W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 12, 2017 – 08:21 pm GMT

|		
PDB ID	:	4YB0
Title	:	3',3'-cGAMP riboswitch bound with c-di-GMP
Authors	:	Ren, A.M.; Patel, D.J.; Rajashankar, R.K.
Deposited on	:	2015-02-18
Resolution	:	2.12 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	Percentile Ranks	Value
Rfree		0.260
Clashscore		5
RSRZ outliers		3.6%
RNA backbone		0.54

Worse   *Better*

▌ Percentile relative to all X-ray structures
⫿ Percentile relative to X-ray structures of similar resolution
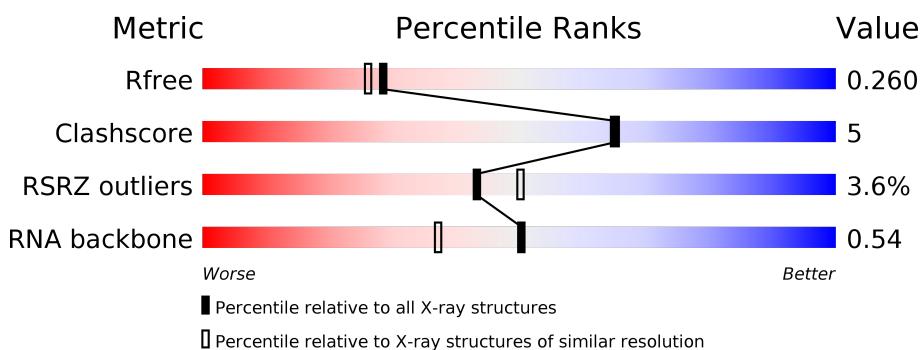
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4988 (2.14-2.10)
Clashscore	112137	5557 (2.14-2.10)
RSRZ outliers	101464	5021 (2.14-2.10)
RNA backbone	2435	1042 (2.70-1.54)

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 >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	83	4% 66% 30% •
1	R	83	4% 64% 29% 6% •
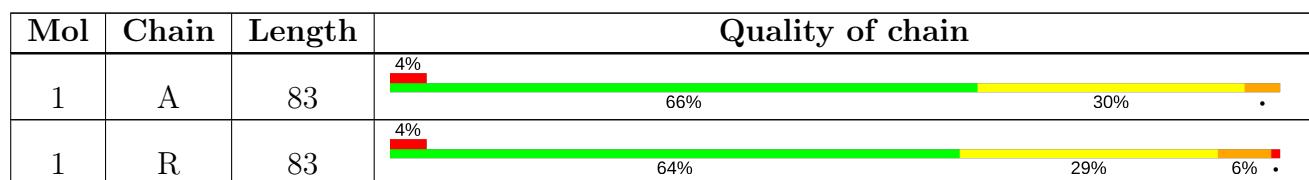
2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 3757 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RNA (84-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	83	Total	C	N	O	P	0	0	0
			1780	795	333	569	83			
1	A	83	Total	C	N	O	P	0	0	0
			1780	795	333	569	83			

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).
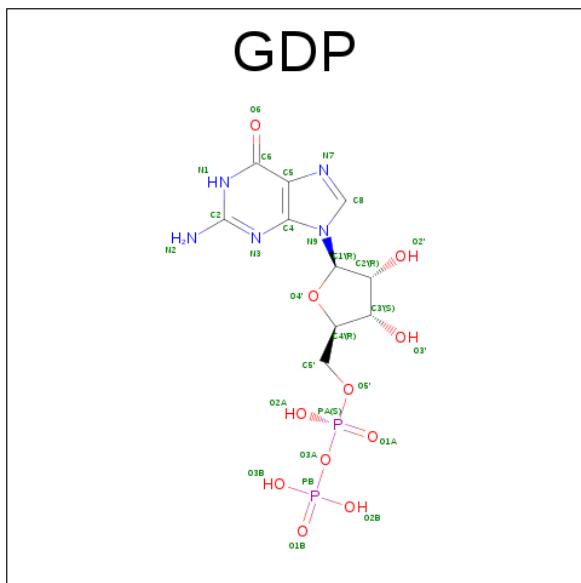
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	R	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 3 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5 ,12-dioxidooctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclodode cine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula:

$C_{20}H_{24}N_{10}O_{14}P_2$).
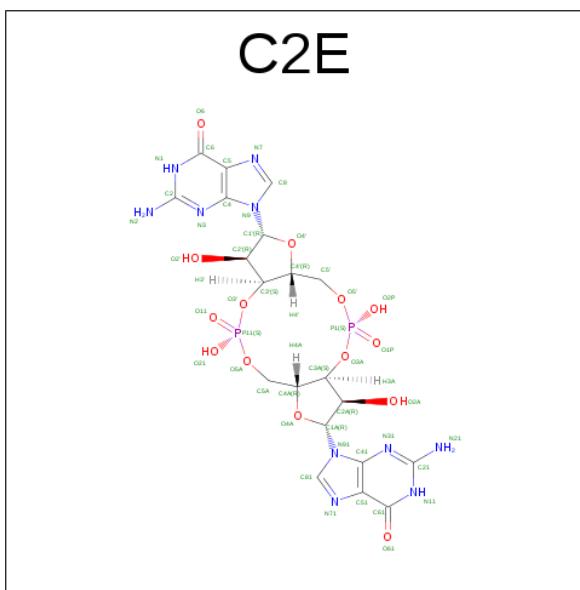
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	R	1	Total 46	C 20	N 10	O 14	P 2	0	0
3	A	1	Total 46	C 20	N 10	O 14	P 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	R	3	Total 3	Mg 3	0	0
4	A	2	Total 2	Mg 2	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	R	2	Total 2	K 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	R	27	Total 27	O 27	0	0
6	A	15	Total 15	O 15	0	0

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 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.

• Molecule 1: RNA (84-MER)
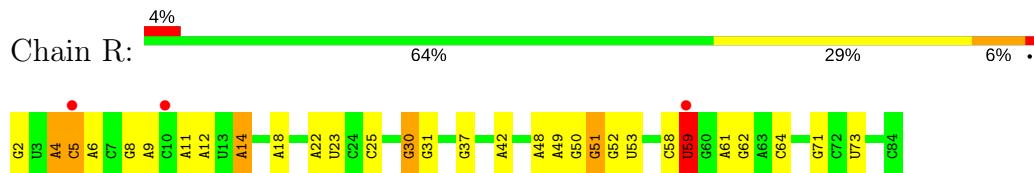
• Molecule 1: RNA (84-MER)
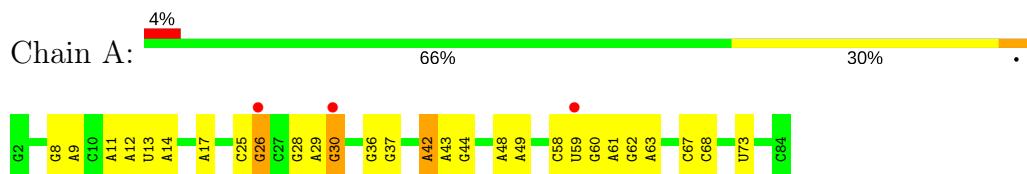
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	174.83Å 44.90Å 68.21Å 90.00° 103.33° 90.00°	Depositor
Resolution (Å)	85.10 – 2.12 85.06 – 2.12	Depositor EDS
% Data completeness (in resolution range)	97.7 (85.10-2.12) 90.7 (85.06-2.12)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.228 , 0.262 0.229 , 0.260	Depositor DCC
R_{free} test set	1466 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	50.5	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 47.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3757	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, K, MG, C2E

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	0.49	0/1993	1.04	1/3106 (0.0%)
1	R	0.69	1/1993 (0.1%)	1.26	18/3106 (0.6%)
All	All	0.60	1/3986 (0.0%)	1.16	19/6212 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	2	G	N9-C8	5.39	1.41	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	59	U	N1-C2-O2	7.82	128.27	122.80
1	R	31	G	C5-C6-O6	-7.62	124.03	128.60
1	R	59	U	N3-C2-O2	-7.37	117.04	122.20
1	R	59	U	C2-N1-C1'	7.14	126.27	117.70
1	R	51	G	C5-C6-O6	-6.60	124.64	128.60
1	R	25	C	O5'-P-OP2	-6.45	99.90	105.70
1	R	30	G	O5'-P-OP2	-6.16	100.15	105.70
1	R	42	A	O4'-C1'-N9	5.92	112.94	108.20
1	R	37	G	O4'-C1'-N9	5.78	112.82	108.20
1	R	51	G	N1-C6-O6	5.68	123.31	119.90
1	R	2	G	C4-C5-N7	5.55	113.02	110.80
1	R	31	G	N1-C6-O6	5.41	123.15	119.90
1	R	64	C	C6-N1-C2	-5.40	118.14	120.30
1	R	2	G	C8-N9-C4	-5.35	104.26	106.40
1	R	37	G	C8-N9-C4	-5.11	104.36	106.40
1	A	42	A	O4'-C1'-N9	5.09	112.27	108.20
1	R	42	A	N1-C6-N6	-5.06	115.56	118.60
1	R	2	G	C5-N7-C8	-5.05	101.78	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	71	G	C5-C6-O6	-5.03	125.58	128.60

There are no chirality outliers.

There are no planarity outliers.

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	A	1780	0	902	14	0
1	R	1780	0	902	11	0
2	A	28	0	11	0	0
2	R	28	0	11	0	0
3	A	46	0	22	1	0
3	R	46	0	22	1	0
4	A	2	0	0	0	0
4	R	3	0	0	0	0
5	R	2	0	0	0	0
6	A	15	0	0	2	0
6	R	27	0	0	2	0
All	All	3757	0	1870	25	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 5.

All (25) 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:A:26:G:N2	1:A:29:A:OP2	2.27	0.65
1:R:4:A:H2'	1:R:6:A:N7	2.17	0.59
1:R:14:A:O3'	6:R:201:HOH:O	2.17	0.58
1:R:11:A:H2'	1:R:12:A:C8	2.39	0.57
1:R:51:G:N7	6:R:211:HOH:O	2.32	0.57
1:A:30:G:H8	6:A:213:HOH:O	1.93	0.52
1:R:52:G:H2'	1:R:53:U:C6	2.46	0.51
1:A:48:A:H5"	1:A:49:A:H3'	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:C:H2'	1:A:26:G:H5"	1.93	0.51
1:A:11:A:H2'	1:A:12:A:C8	2.46	0.51
1:A:8:G:O2'	3:A:102:C2E:H81	2.12	0.50
1:R:4:A:O2'	1:R:5:C:OP1	2.22	0.49
1:A:37:G:OP2	1:A:37:G:N2	2.48	0.46
1:R:48:A:H5'	1:R:50:G:OP1	2.15	0.46
1:R:48:A:H5"	1:R:49:A:H3'	1.98	0.46
1:R:59:U:H2'	1:R:59:U:O2	2.14	0.45
1:R:22:A:H2'	1:R:23:U:C6	2.52	0.45
1:A:42:A:C4	1:A:44:G:C8	3.05	0.44
1:A:26:G:H2'	1:A:28:G:N7	2.32	0.43
1:A:67:C:O2'	1:A:68:C:H5'	2.17	0.43
1:R:8:G:O2'	3:R:102:C2E:H81	2.20	0.42
1:A:17:A:O2'	1:A:36:G:N1	2.52	0.41
1:A:63:A:H4'	6:A:209:HOH:O	2.19	0.41
1:A:13:U:H2'	1:A:14:A:O4'	2.21	0.40
1:A:42:A:O2'	1:A:43:A:H5"	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein molecules in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein molecules in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	82/83 (98%)	9 (10%)	0
1	R	82/83 (98%)	11 (13%)	0
All	All	164/166 (98%)	20 (12%)	0

All (20) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	4	A
1	R	5	C
1	R	9	A
1	R	14	A
1	R	18	A
1	R	30	G
1	R	58	C
1	R	59	U
1	R	61	A
1	R	62	G
1	R	73	U
1	A	9	A
1	A	26	G
1	A	30	G
1	A	58	C
1	A	59	U
1	A	60	G
1	A	61	A
1	A	62	G
1	A	73	U

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 for Mogul analysis.

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	GDP	A	101	1	25,30,30	1.74	6 (24%)	26,47,47	2.49	12 (46%)
3	C2E	A	102	-	44,52,52	1.25	4 (9%)	50,82,82	2.05	15 (30%)
2	GDP	R	101	1	25,30,30	1.23	3 (12%)	26,47,47	2.13	12 (46%)
3	C2E	R	102	-	44,52,52	1.29	4 (9%)	50,82,82	2.16	15 (30%)

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	GDP	A	101	1	-	0/12/32/32	0/3/3/3
3	C2E	A	102	-	-	0/22/62/62	0/6/7/7
2	GDP	R	101	1	-	0/12/32/32	0/3/3/3
3	C2E	R	102	-	-	0/22/62/62	0/6/7/7

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	101	GDP	C8-N7	2.04	1.38	1.34
2	R	101	GDP	O3'-C3'	2.18	1.48	1.43
2	R	101	GDP	O4'-C1'	2.32	1.44	1.41
2	A	101	GDP	C6-C5	2.52	1.46	1.41
2	A	101	GDP	C5-C4	2.69	1.46	1.40
2	A	101	GDP	O4'-C4'	2.81	1.51	1.45
3	A	102	C2E	C5-C4	2.91	1.47	1.40
3	R	102	C2E	C51-C41	2.98	1.47	1.40
3	R	102	C2E	C5-C4	3.01	1.47	1.40
2	A	101	GDP	C8-N7	3.31	1.40	1.34
3	A	102	C2E	C51-C41	3.38	1.48	1.40
2	A	101	GDP	O4'-C1'	3.40	1.46	1.41
2	A	101	GDP	O3'-C3'	3.77	1.51	1.43
3	A	102	C2E	C6-C5	3.83	1.48	1.41
3	R	102	C2E	C61-C51	3.86	1.48	1.41
3	A	102	C2E	C61-C51	4.00	1.49	1.41
3	R	102	C2E	C6-C5	4.72	1.50	1.41

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	101	GDP	C4'-O4'-C1'	-4.79	104.67	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	101	GDP	O3'-C3'-C2'	-4.33	97.98	111.83
3	R	102	C2E	C5-C6-N1	-4.23	117.46	123.48
3	A	102	C2E	C51-C61-N11	-4.22	117.47	123.48
2	A	101	GDP	O2'-C2'-C3'	-4.11	98.65	111.83
3	R	102	C2E	C51-C61-N11	-4.05	117.72	123.48
3	A	102	C2E	C5-C6-N1	-3.95	117.85	123.48
2	A	101	GDP	C6-C5-C4	-3.86	117.01	120.84
3	R	102	C2E	C6-C5-C4	-3.84	117.03	120.84
2	R	101	GDP	O3'-C3'-C2'	-3.64	100.16	111.83
3	R	102	C2E	C4-C5-N7	-3.59	105.94	109.41
2	R	101	GDP	O5'-C5'-C4'	-3.51	96.54	109.00
3	A	102	C2E	C4-C5-N7	-3.41	106.12	109.41
3	A	102	C2E	C61-C51-C41	-3.39	117.47	120.84
3	A	102	C2E	C6-C5-C4	-3.30	117.56	120.84
2	R	101	GDP	C6-C5-C4	-3.17	117.69	120.84
3	A	102	C2E	C41-C51-N71	-3.13	106.38	109.41
3	R	102	C2E	C61-C51-C41	-3.13	117.73	120.84
3	R	102	C2E	N31-C21-N11	-3.03	123.04	127.46
3	R	102	C2E	C41-C51-N71	-3.00	106.51	109.41
2	A	101	GDP	N3-C2-N1	-2.91	123.21	127.46
2	A	101	GDP	O4'-C4'-C3'	-2.79	99.61	105.17
3	R	102	C2E	N3-C2-N1	-2.78	123.40	127.46
3	A	102	C2E	N3-C2-N1	-2.69	123.53	127.46
3	A	102	C2E	N31-C21-N11	-2.64	123.60	127.46
2	A	101	GDP	O3A-PB-O1B	-2.61	95.38	111.44
2	A	101	GDP	C5-C6-N1	-2.43	120.02	123.48
2	R	101	GDP	O2'-C2'-C3'	-2.33	104.36	111.83
2	R	101	GDP	C5-C6-N1	-2.32	120.18	123.48
2	R	101	GDP	O4'-C4'-C3'	-2.25	100.69	105.17
2	R	101	GDP	N3-C2-N1	-2.16	124.31	127.46
2	A	101	GDP	O2A-PA-O1A	-2.07	101.56	112.28
2	A	101	GDP	C4-C5-N7	-2.04	107.44	109.41
2	R	101	GDP	O3B-PB-O1B	-2.03	102.55	110.50
2	R	101	GDP	O5'-PA-O1A	2.03	117.44	109.25
2	R	101	GDP	O2A-PA-O1A	2.08	123.06	112.28
3	A	102	C2E	C4'-O4'-C1'	2.37	112.29	109.77
3	A	102	C2E	C3A-C2A-C1A	2.42	105.39	99.95
3	R	102	C2E	C4A-O4A-C1A	2.53	112.46	109.77
3	A	102	C2E	C3'-C2'-C1'	2.54	105.65	99.95
3	R	102	C2E	C3'-C2'-C1'	2.62	105.83	99.95
3	R	102	C2E	C3A-C2A-C1A	2.62	105.83	99.95
2	R	101	GDP	C2-N3-C4	3.14	118.82	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	101	GDP	O3'-C3'-C4'	3.15	120.30	111.09
2	A	101	GDP	C6-N1-C2	3.22	120.68	116.06
3	A	102	C2E	C6-N1-C2	3.88	121.64	116.06
3	R	102	C2E	C61-N11-C21	4.25	122.18	116.06
3	R	102	C2E	C6-N1-C2	4.33	122.30	116.06
3	A	102	C2E	C61-N11-C21	4.42	122.42	116.06
3	A	102	C2E	C21-N31-C41	4.70	120.65	115.16
3	R	102	C2E	C21-N31-C41	4.93	120.91	115.16
3	A	102	C2E	C2-N3-C4	4.94	120.93	115.16
3	R	102	C2E	C2-N3-C4	5.02	121.02	115.16
2	A	101	GDP	C2-N3-C4	5.84	121.98	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	102	C2E	1	0
3	R	102	C2E	1	0

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.

6   Fit of model and data   ⓘ

6.1   Protein, DNA and RNA chains   ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	83/83 (100%)	0.67	3 (3%)	43	50	57, 79, 110, 131	0
1	R	83/83 (100%)	0.44	3 (3%)	43	50	40, 52, 87, 109	0
All	All	166/166 (100%)	0.55	6 (3%)	43	50	40, 70, 106, 131	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	10	C	3.0
1	A	30	G	2.9
1	A	59	U	2.5
1	R	59	U	2.5
1	A	26	G	2.3
1	R	5	C	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3   Carbohydrates   ⓘ

There are no carbohydrates in this entry.

6.4   Ligands   ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	C2E	A	102	46/46	0.94	0.22	0.53	53,57,67,75	0
3	C2E	R	102	46/46	0.91	0.23	0.33	40,53,70,80	0
4	MG	A	104	1/1	0.86	0.19	-0.75	59,59,59,59	0
5	K	R	106	1/1	0.92	0.14	-2.12	57,57,57,57	0
2	GDP	A	101	28/28	0.75	0.26	-	61,68,93,117	0
4	MG	R	103	1/1	0.55	0.40	-	73,73,73,73	0
4	MG	A	103	1/1	0.65	0.10	-	108,108,108,108	0
5	K	R	107	1/1	0.94	0.22	-	62,62,62,62	0
4	MG	R	104	1/1	0.91	0.25	-	81,81,81,81	0
4	MG	R	105	1/1	0.92	0.20	-	52,52,52,52	0
2	GDP	R	101	28/28	0.79	0.28	-	77,80,91,92	0

6.5 Other polymers (i)

There are no such residues in this entry.