:O2'	1:D:4:G:H5'	1.74	0.87
1:D:47:U:H2'	1:D:50:U:OP1	1.75	0.87
1:D:52:U:C4'	4:A:326:GLU:CA	2.52	0.87
4:A:90:LYS:CA	4:A:346:THR:N	2.39	0.86
1:D:38:A:H2'	1:D:39:PSU:O4'	1.76	0.85
4:A:301:GLY:CA	4:A:379:ALA:H	1.90	0.85
4:A:301:GLY:O	4:A:378:VAL:C	2.14	0.85
1:D:37:YG:HN2	1:D:37:YG:H101	1.40	0.84
1:D:52:U:O4'	4:A:326:GLU:CA	2.25	0.84
1:D:66:A:H3'	4:A:392:GLY:N	1.53	0.84
1:C:10:2MG:C5	1:C:26:M2G:HM12	2.12	0.83
1:D:68:U:H2'	1:D:69:U:H6	1.44	0.82
1:D:12:U:H1'	5:O:47:ALA:CA	2.09	0.82
1:C:25:C:H2'	1:C:26:M2G:O4'	1.80	0.82
1:C:33:U:O2	1:C:35:A:H3'	1.80	0.82
1:D:14:A:C3'	1:D:15:G:H5'	2.10	0.82
1:D:30:G:O2'	1:D:31:A:H5'	1.81	0.81
1:D:75:C:O2	1:D:75:C:H2'	1.80	0.80
1:C:1:G:H22	1:C:2:C:H41	1.25	0.80
4:A:301:GLY:O	4:A:379:ALA:N	2.15	0.79
1:D:37:YG:C2'	1:D:37:YG:H31	2.13	0.79
1:D:37:YG:O17	1:D:37:YG:H243	1.83	0.79
1:D:75:C:H4'	1:D:76:A:OP1	1.85	0.77
1:C:1:G:H21	1:C:2:C:N4	1.80	0.77
4:A:301:GLY:HA2	4:A:379:ALA:H	1.49	0.76
4:A:301:GLY:O	4:A:312:ARG:CA	2.33	0.76
1:D:34:OMG:H2'	1:D:34:OMG:N3	1.98	0.76
1:D:76:A:O3'	4:A:230:THR:O	2.03	0.76
1:D:51:G:C4'	4:A:325:LYS:CA	2.64	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:A:C2'	1:D:15:G:H5'	2.16	0.75
4:A:258:LEU:H	4:A:313:HIS:C	1.90	0.75
4:A:301:GLY:CA	4:A:379:ALA:N	2.50	0.74
1:C:10:2MG:C4	1:C:26:M2G:HM12	2.22	0.74
1:D:70:C:H2'	1:D:71:G:H8	1.52	0.74
1:D:42:G:O2'	1:D:43:G:H5'	1.87	0.73
1:D:68:U:H2'	1:D:69:U:C6	2.23	0.73
1:C:37:YG:C1'	1:C:37:YG:H31	2.19	0.73
1:C:10:2MG:C5	1:C:26:M2G:CM1	2.71	0.73
1:D:34:OMG:H5''	1:D:35:A:OP2	1.88	0.73
1:D:35:A:H2'	1:D:36:A:C1'	2.18	0.73
1:D:51:G:H4'	4:A:325:LYS:CA	2.19	0.72
1:C:37:YG:H31	1:C:37:YG:C2'	2.20	0.72
1:D:37:YG:C1'	1:D:37:YG:H31	2.19	0.72
1:C:11:C:H4'	3:R:5:C:P	2.29	0.72
1:D:16:H2U:OP1	1:D:16:H2U:H51	1.90	0.72
1:C:34:OMG:OP1	1:C:34:OMG:H8	1.71	0.72
4:A:258:LEU:N	4:A:313:HIS:O	2.23	0.71
1:C:37:YG:H101	1:C:37:YG:N20	2.06	0.71
1:D:52:U:H4'	4:A:326:GLU:CA	2.22	0.69
1:C:37:YG:H31	1:C:37:YG:H1'	1.74	0.69
1:D:1:G:C6	1:D:73:A:C2	2.82	0.68
1:C:1:G:N2	1:C:2:C:C4	2.61	0.68
1:D:54:5MU:H73	1:D:55:PSU:C2	2.29	0.68
4:A:301:GLY:HA2	4:A:379:ALA:N	2.09	0.67
1:D:28:C:C2	1:D:29:A:C8	2.82	0.67
4:A:257:GLY:HA3	4:A:312:ARG:O	1.96	0.66
1:C:44:A:C2'	1:C:45:G:H5'	2.25	0.66
4:A:302:GLN:CA	4:A:312:ARG:CA	2.75	0.65
1:C:26:M2G:HM22	1:C:44:A:C2	2.32	0.65
1:C:12:U:OP1	3:R:4:G:P	2.55	0.65
1:D:70:C:C2	1:D:71:G:C8	2.84	0.65
4:A:47:TYR:O	4:A:50:ILE:N	2.27	0.64
4:A:303:VAL:N	4:A:312:ARG:N	2.45	0.64
1:D:28:C:N3	1:D:29:A:N7	2.46	0.64
1:D:16:H2U:H51	1:D:16:H2U:P	2.38	0.64
1:D:31:A:O2'	1:D:32:OMC:H5''	1.98	0.64
1:D:5:A:O2'	1:D:6:U:H5'	1.99	0.63
4:A:54:ARG:O	4:A:58:ALA:N	2.30	0.63
1:D:43:G:O2'	1:D:44:A:H5'	1.99	0.62
1:D:51:G:H4'	4:A:330:ARG:O	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:5MC:H2'	1:C:41:U:H5'	1.82	0.62
1:D:37:YG:C2'	1:D:38:A:H5'	2.29	0.62
1:D:26:M2G:O2'	1:D:27:C:H5'	2.00	0.61
4:A:90:LYS:CA	4:A:346:THR:CA	2.78	0.61
1:D:12:U:O2	5:O:47:ALA:CA	2.48	0.61
1:C:37:YG:C21	1:C:37:YG:H101	2.30	0.61
1:C:41:U:C6	1:C:41:U:H5'	2.27	0.60
1:D:28:C:O2'	1:D:29:A:H5'	2.01	0.60
1:C:44:A:O2'	1:C:45:G:H5'	2.00	0.60
1:D:37:YG:H1'	1:D:37:YG:H31	1.83	0.60
1:D:76:A:O3'	4:A:230:THR:CA	2.49	0.60
1:C:41:U:C5'	1:C:41:U:H6	2.13	0.60
1:D:14:A:H2'	1:D:15:G:H5'	1.84	0.59
1:D:29:A:O2'	1:D:30:G:H5'	2.02	0.59
1:D:41:U:O2'	1:D:42:G:H5'	2.02	0.59
1:D:16:H2U:H4'	1:D:17:H2U:OP1	2.02	0.59
1:D:19:G:C4	1:D:57:G:N2	2.71	0.59
1:D:50:U:O2'	1:D:51:G:H5'	2.03	0.59
1:C:41:U:H2'	1:C:42:G:O4'	2.03	0.58
1:D:24:G:C6	1:D:25:C:C4	2.90	0.58
4:A:253:VAL:N	4:A:265:THR:O	2.29	0.58
4:A:257:GLY:HA3	4:A:312:ARG:C	2.23	0.58
1:C:64:A:H2'	1:C:65:G:O4'	2.04	0.57
1:D:37:YG:O2'	1:D:38:A:H5'	2.04	0.57
1:C:44:A:H2'	1:C:45:G:O4'	2.04	0.57
1:D:50:U:O2'	4:A:331:HIS:CA	2.52	0.57
1:D:66:A:H2'	1:D:67:A:C8	2.40	0.57
1:D:34:OMG:H3'	1:D:35:A:H8	1.69	0.56
4:A:302:GLN:C	4:A:312:ARG:CA	2.73	0.56
1:D:10:2MG:N3	1:D:10:2MG:H2'	2.20	0.56
4:A:302:GLN:C	4:A:312:ARG:N	2.59	0.56
1:D:26:M2G:HM22	1:D:44:A:C2	2.41	0.56
1:D:47:U:O2	1:D:47:U:H2'	2.06	0.55
1:C:29:A:O2'	1:C:30:G:H5'	2.06	0.55
1:D:34:OMG:H3'	1:D:35:A:C8	2.42	0.55
1:D:24:G:C6	1:D:25:C:N3	2.75	0.55
1:D:50:U:HO2'	4:A:331:HIS:H	1.52	0.55
1:D:19:G:H4'	1:D:20:G:OP2	2.07	0.55
1:D:7:U:H4'	1:D:8:U:OP2	2.06	0.55
1:D:2:C:H2'	1:D:2:C:O2	2.06	0.54
1:C:16:H2U:H1'	1:C:17:H2U:OP2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:A:H2'	1:D:67:A:H8	1.72	0.54
1:D:9:A:C2	1:D:45:G:C6	2.96	0.54
1:D:66:A:H8	4:A:392:GLY:CA	2.19	0.53
1:D:51:G:H1'	4:A:325:LYS:O	2.08	0.53
1:D:66:A:C8	4:A:392:GLY:HA3	2.43	0.53
4:A:333:GLY:HA2	4:A:362:VAL:O	2.09	0.53
1:D:67:A:O2'	1:D:68:U:H5'	2.09	0.53
1:D:24:G:C5	1:D:25:C:C4	2.97	0.52
1:D:53:G:H2'	1:D:53:G:N3	2.23	0.52
4:A:40:ARG:C	4:A:42:VAL:H	2.13	0.52
1:D:31:A:C2'	1:D:32:OMC:H5''	2.40	0.52
1:D:66:A:H8	4:A:392:GLY:HA3	1.74	0.52
1:D:50:U:HO2'	4:A:331:HIS:N	2.01	0.51
1:C:69:U:H2'	1:C:70:C:C6	2.46	0.51
1:D:33:U:C2'	1:D:34:OMG:O5'	2.59	0.51
1:D:37:YG:H31	1:D:37:YG:H2'	1.90	0.51
1:D:69:U:H5'	5:O:71:HIS:CA	2.40	0.51
4:A:217:VAL:O	4:A:245:GLY:HA2	2.11	0.50
1:D:51:G:OP1	4:A:331:HIS:O	2.28	0.50
1:C:40:5MC:H2'	1:C:41:U:C5'	2.40	0.50
4:A:301:GLY:HA3	4:A:379:ALA:H	1.72	0.50
1:D:35:A:C2'	1:D:36:A:O4'	2.60	0.50
1:D:29:A:C6	1:D:42:G:C6	3.00	0.49
1:D:33:U:H2'	1:D:34:OMG:O5'	2.13	0.49
1:D:28:C:C4	1:D:29:A:N7	2.80	0.49
1:C:23:A:O2'	1:C:24:G:H5'	2.12	0.49
1:D:76:A:OP2	1:D:76:A:H8	1.95	0.49
1:D:37:YG:H32	1:D:38:A:O4'	2.12	0.49
1:D:51:G:C4'	4:A:330:ARG:O	2.60	0.49
1:D:42:G:O2'	1:D:43:G:C5'	2.59	0.49
1:D:76:A:OP2	1:D:76:A:C8	2.65	0.49
1:C:30:G:O2'	1:C:31:A:H5'	2.12	0.49
1:D:37:YG:H132	1:D:37:YG:O6	2.13	0.48
1:C:16:H2U:O2'	1:C:17:H2U:OP2	2.21	0.48
1:D:47:U:C2'	1:D:50:U:OP1	2.55	0.47
1:D:75:C:O2	1:D:75:C:C2'	2.51	0.47
1:D:16:H2U:OP1	1:D:16:H2U:C5	2.61	0.47
4:A:90:LYS:CA	4:A:346:THR:H	2.26	0.47
1:D:65:G:O2'	1:D:66:A:H5'	2.15	0.47
1:D:31:A:H2'	1:D:32:OMC:C5'	2.45	0.47
1:D:70:C:O3'	5:O:74:GLN:CA	2.59	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:YG:H31	1:C:37:YG:O2'	2.15	0.47
4:A:301:GLY:C	4:A:379:ALA:N	2.68	0.47
1:D:35:A:H2'	1:D:36:A:H1'	1.95	0.47
1:D:8:U:C4	1:D:13:C:C4	3.04	0.46
1:D:31:A:N1	1:D:39:PSU:O2	2.48	0.46
1:D:32:OMC:H2'	1:D:33:U:C6	2.50	0.46
1:D:76:A:O3'	4:A:230:THR:C	2.54	0.46
1:D:35:A:H2'	1:D:36:A:O4'	2.16	0.46
1:D:1:G:C2'	1:D:2:C:H6	2.14	0.46
1:D:30:G:O2'	1:D:31:A:C5'	2.61	0.46
1:D:31:A:C2	1:D:40:5MC:N3	2.84	0.46
1:D:70:C:N3	1:D:71:G:N7	2.64	0.46
4:A:303:VAL:CA	4:A:312:ARG:N	2.79	0.46
1:D:37:YG:H2'	1:D:37:YG:C3	2.45	0.46
1:D:51:G:H2'	1:D:52:U:C6	2.51	0.46
1:D:61:C:H2'	1:D:62:A:H8	1.80	0.46
1:C:33:U:O2	1:C:35:A:H5'	2.13	0.45
1:D:5:A:O2'	1:D:6:U:C5'	2.64	0.45
1:D:70:C:H2'	1:D:71:G:C8	2.41	0.45
1:C:23:A:H2'	1:C:24:G:C8	2.52	0.45
1:D:34:OMG:HM23	1:D:34:OMG:O3'	2.16	0.45
1:D:16:H2U:H62	1:D:16:H2U:H2'	1.67	0.44
1:D:37:YG:C16	1:D:37:YG:H243	2.46	0.44
1:C:50:U:O2'	1:C:51:G:H5'	2.17	0.44
1:D:2:C:C2'	1:D:2:C:O2	2.66	0.44
1:D:43:G:HO2'	1:D:44:A:H5'	1.81	0.44
4:A:256:VAL:O	4:A:312:ARG:O	2.35	0.44
1:D:3:G:N2	1:D:71:G:C4	2.86	0.44
1:C:16:H2U:C2'	1:C:17:H2U:OP2	2.65	0.44
1:D:3:G:C2'	1:D:4:G:H5'	2.47	0.43
1:D:63:C:H2'	1:D:64:A:C8	2.53	0.43
1:D:9:A:H4'	1:D:10:2MG:OP2	2.18	0.43
1:D:28:C:H2'	1:D:29:A:H8	1.84	0.43
1:C:50:U:C2'	1:C:51:G:H5'	2.48	0.43
1:C:43:G:H2'	1:C:44:A:C8	2.53	0.43
1:D:33:U:O2'	1:D:35:A:N7	2.43	0.43
1:C:34:OMG:H3'	1:C:35:A:H5''	2.00	0.42
1:D:70:C:O2'	1:D:71:G:H5'	2.19	0.42
1:C:44:A:C2'	1:C:45:G:C5'	2.96	0.42
1:D:1:G:C4	1:D:2:C:C6	3.07	0.42
1:D:12:U:C2'	1:D:13:C:O5'	2.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:A:C3'	4:A:392:GLY:N	2.27	0.42
1:D:16:H2U:O5'	1:D:16:H2U:C2'	2.68	0.42
1:D:3:G:N1	1:D:71:G:C6	2.88	0.42
1:C:32:OMC:H6	1:C:32:OMC:O5'	2.01	0.42
1:D:12:U:H2'	1:D:13:C:O5'	2.20	0.41
1:D:5:A:C2'	1:D:6:U:O5'	2.68	0.41
4:A:40:ARG:O	4:A:42:VAL:N	2.45	0.41
1:C:37:YG:H32	1:C:38:A:O4'	2.20	0.41
1:D:14:A:C6	1:D:22:G:N3	2.88	0.41
1:D:61:C:H2'	1:D:62:A:C8	2.54	0.41
1:D:30:G:HO2'	1:D:31:A:H5'	1.81	0.41
1:D:14:A:C5	1:D:22:G:C2	3.09	0.41
1:D:19:G:C5	1:D:57:G:N2	2.88	0.41
1:C:52:U:O2'	1:C:53:G:H5'	2.20	0.41
1:D:19:G:C8	1:D:57:G:N2	2.89	0.41
1:D:31:A:C2'	1:D:32:OMC:C5'	2.98	0.41
1:D:35:A:C2'	1:D:36:A:C1'	2.95	0.41
1:D:26:M2G:C2'	1:D:27:C:O5'	2.69	0.40
1:D:47:U:H4'	1:D:48:C:OP2	2.20	0.40
1:D:7:U:C4'	1:D:8:U:OP2	2.68	0.40
1:D:30:G:C2'	1:D:31:A:O5'	2.69	0.40
1:D:66:A:C8	4:A:392:GLY:CA	3.01	0.40
1:D:47:U:O2	1:D:47:U:C2'	2.69	0.40
1:C:39:PSU:N1	1:C:40:5MC:HM52	2.36	0.40
1:C:5:A:H2'	1:C:6:U:O4'	2.21	0.40
1:D:58:1MA:H4'	1:D:59:U:OP1	2.21	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
4	A	401/405 (99%)	371 (92%)	24 (6%)	6 (2%)	12 53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	2	LYS
4	A	41	ASN
4	A	40	ARG
4	A	194	GLU
4	A	58	ALA
4	A	186	ARG

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	75/76 (98%)	13 (17%)	0
1	D	75/76 (98%)	29 (38%)	0
2	Q	0/41	-	-
3	R	0/27	-	-
All	All	150/220 (68%)	42 (28%)	0

All (42) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	D	4	G
1	D	7	U
1	D	9	A
1	D	12	U
1	D	13	C
1	D	15	G
1	D	16	H2U
1	D	17	H2U
1	D	18	G
1	D	19	G
1	D	21	A
1	D	27	C
1	D	33	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	34	OMG
1	D	36	A
1	D	38	A
1	D	40	5MC
1	D	45	G
1	D	46	7MG
1	D	47	U
1	D	48	C
1	D	49	5MC
1	D	53	G
1	D	58	1MA
1	D	60	C
1	D	65	G
1	D	70	C
1	D	73	A
1	D	76	A
1	C	2	C
1	C	3	G
1	C	17	H2U
1	C	18	G
1	C	19	G
1	C	21	A
1	C	34	OMG
1	C	35	A
1	C	36	A
1	C	37	YG
1	C	41	U
1	C	75	C
1	C	76	A

There are no RNA pucker outliers to report.

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

28 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	C	10	1	19,26,27	1.05	1 (5%)	20,38,41	2.53	4 (20%)
1	H2U	C	16	1	17,21,22	0.78	1 (5%)	21,30,33	1.16	3 (14%)
1	H2U	C	17	1	17,21,22	0.77	0	21,30,33	1.03	2 (9%)
1	M2G	C	26	1	20,27,28	1.23	3 (15%)	21,40,43	2.68	4 (19%)
1	OMC	C	32	1	15,22,23	0.86	0	19,31,34	0.61	0
1	OMG	C	34	1	18,26,27	1.30	2 (11%)	22,38,41	2.57	4 (18%)
1	YG	C	37	1	29,42,43	1.04	2 (6%)	29,62,65	2.23	8 (27%)
1	PSU	C	39	1	16,21,22	1.27	2 (12%)	20,30,33	6.11	4 (20%)
1	5MC	C	40	1	15,22,23	0.99	1 (6%)	17,32,35	1.03	2 (11%)
1	7MG	C	46	1	20,26,27	1.19	2 (10%)	22,39,42	2.11	2 (9%)
1	5MC	C	49	1	15,22,23	0.94	0	17,32,35	1.13	2 (11%)
1	5MU	C	54	1	14,22,23	1.26	2 (14%)	16,32,35	4.34	2 (12%)
1	PSU	C	55	1	16,21,22	1.45	3 (18%)	20,30,33	5.96	6 (30%)
1	1MA	C	58	1	16,25,26	2.76	4 (25%)	13,37,40	1.19	1 (7%)
1	2MG	D	10	1	19,26,27	1.02	1 (5%)	20,38,41	3.35	5 (25%)
1	H2U	D	16	1	17,21,22	1.13	1 (5%)	21,30,33	1.16	1 (4%)
1	H2U	D	17	1	17,21,22	0.67	0	21,30,33	0.92	1 (4%)
1	M2G	D	26	1	20,27,28	1.11	2 (10%)	21,40,43	3.21	8 (38%)
1	OMC	D	32	1	15,22,23	1.40	2 (13%)	19,31,34	2.03	1 (5%)
1	OMG	D	34	1	18,26,27	1.24	2 (11%)	22,38,41	2.67	5 (22%)
1	YG	D	37	1	29,42,43	2.94	7 (24%)	29,62,65	2.74	12 (41%)
1	PSU	D	39	1	16,21,22	1.36	2 (12%)	20,30,33	6.18	4 (20%)
1	5MC	D	40	1	15,22,23	1.05	2 (13%)	17,32,35	1.13	2 (11%)
1	7MG	D	46	1	20,26,27	1.64	3 (15%)	22,39,42	1.82	2 (9%)
1	5MC	D	49	1	15,22,23	0.99	2 (13%)	17,32,35	1.18	1 (5%)
1	5MU	D	54	1	14,22,23	0.96	0	16,32,35	2.74	3 (18%)
1	PSU	D	55	1	16,21,22	1.48	3 (18%)	20,30,33	6.51	6 (30%)
1	1MA	D	58	1	16,25,26	1.17	1 (6%)	13,37,40	0.99	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	C	10	1	-	0/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	H2U	C	16	1	-	0/7/38/39	0/2/2/2
1	H2U	C	17	1	-	0/7/38/39	0/2/2/2
1	M2G	C	26	1	-	0/7/29/30	0/3/3/3
1	OMC	C	32	1	-	0/5/27/28	0/2/2/2
1	OMG	C	34	1	-	0/5/27/28	0/3/3/3
1	YG	C	37	1	-	0/20/42/43	0/4/4/4
1	PSU	C	39	1	-	0/7/25/26	0/2/2/2
1	5MC	C	40	1	-	0/3/25/26	0/2/2/2
1	7MG	C	46	1	-	0/7/37/38	0/3/3/3
1	5MC	C	49	1	-	0/3/25/26	0/2/2/2
1	5MU	C	54	1	-	0/3/25/26	0/2/2/2
1	PSU	C	55	1	-	0/7/25/26	0/2/2/2
1	1MA	C	58	1	-	0/3/25/26	0/3/3/3
1	2MG	D	10	1	-	0/5/27/28	0/3/3/3
1	H2U	D	16	1	-	0/7/38/39	0/2/2/2
1	H2U	D	17	1	-	0/7/38/39	0/2/2/2
1	M2G	D	26	1	-	0/7/29/30	0/3/3/3
1	OMC	D	32	1	-	0/5/27/28	0/2/2/2
1	OMG	D	34	1	-	0/5/27/28	0/3/3/3
1	YG	D	37	1	-	0/20/42/43	0/4/4/4
1	PSU	D	39	1	-	0/7/25/26	0/2/2/2
1	5MC	D	40	1	-	0/3/25/26	0/2/2/2
1	7MG	D	46	1	-	0/7/37/38	0/3/3/3
1	5MC	D	49	1	-	0/3/25/26	0/2/2/2
1	5MU	D	54	1	-	0/3/25/26	0/2/2/2
1	PSU	D	55	1	-	0/7/25/26	0/2/2/2
1	1MA	D	58	1	-	0/3/25/26	0/3/3/3

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	37	YG	C3-N3	-9.13	1.36	1.49
1	D	46	7MG	C8-N9	-5.67	1.37	1.45
1	D	32	OMC	O2'-CM2	-3.71	1.28	1.42
1	D	34	OMG	O2'-CM2	-3.47	1.29	1.42
1	C	39	PSU	C6-C5	-3.40	1.33	1.38
1	C	55	PSU	C6-C5	-3.00	1.34	1.38
1	C	58	1MA	O5'-C5'	-2.63	1.41	1.44
1	D	37	YG	C14-C15	-2.63	1.47	1.53
1	D	55	PSU	C6-C5	-2.63	1.34	1.38
1	C	54	5MU	O5'-C5'	-2.60	1.41	1.44
1	D	46	7MG	C8-N7	-2.57	1.32	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	39	PSU	C6-C5	-2.49	1.35	1.38
1	D	55	PSU	O4'-C1'	-2.28	1.41	1.44
1	C	40	5MC	C6-C5	-2.23	1.34	1.40
1	D	26	M2G	CM2-N2	-2.21	1.40	1.45
1	C	26	M2G	C8-N7	-2.18	1.30	1.34
1	D	37	YG	C6-N1	-2.17	1.34	1.37
1	D	40	5MC	C6-C5	-2.06	1.34	1.40
1	C	55	PSU	O4'-C1'	-2.04	1.41	1.44
1	D	49	5MC	C6-C5	-2.04	1.34	1.40
1	C	37	YG	C6-C5	2.00	1.44	1.41
1	C	34	OMG	C2-N1	2.01	1.39	1.35
1	C	26	M2G	C2-N1	2.20	1.38	1.34
1	D	32	OMC	O4'-C1'	2.24	1.44	1.41
1	D	58	1MA	C6-N6	2.26	1.32	1.27
1	D	49	5MC	O4'-C1'	2.29	1.44	1.41
1	C	46	7MG	CM7-N7	2.36	1.50	1.46
1	C	16	H2U	C2-N1	2.48	1.39	1.35
1	D	46	7MG	C6-N1	2.49	1.37	1.33
1	D	40	5MC	O4'-C1'	2.60	1.44	1.41
1	D	10	2MG	C6-N1	2.73	1.38	1.33
1	D	34	OMG	C6-N1	2.76	1.38	1.33
1	D	26	M2G	C6-N1	2.76	1.38	1.33
1	C	37	YG	C6-N1	2.81	1.42	1.37
1	C	39	PSU	C4-N3	3.03	1.38	1.33
1	D	16	H2U	O5'-C5'	3.07	1.49	1.44
1	C	46	7MG	C6-N1	3.17	1.38	1.33
1	D	55	PSU	C4-N3	3.23	1.38	1.33
1	C	54	5MU	C4-N3	3.27	1.39	1.33
1	D	37	YG	O4'-C1'	3.30	1.45	1.41
1	C	58	1MA	C6-C5	3.40	1.47	1.41
1	C	26	M2G	C6-N1	3.47	1.39	1.33
1	D	39	PSU	C4-N3	3.62	1.39	1.33
1	C	10	2MG	C6-N1	3.63	1.39	1.33
1	D	37	YG	O18-C16	3.82	1.42	1.33
1	C	58	1MA	C2-N3	4.02	1.37	1.30
1	C	34	OMG	C6-N1	4.11	1.40	1.33
1	C	55	PSU	C4-N3	4.17	1.40	1.33
1	D	37	YG	O23-C21	5.99	1.43	1.34
1	D	37	YG	C2-N2	8.72	1.48	1.35
1	C	58	1MA	C6-N6	8.89	1.48	1.27

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	55	PSU	N1-C2-N3	-20.12	113.93	128.40
1	D	39	PSU	N1-C2-N3	-19.73	114.21	128.40
1	C	39	PSU	N1-C2-N3	-19.62	114.29	128.40
1	C	55	PSU	N1-C2-N3	-19.48	114.39	128.40
1	D	55	PSU	C5-C4-N3	-13.08	114.70	125.43
1	C	39	PSU	C5-C4-N3	-12.98	114.78	125.43
1	D	39	PSU	C5-C4-N3	-12.74	114.98	125.43
1	C	55	PSU	C5-C4-N3	-12.32	115.33	125.43
1	D	10	2MG	CM2-N2-C2	-12.18	108.82	123.63
1	C	54	5MU	C5-C4-N3	-10.07	114.14	125.24
1	D	26	M2G	CM1-N2-C2	-9.15	112.63	121.34
1	C	34	OMG	C5-C6-N1	-8.57	111.28	123.48
1	C	26	M2G	C5-C6-N1	-8.28	111.69	123.48
1	C	10	2MG	C5-C6-N1	-8.19	111.83	123.48
1	C	46	7MG	C5-C6-N1	-7.01	112.37	123.37
1	D	26	M2G	C5-C6-N1	-6.53	114.19	123.48
1	D	34	OMG	C5-C6-N1	-6.36	114.42	123.48
1	D	10	2MG	C5-C6-N1	-6.18	114.68	123.48
1	D	46	7MG	C5-C6-N1	-6.08	113.83	123.37
1	D	54	5MU	C5-C4-N3	-5.47	119.21	125.24
1	D	55	PSU	C5-C1'-C2'	-5.35	106.31	115.55
1	D	37	YG	C6-C5-C4	-5.32	116.25	119.92
1	D	37	YG	C24-O23-C21	-5.22	109.23	115.68
1	C	37	YG	C13-C12-C11	-4.10	123.54	130.66
1	D	37	YG	O23-C21-O22	-3.91	119.24	124.60
1	D	26	M2G	C2-N3-C4	-3.76	110.83	115.11
1	C	37	YG	O23-C21-O22	-3.61	119.66	124.60
1	D	26	M2G	CM2-N2-C2	-3.27	118.23	121.34
1	D	34	OMG	C6-C5-C4	-3.25	117.61	120.84
1	C	26	M2G	C2-N3-C4	-3.05	111.63	115.11
1	D	10	2MG	C2-N3-C4	-3.01	111.68	115.11
1	C	49	5MC	CM5-C5-C4	-3.00	118.57	121.65
1	C	58	1MA	C2-N3-C4	-2.99	111.82	116.41
1	D	58	1MA	C2-N3-C4	-2.96	111.87	116.41
1	C	10	2MG	C2-N3-C4	-2.84	111.87	115.11
1	D	34	OMG	C2-N3-C4	-2.83	111.86	115.16
1	C	34	OMG	C2-N3-C4	-2.81	111.88	115.16
1	D	16	H2U	O5'-C5'-C4'	-2.79	99.19	109.01
1	D	26	M2G	C6-C5-C4	-2.78	118.08	120.84
1	D	10	2MG	C6-C5-C4	-2.75	118.11	120.84
1	D	37	YG	C13-C12-C11	-2.72	125.92	130.66
1	C	40	5MC	CM5-C5-C4	-2.67	118.90	121.65
1	D	26	M2G	N3-C2-N2	-2.56	114.51	117.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	37	YG	O22-C21-N20	-2.50	120.56	124.87
1	C	34	OMG	N3-C2-N1	-2.49	123.82	127.46
1	C	17	H2U	C5-C4-N3	-2.33	114.41	116.72
1	D	37	YG	O17-C16-C15	-2.23	117.26	123.91
1	C	55	PSU	O2'-C2'-C1'	-2.21	107.22	112.21
1	C	55	PSU	C4-C5-C1'	-2.19	116.91	121.15
1	D	17	H2U	C5-C6-N1	-2.03	108.59	110.70
1	C	16	H2U	C5-C4-N3	-2.02	114.72	116.72
1	D	40	5MC	CM5-C5-C4	-2.02	119.58	121.65
1	C	26	M2G	N3-C2-N2	2.15	119.37	117.15
1	C	17	H2U	C4-N3-C2	2.24	127.74	125.81
1	C	40	5MC	CM5-C5-C6	2.26	123.19	118.67
1	C	37	YG	O18-C16-C15	2.29	117.59	111.54
1	D	40	5MC	N4-C4-N3	2.31	120.41	117.00
1	D	37	YG	C14-C15-N20	2.33	115.73	110.90
1	C	16	H2U	O3'-C3'-C2'	2.39	119.47	111.83
1	C	49	5MC	CM5-C5-C6	2.49	123.64	118.67
1	D	37	YG	C4-C5-N7	2.52	111.84	109.41
1	D	55	PSU	O4'-C1'-C2'	2.59	108.61	104.45
1	D	37	YG	C3-N3-C2	2.67	122.11	118.31
1	C	16	H2U	C4-N3-C2	2.70	128.13	125.81
1	C	37	YG	C19-O18-C16	2.78	122.50	115.97
1	C	37	YG	C3-N3-C2	2.98	122.56	118.31
1	D	49	5MC	O4'-C1'-N1	2.99	114.06	108.08
1	C	10	2MG	N2-C2-N3	3.34	120.20	116.95
1	D	54	5MU	O4'-C1'-N1	3.43	114.94	108.08
1	D	37	YG	O18-C16-C15	3.56	120.94	111.54
1	D	10	2MG	C6-N1-C2	3.67	121.75	115.18
1	C	37	YG	O23-C21-N20	4.01	118.50	110.82
1	D	26	M2G	CM2-N2-CM1	4.05	129.14	116.03
1	D	34	OMG	C6-N1-C2	4.61	122.69	116.06
1	D	37	YG	O23-C21-N20	4.89	120.20	110.82
1	D	46	7MG	C6-N1-C2	4.95	123.19	116.06
1	D	26	M2G	C6-N1-C2	5.01	122.14	116.18
1	D	39	PSU	C6-N1-C2	5.02	123.39	115.36
1	D	55	PSU	C6-N1-C2	5.03	123.41	115.36
1	C	37	YG	C3-N3-C4	5.11	125.59	118.31
1	C	55	PSU	C6-N1-C2	5.19	123.67	115.36
1	C	39	PSU	C6-N1-C2	5.27	123.80	115.36
1	C	10	2MG	C6-N1-C2	5.41	124.86	115.18
1	C	37	YG	C24-O23-C21	5.99	123.08	115.68
1	C	46	7MG	C6-N1-C2	6.00	124.69	116.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	34	OMG	C6-N1-C2	6.44	125.33	116.06
1	D	37	YG	C3-N3-C4	7.11	128.44	118.31
1	C	26	M2G	C6-N1-C2	7.35	124.93	116.18
1	D	34	OMG	CM2-O2'-C2'	7.87	136.06	114.54
1	D	32	OMC	CM2-O2'-C2'	7.94	136.25	114.54
1	D	54	5MU	C4-N3-C2	8.47	122.57	115.16
1	C	55	PSU	C4-N3-C2	11.37	125.11	115.16
1	C	39	PSU	C4-N3-C2	12.35	125.96	115.16
1	D	39	PSU	C4-N3-C2	13.34	126.83	115.16
1	C	54	5MU	C4-N3-C2	13.84	127.26	115.16
1	D	55	PSU	C4-N3-C2	14.02	127.42	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	10	2MG	3	0
1	C	16	H2U	3	0
1	C	17	H2U	3	0
1	C	26	M2G	6	0
1	C	32	OMC	1	0
1	C	34	OMG	2	0
1	C	37	YG	7	0
1	C	39	PSU	1	0
1	C	40	5MC	3	0
1	D	10	2MG	2	0
1	D	16	H2U	6	0
1	D	17	H2U	1	0
1	D	26	M2G	3	0
1	D	32	OMC	5	0
1	D	34	OMG	7	0
1	D	37	YG	13	0
1	D	39	PSU	2	0
1	D	40	5MC	1	0
1	D	54	5MU	1	0
1	D	55	PSU	1	0
1	D	58	1MA	1	0

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.