



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jun 16, 2019 – 04:25 AM EDT

PDB ID : 4CXG
EMDB ID: : EMD-2623
Title : Regulation of the mammalian elongation cycle by 40S subunit rolling: a eukaryotic-specific ribosome rearrangement
Authors : Budkevich, T.V.; Giesebrecht, J.; Behrmann, E.; Loerke, J.; Ramrath, D.J.F.; Mielke, T.; Ismer, J.; Hildebrand, P.; Tung, C.-S.; Nierhaus, K.H.; Sanbonmatsu, K.Y.; Spahn, C.M.T.
Deposited on : 2014-04-07
Resolution : 8.70 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary 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
Mogul : 1.8.0 (224370), CSD as540be (2019)
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) : 2.3.2

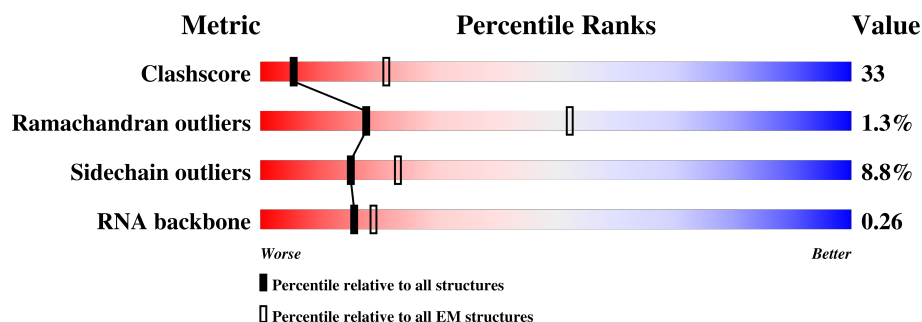
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.70 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. 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	1	135	17% 52% 30% .
2	2	50	18% 30% 52%
3	A	437	75% 19% . .
4	X	143	54% 36% . 6%
5	Y	76	14% 22% 54% 9%
6	a	48	33% 65% .
7	b	17	41% 59%
8	c	19	42% 53% 5%

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Mol	Chain	Length	Quality of chain
9	x	28	<div><div></div><div>36%</div><div>64%</div></div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	2MG	Y	10	-	-	X	-
5	M2G	Y	26	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12269 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 18S RRNA - H44.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	135	Total	C	N	O	P	0	0
			2890	1288	527	940	135		

- Molecule 2 is a RNA chain called 28S RRNA - H89.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	50	Total	C	N	O	P	0	0
			1057	471	176	360	50		

- Molecule 3 is a protein called ELONGATION FACTOR 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	427	Total	C	N	O	S	0	0
			3272	2104	570	585	13		

- Molecule 4 is a protein called 40S RIBOSOMAL PROTEIN US12.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	134	Total	C	N	O	S	0	0
			1046	663	205	176	2		

- Molecule 5 is a RNA chain called TRANSFER RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	Y	76	Total	C	N	O	P	S	0	0
			1636	737	290	532	76	1		

- Molecule 6 is a RNA chain called 18S RRNA - H5-H14.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	a	48	Total	C	N	O	P	0	0
			1024	458	192	326	48		

- Molecule 7 is a RNA chain called 18S RRNA - H8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	b	17	Total	C	N	O	P	0	0
			363	162	63	121	17		

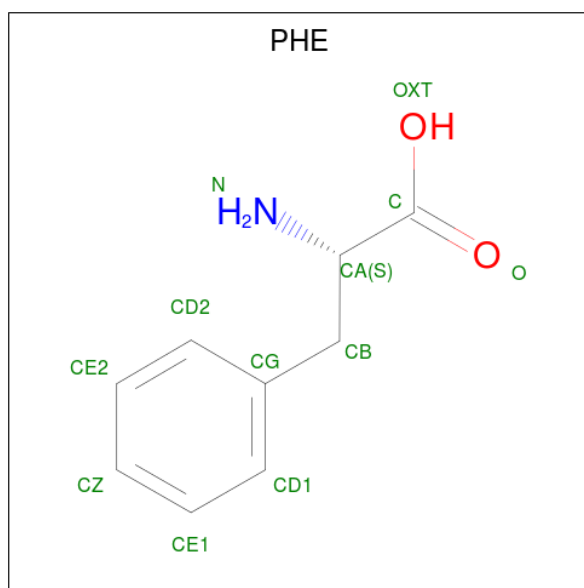
- Molecule 8 is a RNA chain called 28S RRNA - H95.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	c	19	Total	C	N	O	P	0	0
			410	183	78	130	19		

- Molecule 9 is a RNA chain called MESSENGER RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	x	28	Total	C	N	O	P	0	0
			560	252	56	224	28		

- Molecule 10 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).

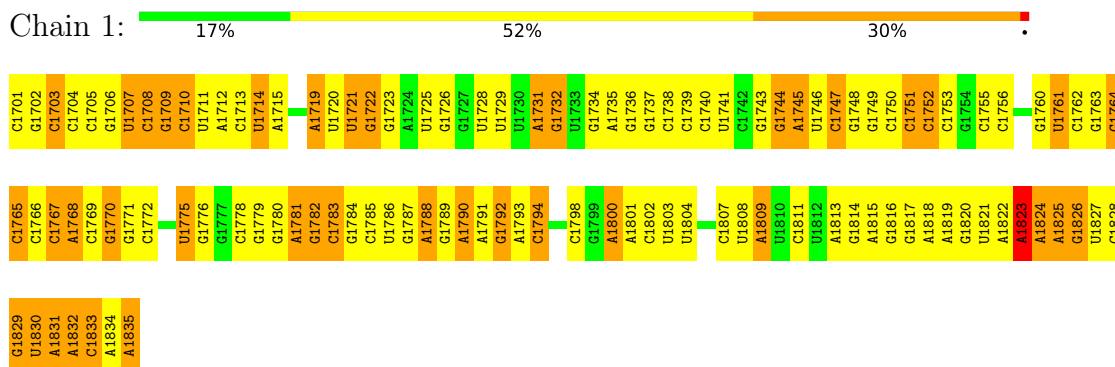


Mol	Chain	Residues	Atoms				AltConf
10	Y	1	Total	C	N	O	0
			11	9	1	1	

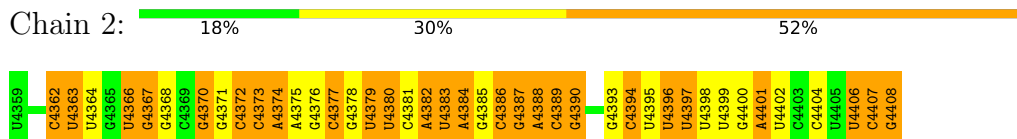
3 Residue-property plots

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.

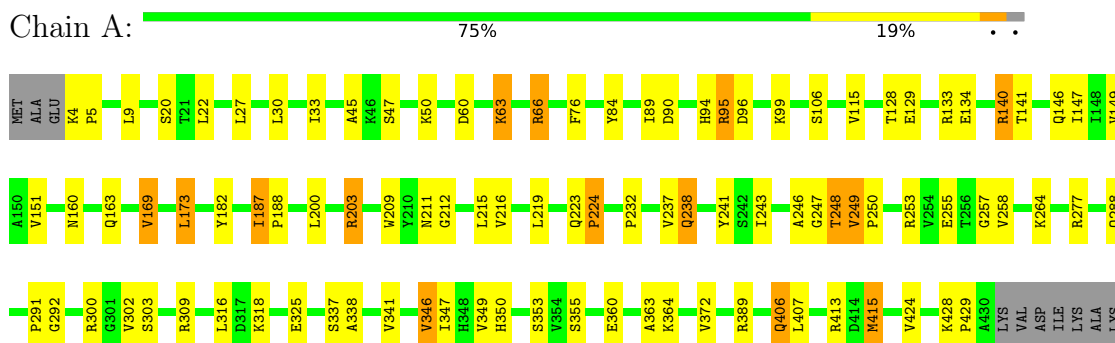
- Molecule 1: 18S RRNA - H44



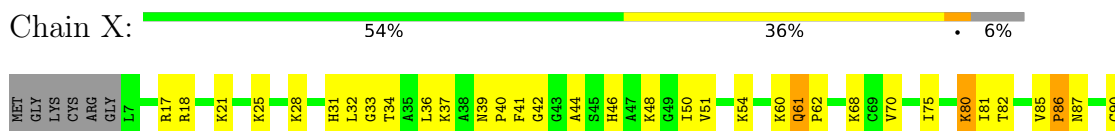
- Molecule 2: 28S RRNA - H89



- Molecule 3: ELONGATION FACTOR 1A



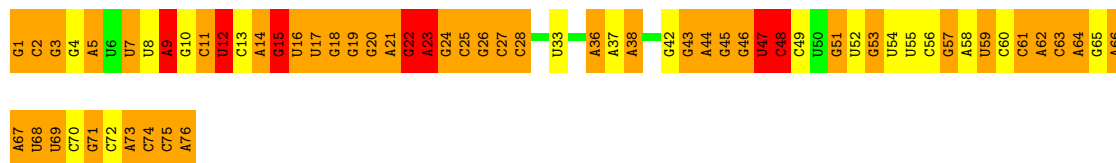
- Molecule 4: 40S RIBOSOMAL PROTEIN US12





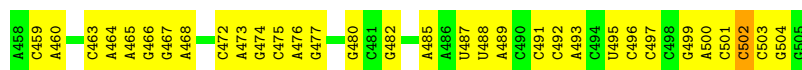
- Molecule 5: TRANSFER RNA

Chain Y: 14% 22% 54% 9%



- Molecule 6: 18S RRNA - H5-H14

Chain a: 33% 65%



- Molecule 7: 18S RRNA - H8

Chain b: 41% 59%



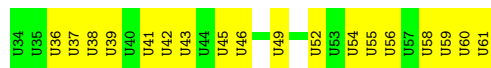
- Molecule 8: 28S RRNA - H95

Chain c: 42% 53% 5%



- Molecule 9: MESSENGER RNA

Chain x: 36% 64%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	79705	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	DEFOCUS GROUP	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	65520	Depositor
Image detector	KODAK SO-163 FILM	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: OMC, 5MU, H2U, MIA, 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	1	0.33	0/3232	0.77	0/5039
2	2	0.34	0/1177	0.81	0/1831
3	A	0.44	0/3346	0.62	0/4542
4	X	0.46	0/1063	0.70	0/1421
5	Y	0.48	1/1550 (0.1%)	1.94	65/2410 (2.7%)
6	a	0.37	0/1145	0.83	1/1782 (0.1%)
7	b	0.35	0/405	0.78	0/629
8	c	0.35	0/459	0.86	1/714 (0.1%)
9	x	0.42	1/615 (0.2%)	1.25	11/948 (1.2%)
All	All	0.40	2/12992 (0.0%)	1.00	78/19316 (0.4%)

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	1	0	1
5	Y	1	1
9	x	1	0
All	All	2	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	1	G	OP3-P	-5.77	1.54	1.61
9	x	60	U	O3'-P	5.07	1.67	1.61

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	22	G	O4'-C1'-N9	29.56	131.85	108.20
5	Y	21	A	N9-C1'-C2'	-20.07	87.90	114.00
5	Y	22	G	N9-C1'-C2'	-18.97	89.33	114.00
5	Y	71	G	O4'-C1'-N9	-17.30	94.36	108.20
5	Y	48	C	O4'-C1'-N1	15.16	120.33	108.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	Y	36	A	C3'
9	x	58	U	C3'

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	1823	A	Sidechain
5	Y	33	U	Sidechain

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	1	2890	0	1462	156	0
2	2	1057	0	535	67	0
3	A	3272	0	3292	88	0
4	X	1046	0	1110	48	0
5	Y	1636	0	848	145	0
6	a	1024	0	525	0	0
7	b	363	0	182	0	0
8	c	410	0	207	0	0
9	x	560	0	281	0	0
10	Y	11	0	8	0	0
All	All	12269	0	8450	464	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 33.

The worst 5 of 464 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)
3:A:249:VAL:CG1	5:Y:76:A:N3	1.70	1.51
3:A:249:VAL:HG11	5:Y:76:A:C2	1.58	1.38
3:A:249:VAL:CG1	5:Y:76:A:C2	2.08	1.37
3:A:243:ILE:O	5:Y:76:A:N6	1.62	1.29
3:A:415:MET:CE	5:Y:51:G:H21	1.46	1.28

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	
3	A	425/437 (97%)	413 (97%)	12 (3%)	0	100	100
4	X	132/143 (92%)	120 (91%)	5 (4%)	7 (5%)	2	25
All	All	557/580 (96%)	533 (96%)	17 (3%)	7 (1%)	18	54

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	X	61	GLN
4	X	106	GLY
4	X	107	ARG
4	X	116	PRO
4	X	33	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
3	A	344/372 (92%)	309 (90%)	35 (10%)	8	30
4	X	108/115 (94%)	103 (95%)	5 (5%)	29	59
All	All	452/487 (93%)	412 (91%)	40 (9%)	15	37

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	187	ILE
3	A	237	VAL
4	X	31	HIS
3	A	211	ASN
3	A	238	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	348	HIS
4	X	77	ASN
4	X	61	GLN
3	A	315	HIS
4	X	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	134/135 (99%)	57 (42%)	7 (5%)
2	2	49/50 (98%)	28 (57%)	4 (8%)
5	Y	74/76 (97%)	29 (39%)	7 (9%)
6	a	47/48 (97%)	32 (68%)	0
7	b	16/17 (94%)	10 (62%)	0
8	c	18/19 (94%)	11 (61%)	0
9	x	27/28 (96%)	15 (55%)	0
All	All	365/373 (97%)	182 (49%)	18 (4%)

5 of 182 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	1702	G
1	1	1703	C
1	1	1707	U

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Mol	Chain	Res	Type
1	1	1708	C
1	1	1709	G

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	4387	G
2	2	4388	A
5	Y	22	G
1	1	1834	A
2	2	4374	A

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

11 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
5	2MG	Y	10	5	18,26,27	1.11	2 (11%)	19,38,41	2.86	6 (31%)
5	H2U	Y	16	5	17,21,22	0.82	0	20,30,33	2.10	4 (20%)
5	H2U	Y	17	5	17,21,22	0.78	1 (5%)	20,30,33	2.09	5 (25%)
5	M2G	Y	26	5	19,27,28	1.51	4 (21%)	20,40,43	3.23	5 (25%)
5	OMC	Y	32	5	15,22,23	0.75	0	20,31,34	1.09	2 (10%)
5	MIA	Y	37	5	22,31,32	1.04	2 (9%)	26,44,47	1.75	5 (19%)
5	7MG	Y	46	5	20,26,27	1.99	3 (15%)	24,39,42	1.94	5 (20%)
5	5MC	Y	49	5	14,22,23	1.04	1 (7%)	17,32,35	3.45	6 (35%)
5	5MU	Y	54	5	13,22,23	7.39	3 (23%)	14,32,35	4.69	5 (35%)
5	PSU	Y	55	5	16,21,22	1.71	3 (18%)	20,30,33	5.57	6 (30%)
5	1MA	Y	58	5	14,25,26	0.84	0	13,37,40	1.18	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
5	2MG	Y	10	5	-	2/5/27/28	0/3/3/3
5	H2U	Y	16	5	-	6/7/38/39	0/2/2/2
5	H2U	Y	17	5	-	6/7/38/39	0/2/2/2
5	M2G	Y	26	5	-	2/7/29/30	0/3/3/3
5	OMC	Y	32	5	-	0/5/27/28	0/2/2/2
5	MIA	Y	37	5	-	3/11/33/34	0/3/3/3
5	7MG	Y	46	5	-	2/7/37/38	0/3/3/3
5	5MC	Y	49	5	-	0/3/25/26	0/2/2/2
5	5MU	Y	54	5	-	0/3/25/26	0/2/2/2
5	PSU	Y	55	5	-	0/7/25/26	0/2/2/2
5	1MA	Y	58	5	-	2/3/25/26	0/3/3/3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	54	5MU	C5M-C5	-26.30	1.02	1.51
5	Y	46	7MG	CM7-N7	7.04	1.58	1.46
5	Y	55	PSU	C5-C1'	-4.34	1.48	1.52
5	Y	10	2MG	C6-N1	3.64	1.39	1.33
5	Y	46	7MG	C8-N9	-3.52	1.37	1.45

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	55	PSU	N1-C2-N3	-16.90	114.99	128.43
5	Y	55	PSU	C4-N3-C2	14.09	127.03	115.14
5	Y	54	5MU	C4-N3-C2	13.87	126.86	115.14
5	Y	49	5MC	CM5-C5-C4	-11.53	110.16	121.68
5	Y	10	2MG	C5-C6-N1	-8.58	111.53	123.47

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Y	17	H2U	O4'-C4'-C5'-O5'
5	Y	17	H2U	C3'-C4'-C5'-O5'
5	Y	46	7MG	O4'-C4'-C5'-O5'
5	Y	46	7MG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	Y	16	H2U	O4'-C1'-N1-C6

There are no ring outliers.

10 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	10	2MG	10	0
5	Y	16	H2U	5	0
5	Y	17	H2U	3	0
5	Y	26	M2G	26	0
5	Y	37	MIA	1	0
5	Y	46	7MG	2	0
5	Y	49	5MC	1	0
5	Y	54	5MU	1	0
5	Y	55	PSU	1	0
5	Y	58	1MA	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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 ⓘ

There are no chain breaks in this entry.