



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:20 PM GMT

PDB ID : 1JGO  
Title : The Path of Messenger RNA Through the Ribosome. THIS FILE, 1JGO, CONTAINS THE 30S RIBOSOME SUBUNIT, THREE TRNA, AND MRNA MOLECULES. 50S RIBOSOME SUBUNIT IS IN THE FILE 1GIY  
Authors : Yusupova, G.Z.; Yusupov, M.M.; Cate, J.H.D.; Noller, H.F.  
Deposited on : 2001-06-26  
Resolution : 5.60 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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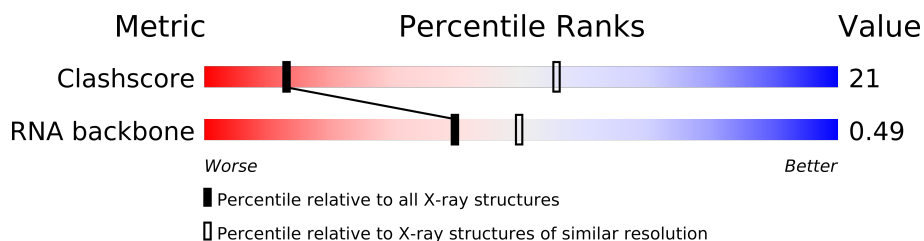
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : NOT EXECUTED  
EDS : NOT EXECUTED  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 5.60 Å.





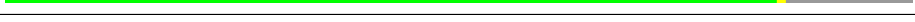


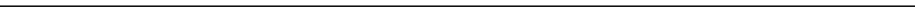








Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1018 (7.66-3.52)
RNA backbone	1838	1040 (7.50-2.80)








The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1522	
2	B	76	
2	C	76	
3	D	74	
4	1	27	
5	E	256	
6	F	239	
7	G	209	
8	H	162	
9	I	101	
10	J	156	
11	K	138	
12	L	128	
13	M	105	
14	N	129	
15	O	135	
16	P	126	
17	Q	61	

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Mol	Chain	Length	Quality of chain
18	R	89	
19	S	91	
20	T	105	
21	U	88	
22	V	93	
23	W	106	
24	X	26	

## 2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 8930 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 30S 16S ribosomal RNA.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	1519	Total	P	0	0	1519
			1519	1519			

- Molecule 2 is a RNA chain called tRNA(Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	P	0	0	0
			1652	746	294	536	76			
2	C	76	Total	C	N	O	P	0	0	0
			1652	746	294	536	76			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	2MG	G	TRNA MODIFICATION	GB 176479
B	16	H2U	U	TRNA MODIFICATION	GB 176479
B	17	H2U	U	TRNA MODIFICATION	GB 176479
B	26	M2G	G	TRNA MODIFICATION	GB 176479
B	32	OMC	C	TRNA MODIFICATION	GB 176479
B	34	OMG	G	TRNA MODIFICATION	GB 176479
B	37	YG	G	TRNA MODIFICATION	GB 176479
B	39	PSU	U	TRNA MODIFICATION	GB 176479
B	40	5MC	C	TRNA MODIFICATION	GB 176479
B	46	7MG	G	TRNA MODIFICATION	GB 176479
B	49	5MC	C	TRNA MODIFICATION	GB 176479
B	54	5MU	U	TRNA MODIFICATION	GB 176479
B	55	PSU	U	TRNA MODIFICATION	GB 176479
B	58	1MA	A	TRNA MODIFICATION	GB 176479
C	10	2MG	G	TRNA MODIFICATION	GB 176479
C	16	H2U	U	TRNA MODIFICATION	GB 176479
C	17	H2U	U	TRNA MODIFICATION	GB 176479
C	26	M2G	G	TRNA MODIFICATION	GB 176479

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Chain	Residue	Modelled	Actual	Comment	Reference
C	32	OMC	C	TRNA MODIFICATION	GB 176479
C	34	OMG	G	TRNA MODIFICATION	GB 176479
C	37	YG	G	TRNA MODIFICATION	GB 176479
C	39	PSU	U	TRNA MODIFICATION	GB 176479
C	40	5MC	C	TRNA MODIFICATION	GB 176479
C	46	7MG	G	TRNA MODIFICATION	GB 176479
C	49	5MC	C	TRNA MODIFICATION	GB 176479
C	54	5MU	U	TRNA MODIFICATION	GB 176479
C	55	PSU	U	TRNA MODIFICATION	GB 176479
C	58	1MA	A	TRNA MODIFICATION	GB 176479

- Molecule 3 is a RNA chain called tRNA(Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
3	D	74	Total	C	N	O	P	S	0	0	0
			1570	702	269	524	74	1			

- Molecule 4 is a RNA chain called MESSENGER RNA MK27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	1	27	Total	C	N	O	P	0	0	21
			141	54	12	48	27			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
5	E	234	Total	C	0	0	234
			234	234			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
6	F	206	Total	C	0	0	206
			206	206			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
7	G	208	Total	C	0	0	208
			208	208			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
8	H	150	Total 150	C 150	0	0	150

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
9	I	101	Total 101	C 101	0	0	101

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
10	J	155	Total 155	C 155	0	0	155

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
11	K	138	Total 138	C 138	0	0	138

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
12	L	127	Total 127	C 127	0	0	127

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
13	M	98	Total 98	C 98	0	0	98

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
14	N	119	Total 119	C 119	0	0	119

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
15	O	124	Total 124	C 124	0	0	124

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
16	P	125	Total 125	C 125	0	0	125

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
17	Q	60	Total 60	C 60	0	0	60

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
18	R	88	Total 88	C 88	0	0	88

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
19	S	83	Total 83	C 83	0	0	83

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
20	T	104	Total 104	C 104	0	0	104

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
21	U	73	Total 73	C 73	0	0	73

- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	V	80	Total C 80 80	0	0	80

- Molecule 23 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	W	99	Total C 99 99	0	0	99

- Molecule 24 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	X	24	Total C 24 24	0	0	24



### 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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

Note EDS was not executed.

- Molecule 1: 30S 16S ribosomal RNA

Chain A: 



- Molecule 2: tRNA(Phe)

Chain B: 



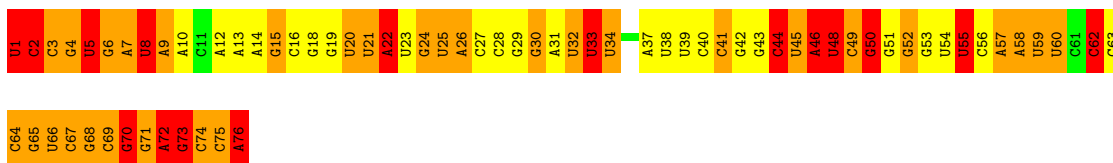
- Molecule 2: tRNA(Phe)

Chain C: 



- Molecule 3: tRNA(Phe)

Chain D: 



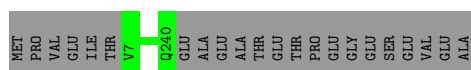
- Molecule 4: MESSENGER RNA MK27

Chain 1: 



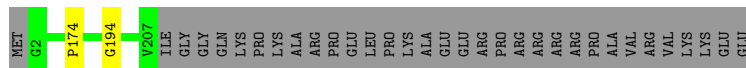
- Molecule 5: 30S RIBOSOMAL PROTEIN S2

Chain E: 



- Molecule 6: 30S RIBOSOMAL PROTEIN S3

Chain F:



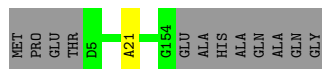
- Molecule 7: 30S RIBOSOMAL PROTEIN S4

Chain G:



- Molecule 8: 30S RIBOSOMAL PROTEIN S5

Chain H:



- Molecule 9: 30S RIBOSOMAL PROTEIN S6

Chain I:

There are no outlier residues recorded for this chain.

- Molecule 10: 30S RIBOSOMAL PROTEIN S7

Chain J:



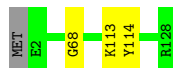
- Molecule 11: 30S RIBOSOMAL PROTEIN S8

Chain K:

There are no outlier residues recorded for this chain.

- Molecule 12: 30S RIBOSOMAL PROTEIN S9

Chain L:



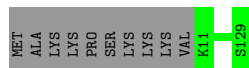
- Molecule 13: 30S RIBOSOMAL PROTEIN S10

Chain M:



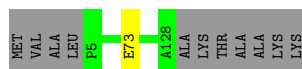
- Molecule 14: 30S RIBOSOMAL PROTEIN S11

Chain N: 



- Molecule 15: 30S RIBOSOMAL PROTEIN S12

Chain O: 



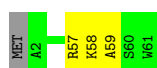
- Molecule 16: 30S RIBOSOMAL PROTEIN S13

Chain P: 



- Molecule 17: 30S RIBOSOMAL PROTEIN S14

Chain Q: 



- Molecule 18: 30S RIBOSOMAL PROTEIN S15

Chain R: 



- Molecule 19: 30S RIBOSOMAL PROTEIN S16

Chain S: 



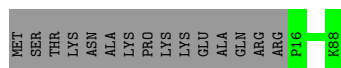
- Molecule 20: 30S RIBOSOMAL PROTEIN S17

Chain T: 



- Molecule 21: 30S RIBOSOMAL PROTEIN S18

Chain U: 



- Molecule 22: 30S RIBOSOMAL PROTEIN S19

Chain V: 

MET	P2	R81	GLY	HIS	GLY	LYS	GLU	ALA	LYS	ALA	THR	LYS	LYS
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- Molecule 23: 30S RIBOSOMAL PROTEIN S20

Chain W: 

MET	ALA	GLN	LYS	LYS	PRO	LYS	R8	A106
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- Molecule 24: 30S RIBOSOMAL PROTEIN THX

Chain X: 

G2	K25	LYS	LYS
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## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	507.20Å 507.20Å 803.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	250.00 – 5.60	Depositor
% Data completeness (in resolution range)	97.7 (250.00-5.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
Refinement program	O	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8930	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	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: OMC, 5MU, M2G, OMG, H2U, YG, 2MG, 5MC, 1MA, 4SU, 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  > 5$	RMSZ	# $ Z  > 5$
2	B	1.21	4/1486 (0.3%)	1.43	13/2311 (0.6%)
2	C	1.44	7/1487 (0.5%)	1.47	22/2315 (1.0%)
3	D	1.95	17/1616 (1.1%)	2.85	154/2512 (6.1%)
4	1	2.35	5/131 (3.8%)	2.46	3/200 (1.5%)
All	All	1.60	33/4720 (0.7%)	2.07	192/7338 (2.6%)

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
2	B	0	3
2	C	0	3
All	All	0	6

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	33	U	O3'-P	31.20	1.98	1.61
2	C	74	C	O3'-P	-27.00	1.28	1.61
2	B	75	C	O3'-P	-26.77	1.29	1.61
2	C	75	C	O3'-P	-25.61	1.30	1.61
3	D	15	G	O3'-P	24.09	1.90	1.61

The worst 5 of 192 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	35	A	P-O3'-C3'	41.11	169.03	119.70
3	D	25	U	P-O3'-C3'	31.41	157.40	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	75	C	P-O3'-C3'	-29.51	84.29	119.70
4	1	18	U	P-O3'-C3'	27.61	152.83	119.70
3	D	8	4SU	O3'-P-O5'	-27.11	52.48	104.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

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

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1519	0	0	15	0
2	B	1652	0	862	56	0
2	C	1652	0	862	53	0
3	D	1570	0	801	105	0
4	1	141	0	61	6	0
5	E	234	0	0	0	0
6	F	206	0	0	2	0
7	G	208	0	0	2	0
8	H	150	0	0	1	0
9	I	101	0	0	0	0
10	J	155	0	0	4	0
11	K	138	0	0	0	0
12	L	127	0	0	3	0
13	M	98	0	0	5	0
14	N	119	0	0	0	0
15	O	124	0	0	1	0
16	P	125	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	60	0	0	4	0
18	R	88	0	0	0	0
19	S	83	0	0	0	0
20	T	104	0	0	0	0
21	U	73	0	0	0	0
22	V	80	0	0	0	0
23	W	99	0	0	0	0
24	X	24	0	0	0	0
All	All	8930	0	2586	237	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

The worst 5 of 237 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:1:G:N2	2:C:2:C:H41	1.22	1.34
1:A:430:A:P	7:G:7:PRO:CA	2.16	1.32
3:D:75:C:C2'	3:D:76:A:H5'	1.59	1.30
2:C:1:G:N2	2:C:2:C:N4	1.77	1.29
3:D:75:C:H2'	3:D:76:A:C5'	1.62	1.27

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

### 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	A	0/1522	-	-
2	B	74/76 (97%)	13 (17%)	3 (4%)
2	C	75/76 (98%)	13 (17%)	3 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	D	73/74 (98%)	26 (35%)	2 (2%)
4	1	5/27 (18%)	1 (20%)	0
All	All	227/1775 (12%)	53 (23%)	8 (3%)

5 of 53 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	C
2	B	3	G
2	B	17	H2U
2	B	18	G
2	B	19	G

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	16	H2U
3	D	33	U
2	C	35	A
2	B	35	A
2	C	18	G

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

34 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	$\# Z  > 2$
2	2MG	B	10	2	24,26,27	0.78	1 (4%)	32,38,41	5.50	3 (9%)
2	H2U	B	16	2	19,21,22	0.90	2 (10%)	27,30,33	1.08	3 (11%)
2	H2U	B	17	2	19,21,22	0.84	1 (5%)	27,30,33	1.01	2 (7%)
2	M2G	B	26	2	25,27,28	0.83	1 (4%)	34,40,43	5.44	3 (8%)
2	OMC	B	32	2	20,22,23	0.82	1 (5%)	25,31,34	0.89	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OMG	B	34	2,4	24,26,27	0.98	2 (8%)	32,38,41	5.23	3 (9%)
2	YG	B	37	2	40,42,43	1.08	4 (10%)	50,62,65	11.04	11 (22%)
2	PSU	B	39	2	19,21,22	0.91	1 (5%)	23,30,33	0.88	1 (4%)
2	5MC	B	40	2	20,22,23	0.88	2 (10%)	26,32,35	1.45	4 (15%)
2	7MG	B	46	2	24,26,27	1.12	4 (16%)	34,39,42	1.52	5 (14%)
2	5MC	B	49	2	20,22,23	1.34	2 (10%)	26,32,35	1.49	4 (15%)
2	5MU	B	54	2	20,22,23	0.93	1 (5%)	25,32,35	1.42	3 (12%)
2	PSU	B	55	2	19,21,22	1.16	3 (15%)	23,30,33	1.06	2 (8%)
2	1MA	B	58	2	23,25,26	2.04	4 (17%)	32,37,40	2.07	6 (18%)
2	2MG	C	10	2	24,26,27	0.79	1 (4%)	32,38,41	5.58	3 (9%)
2	H2U	C	16	2	19,21,22	0.89	2 (10%)	27,30,33	1.08	3 (11%)
2	H2U	C	17	2	19,21,22	0.85	1 (5%)	27,30,33	1.02	2 (7%)
2	M2G	C	26	2	25,27,28	0.83	1 (4%)	34,40,43	5.44	3 (8%)
2	OMC	C	32	2	20,22,23	0.81	1 (5%)	25,31,34	0.89	1 (4%)
2	OMG	C	34	2,4	24,26,27	0.97	1 (4%)	32,38,41	5.19	3 (9%)
2	YG	C	37	2	40,42,43	1.09	4 (10%)	50,62,65	11.19	11 (22%)
2	PSU	C	39	2	19,21,22	0.90	1 (5%)	23,30,33	0.88	1 (4%)
2	5MC	C	40	2	20,22,23	0.87	2 (10%)	26,32,35	1.44	4 (15%)
2	7MG	C	46	2	24,26,27	1.11	3 (12%)	34,39,42	1.51	5 (14%)
2	5MC	C	49	2	20,22,23	1.35	2 (10%)	26,32,35	1.51	4 (15%)
2	5MU	C	54	2	20,22,23	0.91	1 (5%)	25,32,35	1.39	3 (12%)
2	PSU	C	55	2	19,21,22	1.14	3 (15%)	23,30,33	1.06	2 (8%)
2	1MA	C	58	2	23,25,26	2.04	4 (17%)	32,37,40	2.06	5 (15%)
3	H2U	D	20	3	19,21,22	0.58	1 (5%)	27,30,33	0.71	1 (3%)
3	H2U	D	21	3	19,21,22	0.69	0	27,30,33	0.64	0
3	5MC	D	49	3	20,22,23	0.94	2 (10%)	26,32,35	2.05	3 (11%)
3	5MU	D	54	3	20,22,23	1.10	2 (10%)	25,32,35	1.80	2 (8%)
3	PSU	D	55	3	19,21,22	1.49	2 (10%)	23,30,33	1.16	3 (13%)
3	4SU	D	8	3	19,21,22	1.04	1 (5%)	23,30,33	26.94	1 (4%)

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
2	2MG	B	10	2	-	0/10/27/28	0/1/3/3
2	H2U	B	16	2	-	0/8/38/39	0/2/2/2
2	H2U	B	17	2	-	0/8/38/39	0/2/2/2
2	M2G	B	26	2	-	0/12/29/30	0/1/3/3
2	OMC	B	32	2	-	0/8/27/28	0/2/2/2
2	OMG	B	34	2,4	-	1/10/27/28	0/1/3/3
2	YG	B	37	2	-	0/25/42/43	0/1/4/4
2	PSU	B	39	2	-	0/8/25/26	0/2/2/2
2	5MC	B	40	2	-	0/6/25/26	0/2/2/2
2	7MG	B	46	2	-	0/8/37/38	0/1/3/3
2	5MC	B	49	2	-	0/6/25/26	0/2/2/2
2	5MU	B	54	2	-	0/6/25/26	0/2/2/2
2	PSU	B	55	2	-	0/8/25/26	0/2/2/2
2	1MA	B	58	2	-	0/8/25/26	0/1/3/3
2	2MG	C	10	2	-	0/10/27/28	0/1/3/3
2	H2U	C	16	2	-	0/8/38/39	0/2/2/2
2	H2U	C	17	2	-	0/8/38/39	0/2/2/2
2	M2G	C	26	2	-	0/12/29/30	0/1/3/3
2	OMC	C	32	2	-	0/8/27/28	0/2/2/2
2	OMG	C	34	2,4	-	1/10/27/28	0/1/3/3
2	YG	C	37	2	-	0/25/42/43	0/1/4/4
2	PSU	C	39	2	-	0/8/25/26	0/2/2/2
2	5MC	C	40	2	-	0/6/25/26	0/2/2/2
2	7MG	C	46	2	-	0/8/37/38	0/1/3/3
2	5MC	C	49	2	-	0/6/25/26	0/2/2/2
2	5MU	C	54	2	-	0/6/25/26	0/2/2/2
2	PSU	C	55	2	-	0/8/25/26	0/2/2/2
2	1MA	C	58	2	-	0/8/25/26	0/1/3/3
3	H2U	D	20	3	-	0/8/38/39	0/2/2/2
3	H2U	D	21	3	-	0/8/38/39	0/2/2/2
3	5MC	D	49	3	-	1/6/25/26	0/2/2/2
3	5MU	D	54	3	-	0/6/25/26	0/2/2/2
3	PSU	D	55	3	-	0/8/25/26	0/2/2/2
3	4SU	D	8	3	-	0/6/25/26	0/2/2/2

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	58	1MA	C6-N6	6.15	1.48	1.28
2	B	58	1MA	C6-N6	6.11	1.48	1.28
2	B	58	1MA	C6-N1	4.91	1.45	1.38
2	C	58	1MA	C6-N1	4.89	1.45	1.38
3	D	55	PSU	C6-N1	4.63	1.36	1.32

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	8	4SU	C4-N3-C2	129.19	127.13	121.60
2	C	37	YG	C6-C5-N7	-75.95	130.20	134.24
2	B	37	YG	C6-C5-N7	-74.86	130.25	134.24
2	C	10	2MG	C6-C5-N7	-31.05	129.96	134.14
2	C	26	M2G	C6-C5-N7	-30.66	130.01	134.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	34	OMG	OP2-P-O5'-C5'
2	B	34	OMG	OP2-P-O5'-C5'
3	D	49	5MC	OP2-P-O5'-C5'

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers

EDS was not executed - this section will therefore be empty.