wwPDB EM Validation Summary Report

Jan 29, 2024 – 09:22 PM EST

PDB ID	:	1FCW
Title	:	TRNA POSITIONS DURING THE ELONGATION CYCLE
Authors	:	Agrawal, R.K.; Spahn, C.M.T.; Penczek, P.; Grassucci, R.A.; Nierhaus, K.H.; Frank, J.
Deposited on	:	2000-07-19
Resolution	:	17.00 Å(reported)

This is a wwPDB EM 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

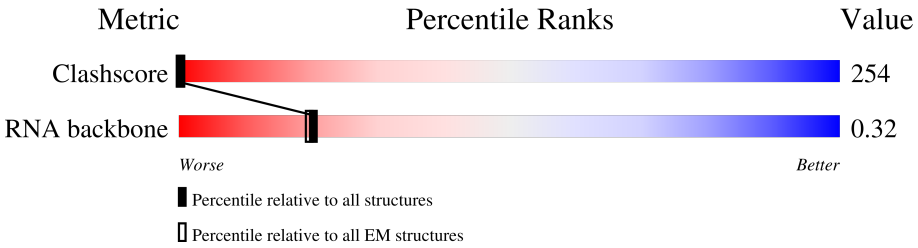
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 17.00 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	158937	4297
RNA backbone	4643	859

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 of 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	76	7% 62% 32%
1	B	76	• • 62% 33%
1	C	76	• 32% 37% 30%
1	D	76	• 13% 55% 30%
1	E	76	14% 57% 29%

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
1	H2U	A	16	-	-	X	-
1	H2U	A	17	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	M2G	A	26	-	-	X	-
1	OMC	A	32	-	-	X	-
1	OMG	A	34	-	-	X	-
1	YG	A	37	X	-	X	-
1	PSU	A	39	-	-	X	-
1	5MC	A	40	-	-	X	-
1	7MG	A	46	-	-	X	-
1	5MC	A	49	-	-	X	-
1	5MU	A	54	-	-	X	-
1	PSU	A	55	-	-	X	-
1	1MA	A	58	-	-	X	-
1	2MG	B	10	-	-	X	-
1	H2U	B	16	-	-	X	-
1	H2U	B	17	-	-	X	-
1	M2G	B	26	-	-	X	-
1	OMC	B	32	-	-	X	-
1	OMG	B	34	-	-	X	-
1	YG	B	37	X	-	X	-
1	PSU	B	39	-	-	X	-
1	5MC	B	40	-	-	X	-
1	7MG	B	46	-	-	X	-
1	5MC	B	49	-	-	X	-
1	5MU	B	54	-	-	X	-
1	PSU	B	55	-	-	X	-
1	1MA	B	58	-	-	X	-
1	YG	C	37	X	-	-	-
1	2MG	D	10	-	-	X	-
1	H2U	D	17	-	-	X	-
1	M2G	D	26	-	-	X	-
1	YG	D	37	X	-	-	-
1	7MG	D	46	-	-	X	-
1	5MC	D	49	-	-	X	-
1	5MU	D	54	-	-	X	-
1	PSU	D	55	-	-	X	-
1	1MA	D	58	-	-	X	-
1	H2U	E	17	-	-	X	-
1	YG	E	37	X	-	-	-
1	5MC	E	49	-	-	X	-
1	5MU	E	54	-	-	X	-
1	1MA	E	58	-	-	X	-

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8260 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 TRNAPHE.

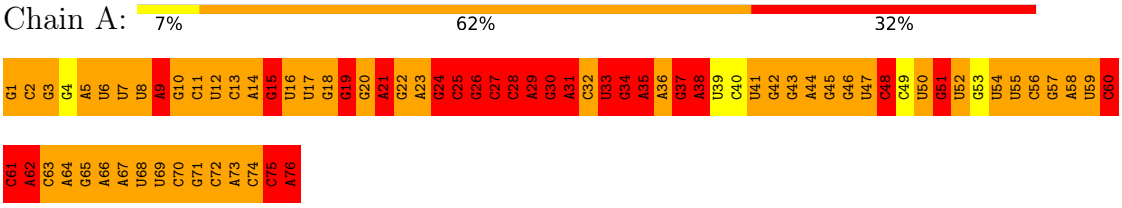
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	76	Total	C	N	O	P	0	0
			1652	746	294	536	76		
1	B	76	Total	C	N	O	P	0	0
			1652	746	294	536	76		
1	C	76	Total	C	N	O	P	0	0
			1652	746	294	536	76		
1	D	76	Total	C	N	O	P	0	0
			1652	746	294	536	76		
1	E	76	Total	C	N	O	P	0	0
			1652	746	294	536	76		

3 Residue-property plots

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

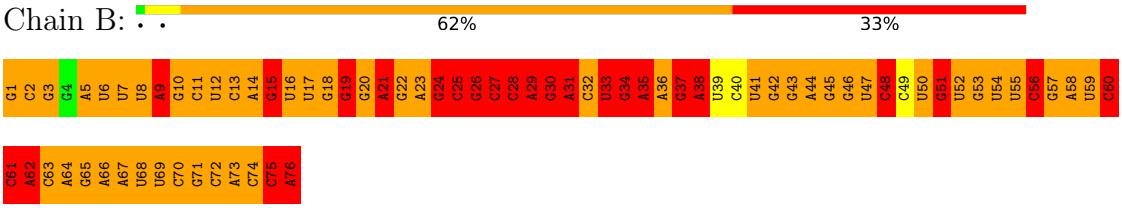
- Molecule 1: TRNAPHE

Chain A:



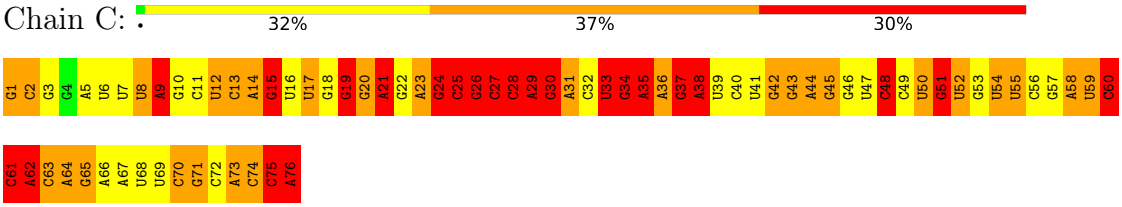
- Molecule 1: TRNAPHE

Chain B:



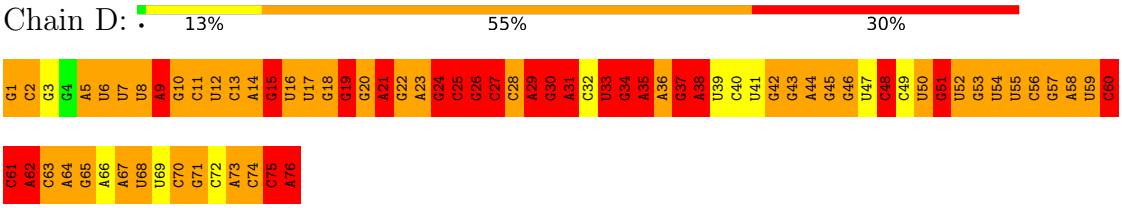
- Molecule 1: TRNAPHE

Chain C:



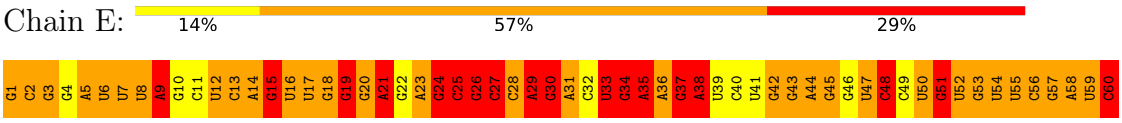
- Molecule 1: TRNAPHE

Chain D:



- Molecule 1: TRNAPHE

Chain E:




C61
A62
C63
A64
G65
A66
A67
U68
U69
C70
G71
C72
A73
C74
C75
A76

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 17.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-17.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8260	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

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: 1MA, H2U, PSU, 2MG, 5MU, OMG, OMC, YG, 7MG, 5MC, M2G

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	1.34	2/1487 (0.1%)	2.55	176/2315 (7.6%)
1	B	1.33	2/1487 (0.1%)	2.55	176/2315 (7.6%)
1	C	1.33	3/1487 (0.2%)	2.55	175/2315 (7.6%)
1	D	1.33	2/1487 (0.1%)	2.55	178/2315 (7.7%)
1	E	1.32	3/1487 (0.2%)	2.55	175/2315 (7.6%)
All	All	1.33	12/7435 (0.2%)	2.55	880/11575 (7.6%)

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	A	1	0
1	B	1	0
1	C	1	0
1	D	1	0
1	E	1	0
All	All	5	0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	U	C4-O4	5.57	1.28	1.23
1	B	59	U	C4-O4	5.56	1.28	1.23
1	D	59	U	C4-O4	5.54	1.28	1.23
1	E	19	G	C2'-C1'	-5.53	1.47	1.53
1	E	59	U	C4-O4	5.37	1.27	1.23

The worst 5 of 880 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	18	G	P-O3'-C3'	13.16	135.49	119.70
1	B	18	G	P-O3'-C3'	13.13	135.45	119.70
1	D	18	G	P-O3'-C3'	13.03	135.33	119.70
1	E	18	G	P-O3'-C3'	13.02	135.32	119.70
1	C	18	G	P-O3'-C3'	12.99	135.29	119.70

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	37	YG	C15
1	B	37	YG	C15
1	C	37	YG	C15
1	D	37	YG	C15
1	E	37	YG	C15

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	1652	0	737	2017	0
1	B	1652	0	728	2071	0
1	C	1652	0	860	140	0
1	D	1652	0	814	809	0
1	E	1652	0	810	805	0
All	All	8260	0	3949	3083	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 254.

The worst 5 of 3083 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:B:73:A:P	1:C:75:C:H3'	1.34	1.68
1:A:70:C:C4'	1:B:69:U:H3'	1.23	1.63
1:A:37:YG:C8	1:B:36:A:H2'	1.20	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:C:H2'	1:B:29:A:C5'	1.28	1.60
1:A:37:YG:C13	1:B:37:YG:H142	1.19	1.60

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein molecules in this entry.

5.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	75/76 (98%)	28 (37%)	1 (1%)
1	B	75/76 (98%)	29 (38%)	1 (1%)
1	C	75/76 (98%)	28 (37%)	1 (1%)
1	D	75/76 (98%)	28 (37%)	1 (1%)
1	E	75/76 (98%)	28 (37%)	1 (1%)
All	All	375/380 (98%)	141 (37%)	5 (1%)

5 of 141 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	A
1	A	15	G
1	A	16	H2U
1	A	17	H2U
1	A	19	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	75	C

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Mol	Chain	Res	Type
1	B	75	C
1	C	75	C
1	D	75	C
1	E	75	C

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

70 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	7MG	C	46	1	22,26,27	3.56	2 (9%)	29,39,42	1.77	3 (10%)
1	YG	E	37	1	31,42,43	2.24	7 (22%)	33,62,65	2.43	13 (39%)
1	H2U	B	17	1	18,21,22	0.65	0	21,30,33	0.80	0
1	7MG	A	46	1	22,26,27	3.54	2 (9%)	29,39,42	1.76	3 (10%)
1	M2G	C	26	1	20,27,28	1.19	3 (15%)	22,40,43	1.53	3 (13%)
1	2MG	C	10	1	18,26,27	1.35	3 (16%)	16,38,41	1.91	1 (6%)
1	2MG	E	10	1	18,26,27	1.33	3 (16%)	16,38,41	1.92	1 (6%)
1	7MG	E	46	1	22,26,27	3.50	2 (9%)	29,39,42	1.78	3 (10%)
1	5MC	A	49	1	18,22,23	0.60	0	26,32,35	0.90	0
1	PSU	A	55	1	18,21,22	0.53	0	22,30,33	0.82	0
1	OMG	C	34	1	18,26,27	1.47	4 (22%)	19,38,41	2.12	1 (5%)
1	1MA	C	58	1	16,25,26	1.62	5 (31%)	18,37,40	0.75	0
1	M2G	D	26	1	20,27,28	1.19	3 (15%)	22,40,43	1.52	3 (13%)
1	5MC	D	49	1	18,22,23	0.60	0	26,32,35	0.90	0
1	OMG	D	34	1	18,26,27	1.48	4 (22%)	19,38,41	2.12	1 (5%)
1	H2U	C	16	1	18,21,22	0.71	0	21,30,33	0.84	0
1	H2U	E	16	1	18,21,22	0.68	0	21,30,33	0.83	0
1	5MC	D	40	1	18,22,23	0.54	0	26,32,35	0.81	0
1	M2G	E	26	1	20,27,28	1.18	3 (15%)	22,40,43	1.50	3 (13%)
1	5MC	E	49	1	18,22,23	0.60	0	26,32,35	0.89	0
1	OMG	A	34	1	18,26,27	1.49	4 (22%)	19,38,41	2.12	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5MC	B	40	1	18,22,23	0.52	0	26,32,35	0.83	0
1	OMG	E	34	1	18,26,27	1.48	4 (22%)	19,38,41	2.13	1 (5%)
1	7MG	B	46	1	22,26,27	3.54	2 (9%)	29,39,42	1.76	3 (10%)
1	7MG	D	46	1	22,26,27	3.55	2 (9%)	29,39,42	1.78	3 (10%)
1	PSU	C	55	1	18,21,22	0.54	0	22,30,33	0.81	0
1	5MU	C	54	1	19,22,23	0.72	0	28,32,35	1.43	2 (7%)
1	5MU	B	54	1	19,22,23	0.70	0	28,32,35	1.43	2 (7%)
1	H2U	C	17	1	18,21,22	0.66	0	21,30,33	0.80	0
1	PSU	B	55	1	18,21,22	0.53	0	22,30,33	0.81	0
1	YG	C	37	1	31,42,43	2.24	7 (22%)	33,62,65	2.41	13 (39%)
1	H2U	D	16	1	18,21,22	0.73	0	21,30,33	0.84	0
1	PSU	D	55	1	18,21,22	0.53	0	22,30,33	0.80	0
1	OMC	B	32	1	19,22,23	0.92	1 (5%)	26,31,34	1.97	3 (11%)
1	PSU	D	39	1	18,21,22	0.54	0	22,30,33	0.70	0
1	YG	A	37	1	31,42,43	2.25	7 (22%)	33,62,65	2.44	12 (36%)
1	2MG	D	10	1	18,26,27	1.34	3 (16%)	16,38,41	1.92	1 (6%)
1	5MU	A	54	1	19,22,23	0.71	0	28,32,35	1.43	2 (7%)
1	5MC	C	49	1	18,22,23	0.58	0	26,32,35	0.90	0
1	PSU	E	55	1	18,21,22	0.56	0	22,30,33	0.80	0
1	PSU	C	39	1	18,21,22	0.57	0	22,30,33	0.72	0
1	M2G	B	26	1	20,27,28	1.18	3 (15%)	22,40,43	1.51	3 (13%)
1	5MC	B	49	1	18,22,23	0.61	0	26,32,35	0.90	0
1	OMC	A	32	1	19,22,23	0.93	1 (5%)	26,31,34	1.97	2 (7%)
1	2MG	B	10	1	18,26,27	1.36	3 (16%)	16,38,41	1.94	1 (6%)
1	H2U	E	17	1	18,21,22	0.65	0	21,30,33	0.82	0
1	2MG	A	10	1	18,26,27	1.36	3 (16%)	16,38,41	1.94	1 (6%)
1	H2U	A	16	1	18,21,22	0.73	0	21,30,33	0.81	0
1	PSU	A	39	1	18,21,22	0.57	0	22,30,33	0.73	0
1	OMG	B	34	1	18,26,27	1.48	4 (22%)	19,38,41	2.12	1 (5%)
1	M2G	A	26	1	20,27,28	1.17	3 (15%)	22,40,43	1.51	3 (13%)
1	5MC	C	40	1	18,22,23	0.55	0	26,32,35	0.82	0
1	1MA	B	58	1	16,25,26	1.61	4 (25%)	18,37,40	0.74	0
1	H2U	A	17	1	18,21,22	0.65	0	21,30,33	0.80	0
1	PSU	E	39	1	18,21,22	0.60	0	22,30,33	0.70	0
1	YG	B	37	1	31,42,43	2.24	7 (22%)	33,62,65	2.44	12 (36%)
1	5MC	E	40	1	18,22,23	0.55	0	26,32,35	0.80	0
1	YG	D	37	1	31,42,43	2.24	7 (22%)	33,62,65	2.43	13 (39%)
1	OMC	C	32	1	19,22,23	0.92	1 (5%)	26,31,34	1.96	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	H2U	B	16	1	18,21,22	0.72	0	21,30,33	0.81	0
1	H2U	D	17	1	18,21,22	0.65	0	21,30,33	0.77	0
1	5MU	D	54	1	19,22,23	0.71	0	28,32,35	1.44	2 (7%)
1	OMC	D	32	1	19,22,23	0.93	1 (5%)	26,31,34	1.97	3 (11%)
1	1MA	A	58	1	16,25,26	1.61	4 (25%)	18,37,40	0.74	0
1	5MU	E	54	1	19,22,23	0.71	0	28,32,35	1.46	3 (10%)
1	1MA	D	58	1	16,25,26	1.60	4 (25%)	18,37,40	0.75	0
1	5MC	A	40	1	18,22,23	0.51	0	26,32,35	0.83	0
1	PSU	B	39	1	18,21,22	0.57	0	22,30,33	0.71	0
1	1MA	E	58	1	16,25,26	1.64	4 (25%)	18,37,40	0.75	0
1	OMC	E	32	1	19,22,23	0.93	1 (5%)	26,31,34	1.97	3 (11%)

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	7MG	C	46	1	-	1/7/37/38	0/3/3/3
1	YG	E	37	1	1/1/8/9	12/20/42/43	0/3/4/4
1	H2U	B	17	1	-	2/7/38/39	0/2/2/2
1	7MG	A	46	1	-	1/7/37/38	0/3/3/3
1	M2G	C	26	1	-	2/7/29/30	0/3/3/3
1	2MG	C	10	1	-	2/5/27/28	0/3/3/3
1	2MG	E	10	1	-	2/5/27/28	0/3/3/3
1	7MG	E	46	1	-	1/7/37/38	0/3/3/3
1	5MC	A	49	1	-	0/7/25/26	0/2/2/2
1	PSU	A	55	1	-	2/7/25/26	0/2/2/2
1	OMG	C	34	1	-	3/5/27/28	0/3/3/3
1	1MA	C	58	1	-	0/3/25/26	0/3/3/3
1	M2G	D	26	1	-	2/7/29/30	0/3/3/3
1	5MC	D	49	1	-	0/7/25/26	0/2/2/2
1	OMG	D	34	1	-	3/5/27/28	0/3/3/3
1	H2U	C	16	1	-	6/7/38/39	0/2/2/2
1	H2U	E	16	1	-	6/7/38/39	0/2/2/2
1	5MC	D	40	1	-	0/7/25/26	0/2/2/2
1	M2G	E	26	1	-	2/7/29/30	0/3/3/3
1	5MC	E	49	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	A	34	1	-	3/5/27/28	0/3/3/3
1	5MC	B	40	1	-	0/7/25/26	0/2/2/2
1	OMG	E	34	1	-	3/5/27/28	0/3/3/3
1	7MG	B	46	1	-	1/7/37/38	0/3/3/3
1	7MG	D	46	1	-	1/7/37/38	0/3/3/3
1	PSU	C	55	1	-	2/7/25/26	0/2/2/2
1	5MU	C	54	1	-	0/7/25/26	0/2/2/2
1	5MU	B	54	1	-	0/7/25/26	0/2/2/2
1	H2U	C	17	1	-	2/7/38/39	0/2/2/2
1	YG	C	37	1	1/1/8/9	12/20/42/43	0/3/4/4
1	PSU	B	55	1	-	2/7/25/26	0/2/2/2
1	H2U	D	16	1	-	6/7/38/39	0/2/2/2
1	PSU	D	55	1	-	2/7/25/26	0/2/2/2
1	OMC	B	32	1	-	0/9/27/28	0/2/2/2
1	PSU	D	39	1	-	0/7/25/26	0/2/2/2
1	YG	A	37	1	1/1/8/9	12/20/42/43	0/3/4/4
1	2MG	D	10	1	-	2/5/27/28	0/3/3/3
1	5MU	A	54	1	-	0/7/25/26	0/2/2/2
1	5MC	C	49	1	-	0/7/25/26	0/2/2/2
1	PSU	E	55	1	-	2/7/25/26	0/2/2/2
1	PSU	C	39	1	-	0/7/25/26	0/2/2/2
1	M2G	B	26	1	-	2/7/29/30	0/3/3/3
1	5MC	B	49	1	-	0/7/25/26	0/2/2/2
1	OMC	A	32	1	-	0/9/27/28	0/2/2/2
1	2MG	B	10	1	-	2/5/27/28	0/3/3/3
1	H2U	E	17	1	-	2/7/38/39	0/2/2/2
1	2MG	A	10	1	-	2/5/27/28	0/3/3/3
1	H2U	A	16	1	-	6/7/38/39	0/2/2/2
1	PSU	A	39	1	-	0/7/25/26	0/2/2/2
1	OMG	B	34	1	-	3/5/27/28	0/3/3/3
1	M2G	A	26	1	-	2/7/29/30	0/3/3/3
1	5MC	C	40	1	-	0/7/25/26	0/2/2/2
1	1MA	B	58	1	-	0/3/25/26	0/3/3/3
1	H2U	A	17	1	-	2/7/38/39	0/2/2/2
1	PSU	E	39	1	-	0/7/25/26	0/2/2/2
1	YG	B	37	1	1/1/8/9	12/20/42/43	0/3/4/4
1	5MC	E	40	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	YG	D	37	1	1/1/8/9	12/20/42/43	0/3/4/4
1	OMC	C	32	1	-	0/9/27/28	0/2/2/2
1	H2U	B	16	1	-	6/7/38/39	0/2/2/2
1	H2U	D	17	1	-	2/7/38/39	0/2/2/2
1	5MU	D	54	1	-	0/7/25/26	0/2/2/2
1	OMC	D	32	1	-	0/9/27/28	0/2/2/2
1	1MA	A	58	1	-	0/3/25/26	0/3/3/3
1	5MU	E	54	1	-	0/7/25/26	0/2/2/2
1	1MA	D	58	1	-	0/3/25/26	0/3/3/3
1	5MC	A	40	1	-	0/7/25/26	0/2/2/2
1	PSU	B	39	1	-	0/7/25/26	0/2/2/2
1	1MA	E	58	1	-	0/3/25/26	0/3/3/3
1	OMC	E	32	1	-	0/9/27/28	0/2/2/2

The worst 5 of 121 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	7MG	C8-N9	-16.09	1.37	1.46
1	D	46	7MG	C8-N9	-16.09	1.37	1.46
1	B	46	7MG	C8-N9	-15.99	1.37	1.46
1	A	46	7MG	C8-N9	-15.97	1.37	1.46
1	E	46	7MG	C8-N9	-15.80	1.37	1.46

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	34	OMG	CM2-O2'-C2'	8.43	136.63	114.52
1	E	32	OMC	CM2-O2'-C2'	8.42	136.61	114.52
1	C	34	OMG	CM2-O2'-C2'	8.41	136.58	114.52
1	D	32	OMC	CM2-O2'-C2'	8.39	136.55	114.52
1	D	34	OMG	CM2-O2'-C2'	8.39	136.54	114.52

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	37	YG	C15
1	B	37	YG	C15
1	C	37	YG	C15
1	D	37	YG	C15
1	E	37	YG	C15

5 of 150 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	16	H2U	O4'-C1'-N1-C6
1	A	16	H2U	C2'-C1'-N1-C2
1	A	34	OMG	C1'-C2'-O2'-CM2
1	A	37	YG	C12-C13-C14-C15
1	A	37	YG	N20-C21-O23-C24

There are no ring outliers.

62 monomers are involved in 984 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	37	YG	8	0
1	B	17	H2U	30	0
1	A	46	7MG	28	0
1	C	26	M2G	4	0
1	A	49	5MC	8	0
1	A	55	PSU	18	0
1	C	34	OMG	2	0
1	C	58	1MA	3	0
1	D	26	M2G	12	0
1	D	49	5MC	18	0
1	D	34	OMG	2	0
1	E	16	H2U	6	0
1	D	40	5MC	4	0
1	E	26	M2G	4	0
1	E	49	5MC	39	0
1	A	34	OMG	35	0
1	B	40	5MC	65	0
1	E	34	OMG	2	0
1	B	46	7MG	45	0
1	D	46	7MG	22	0
1	C	55	PSU	2	0
1	C	54	5MU	2	0
1	B	54	5MU	10	0
1	C	17	H2U	2	0
1	B	55	PSU	7	0
1	C	37	YG	8	0
1	D	16	H2U	6	0
1	D	55	PSU	11	0
1	B	32	OMC	36	0
1	D	39	PSU	4	0
1	A	37	YG	119	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	10	2MG	12	0
1	A	54	5MU	8	0
1	C	49	5MC	2	0
1	E	55	PSU	5	0
1	C	39	PSU	4	0
1	B	26	M2G	14	0
1	B	49	5MC	32	0
1	A	32	OMC	35	0
1	B	10	2MG	25	0
1	E	17	H2U	55	0
1	A	10	2MG	4	0
1	A	16	H2U	25	0
1	A	39	PSU	40	0
1	B	34	OMG	50	0
1	A	26	M2G	19	0
1	C	40	5MC	4	0
1	B	58	1MA	32	0
1	A	17	H2U	34	0
1	E	39	PSU	4	0
1	B	37	YG	106	0
1	E	40	5MC	4	0
1	D	37	YG	8	0
1	B	16	H2U	16	0
1	D	17	H2U	13	0
1	D	54	5MU	15	0
1	A	58	1MA	32	0
1	E	54	5MU	23	0
1	D	58	1MA	47	0
1	A	40	5MC	83	0
1	B	39	PSU	42	0
1	E	58	1MA	28	0

5.5 Carbohydrates (i)

There are no monosaccharides 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.