



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:03 PM GMT

PDB ID : 3O0Q
Title : Thermotoga maritima Ribonucleotide Reductase, NrdJ, in complex with dTTP, GDP and Adenosine
Authors : Larsson, K.-M.; Logan, D.T.; Nordlund, P.
Deposited on : 2010-07-19
Resolution : 1.80 Å(reported)

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

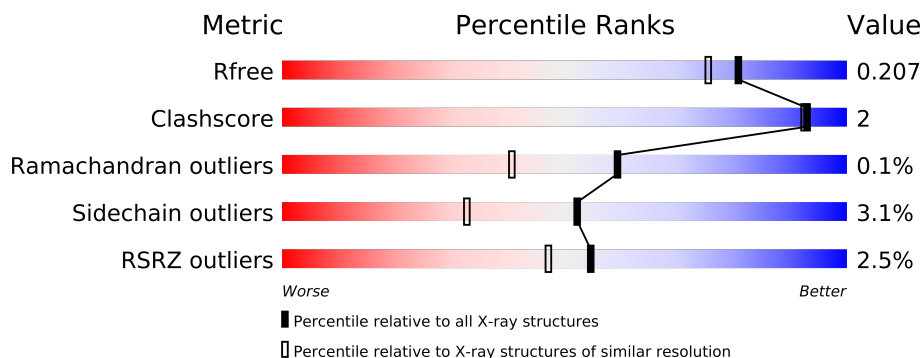
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
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 1.80 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))
R_{free}	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	644	
1	B	644	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	A	1002	-	X
3	MG	B	1002	-	X
5	ADN	A	1004	-	X
5	ADN	B	1004	-	X

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 11000 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.

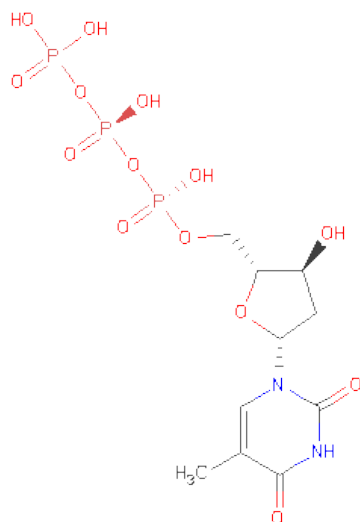
- Molecule 1 is a protein called Ribonucleoside-diphosphatereductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	617	Total	C	N	O	S	0	2	0
			4973	3186	852	915	20			
1	B	617	Total	C	N	O	S	0	1	0
			4967	3183	851	913	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	SER	TYR	SEE REMARK 999	UNP O33839
B	205	SER	TYR	SEE REMARK 999	UNP O33839

- Molecule 2 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

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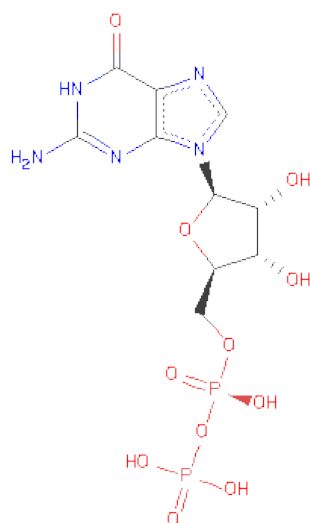
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

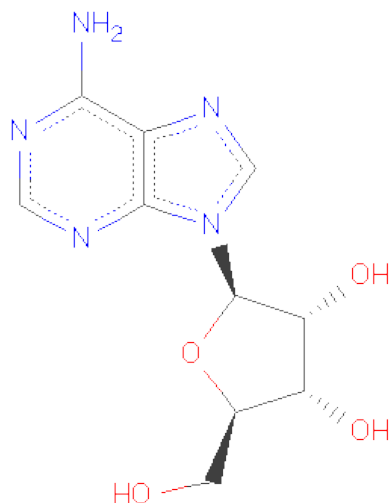
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
4	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 5 is ADENOSINE (three-letter code: ADN) (formula: C₁₀H₁₃N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			19	10	5	4		
5	B	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

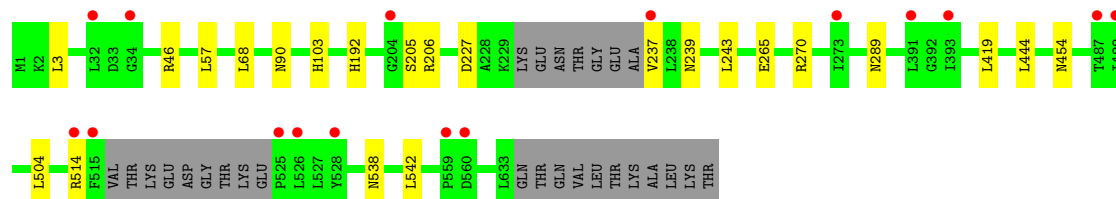
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	465	Total	O	0	0
			465	465		
7	B	440	Total	O	0	0
			440	440		

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.

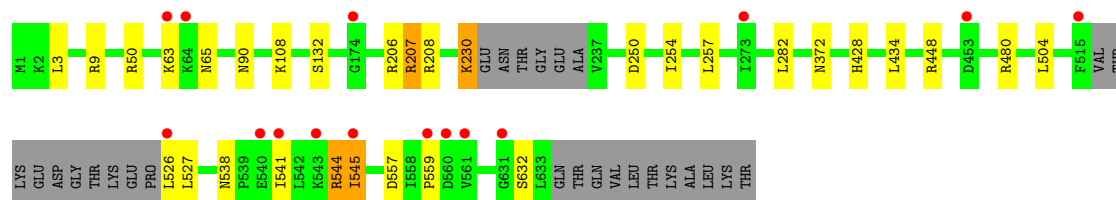
- Molecule 1: Ribonucleoside-diphosphatereductase

Chain A: 



- Molecule 1: Ribonucleoside-diphosphatereductase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.12Å 124.38Å 106.82Å 90.00° 103.43° 90.00°	Depositor
Resolution (Å)	23.12 – 1.80 37.52 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (23.12-1.80) 99.0 (37.52-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 1.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.176 , 0.210 0.173 , 0.207	Depositor DCC
R_{free} test set	6939 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 138418 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11000	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, ADN, MG, TTP, CL

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	0.34	0/5075	0.50	0/6849
1	B	0.36	0/5068	0.52	0/6838
All	All	0.35	0/10143	0.51	0/13687

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4973	0	0	6	0
1	B	4967	0	0	10	0
2	A	29	0	13	0	0
2	B	29	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	28	0	12	0	0
4	B	28	0	12	0	0
5	A	19	0	13	0	0
5	B	19	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
7	A	465	0	0	4	0
7	B	440	0	0	6	0
All	All	11000	0	76	17	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 2.

All (17) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:1004:ADN:H5'2	7:B:760:HOH:O	1.85	0.76
1:B:428:HIS:CD2	1:B:480:ARG:NH2	2.72	0.58
1:B:544:ARG:NH2	1:B:559:PRO:O	2.37	0.57
1:B:132:SER:OG	1:B:372:ASN:ND2	2.43	0.52
1:A:227:ASP:OD1	1:A:289[B]:ASN:ND2	2.46	0.49
1:B:230:LYS:NZ	7:B:893:HOH:O	2.46	0.48
1:B:207:ARG:NH2	7:B:646:HOH:O	2.46	0.47
1:A:454:ASN:N	7:A:728:HOH:O	2.48	0.46
1:B:448:ARG:NH2	7:B:748:HOH:O	2.49	0.46
1:A:103:HIS:CE1	7:A:771:HOH:O	2.68	0.45
1:B:206:ARG:NH1	7:B:738:HOH:O	2.52	0.43
1:B:526:LEU:CG	1:B:527:LEU:N	2.83	0.42
1:A:46:ARG:NE	7:A:845:HOH:O	2.51	0.42
1:B:50:ARG:NH2	1:B:108:LYS:O	2.53	0.42
1:A:192:HIS:CE1	1:A:237:VAL:CG2	3.03	0.41
1:B:9:ARG:NH1	7:B:851:HOH:O	2.53	0.41
1:A:205:SER:N	7:A:689:HOH:O	2.53	0.41

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 X-ray entries followed by that with respect to entries of similar resolution. 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
1	A	613/644 (95%)	602 (98%)	11 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	612/644 (95%)	595 (97%)	16 (3%)	1 (0%)	56 38
All	All	1225/1288 (95%)	1197 (98%)	27 (2%)	1 (0%)	59 41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	545	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. 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
1	A	545/566 (96%)	530 (97%)	15 (3%)	56 38
1	B	544/566 (96%)	525 (96%)	19 (4%)	48 28
All	All	1089/1132 (96%)	1055 (97%)	34 (3%)	52 33

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	57	LEU
1	A	68	LEU
1	A	90	ASN
1	A	206	ARG
1	A	239	ASN
1	A	243	LEU
1	A	265	GLU
1	A	270	ARG
1	A	419	LEU
1	A	444	LEU
1	A	504	LEU
1	A	514	ARG
1	A	538	ASN
1	A	542	LEU
1	B	3	LEU
1	B	63	LYS

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Mol	Chain	Res	Type
1	B	65	ASN
1	B	90	ASN
1	B	207	ARG
1	B	208	ARG
1	B	230	LYS
1	B	250	ASP
1	B	254	ILE
1	B	257	LEU
1	B	282	LEU
1	B	434	LEU
1	B	504	LEU
1	B	538	ASN
1	B	541	ILE
1	B	544	ARG
1	B	545	ILE
1	B	557	ASP
1	B	632	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	TTP	A	1001	3	30,30,30	0.94	2 (6%)	42,47,47	1.75	7 (16%)
4	GDP	A	1003	-	30,30,30	1.48	5 (16%)	44,47,47	3.29	7 (15%)
5	ADN	A	1004	-	21,21,21	2.70	5 (23%)	31,31,31	2.21	4 (12%)
2	TTP	B	1001	3	30,30,30	1.12	3 (10%)	42,47,47	1.66	7 (16%)
4	GDP	B	1003	-	30,30,30	1.40	4 (13%)	44,47,47	2.76	10 (22%)
5	ADN	B	1004	-	21,21,21	2.73	5 (23%)	31,31,31	2.19	4 (12%)

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	TTP	A	1001	3	-	0/19/34/34	0/2/2/2
4	GDP	A	1003	-	-	0/16/32/32	0/1/3/3
5	ADN	A	1004	-	-	0/6/22/22	0/1/3/3
2	TTP	B	1001	3	-	0/19/34/34	0/2/2/2
4	GDP	B	1003	-	-	0/16/32/32	0/1/3/3
5	ADN	B	1004	-	-	0/6/22/22	0/1/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1004	ADN	C4-N3	7.22	1.46	1.35
5	A	1004	ADN	C4-N3	7.14	1.46	1.35
5	B	1004	ADN	C8-N9	5.90	1.45	1.36
5	A	1004	ADN	C8-N9	5.70	1.45	1.36
5	B	1004	ADN	C2-N1	5.45	1.44	1.33
5	A	1004	ADN	C2-N1	5.38	1.44	1.33
5	B	1004	ADN	C2-N3	4.77	1.41	1.32
5	A	1004	ADN	C2-N3	4.61	1.41	1.32
4	A	1003	GDP	C6-C5	4.58	1.48	1.41
4	B	1003	GDP	C6-C5	3.86	1.47	1.41
5	A	1004	ADN	C6-N6	3.76	1.47	1.35
5	B	1004	ADN	C6-N6	3.55	1.46	1.35
4	B	1003	GDP	C4-N9	-3.18	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1003	GDP	C5-C4	3.03	1.47	1.40
4	A	1003	GDP	C2-N2	2.99	1.37	1.32
2	B	1001	TTP	C2-N1	2.96	1.41	1.38
4	B	1003	GDP	C2-N2	2.93	1.37	1.32
4	A	1003	GDP	C5-C4	2.91	1.47	1.40
2	A	1001	TTP	C2-N1	2.67	1.41	1.38
2	B	1001	TTP	C4-C5	2.67	1.48	1.42
4	A	1003	GDP	C4-N9	-2.65	1.33	1.37
2	A	1001	TTP	C4-C5	2.60	1.48	1.42
2	B	1001	TTP	PB-O3A	2.28	1.64	1.59
4	A	1003	GDP	C2-N3	2.15	1.36	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	GDP	C6-C5-N7	19.18	136.72	134.14
4	B	1003	GDP	C6-C5-N7	14.73	136.12	134.14
5	B	1004	ADN	N3-C2-N1	-10.50	119.93	128.71
5	A	1004	ADN	N3-C2-N1	-10.50	119.93	128.71
2	A	1001	TTP	N3-C2-N1	6.44	121.35	115.97
2	B	1001	TTP	N3-C2-N1	6.16	121.11	115.97
2	A	1001	TTP	C6-N1-C2	-5.61	120.81	122.41
4	B	1003	GDP	N3-C4-N9	4.92	134.12	126.91
4	A	1003	GDP	N3-C4-N9	4.87	134.06	126.91
4	A	1003	GDP	C5-C4-N3	-4.08	120.03	125.94
4	A	1003	GDP	C2-N3-C4	3.77	120.39	115.09
2	B	1001	TTP	PB-O3B-PG	-3.76	120.67	131.68
4	B	1003	GDP	C5-C4-N3	-3.65	120.65	125.94
5	B	1004	ADN	N3-C4-N9	3.59	131.91	125.43
4	B	1003	GDP	C8-N9-C4	3.53	109.60	106.90
4	B	1003	GDP	C2-N3-C4	3.42	119.89	115.09
4	A	1003	GDP	C8-N9-C4	3.31	109.43	106.90
5	A	1004	ADN	N3-C4-N9	3.22	131.25	125.43
2	A	1001	TTP	PB-O3B-PG	-3.21	122.28	131.68
2	B	1001	TTP	PB-O3A-PA	-3.20	122.30	131.68
4	A	1003	GDP	C4-C5-N7	-3.06	106.90	109.52
4	B	1003	GDP	C2'-C1'-N9	-3.03	105.50	113.27
2	B	1001	TTP	C6-N1-C2	-2.93	121.57	122.41
2	B	1001	TTP	C5-C6-N1	-2.86	118.81	121.59
4	B	1003	GDP	O3B-PB-O2B	2.68	118.06	107.61
4	B	1003	GDP	C6-N1-C2	2.64	124.12	119.51
2	B	1001	TTP	C4-N3-C2	-2.47	120.33	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1003	GDP	C4-C5-N7	-2.44	107.43	109.52
2	A	1001	TTP	C5-C6-N1	-2.44	119.21	121.59
2	A	1001	TTP	O2B-PB-O3A	2.38	116.41	105.14
5	A	1004	ADN	N7-C8-N9	-2.28	107.91	114.36
5	B	1004	ADN	C5-C4-N3	-2.27	120.75	125.70
5	A	1004	ADN	C5-C4-N3	-2.25	120.79	125.70
2	A	1001	TTP	PB-O3A-PA	-2.17	125.32	131.68
2	A	1001	TTP	C4-N3-C2	-2.11	121.06	125.39
4	B	1003	GDP	N2-C2-N1	2.08	120.15	117.86
5	B	1004	ADN	N7-C8-N9	-2.08	108.49	114.36
4	A	1003	GDP	C6-N1-C2	2.04	123.08	119.51
2	B	1001	TTP	O2B-PB-O3A	2.01	114.69	105.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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(Å ²)	Q<0.9
1	A	617/644 (95%)	-0.09	16 (2%)	53 46	16, 27, 57, 100	0
1	B	617/644 (95%)	-0.14	15 (2%)	56 49	14, 26, 63, 119	0
All	All	1234/1288 (95%)	-0.12	31 (2%)	54 47	14, 27, 60, 119	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	515	PHE	7.1
1	A	526	LEU	5.2
1	B	541	ILE	4.9
1	B	540	GLU	4.5
1	B	273	ILE	4.1
1	B	545	ILE	3.9
1	B	561	VAL	3.7
1	B	560	ASP	3.4
1	A	525	PRO	3.4
1	B	559	PRO	3.2
1	B	453	ASP	3.2
1	B	64	LYS	3.0
1	B	515	PHE	2.9
1	A	488	ILE	2.8
1	A	237	VAL	2.7
1	A	560	ASP	2.7
1	A	204	GLY	2.7
1	B	63	LYS	2.4
1	B	526	LEU	2.3
1	A	487	THR	2.3
1	A	391	LEU	2.3
1	A	514	ARG	2.3
1	A	273	ILE	2.3
1	B	174	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	32	LEU	2.2
1	A	34	GLY	2.2
1	A	393	ILE	2.1
1	B	543	LYS	2.1
1	A	559	PRO	2.1
1	A	528	TYR	2.1
1	B	631	GLY	2.1

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MG	B	1002	1/1	0.23	10.49	46,46,46,46	0
5	ADN	B	1004	19/19	0.19	4.64	22,34,60,61	19
3	MG	A	1002	1/1	0.09	2.71	27,27,27,27	0
5	ADN	A	1004	19/19	0.18	2.33	18,35,51,56	19
2	TTP	B	1001	29/29	0.09	-0.21	20,24,44,46	0
2	TTP	A	1001	29/29	0.06	-0.60	15,21,27,27	0
4	GDP	B	1003	28/28	0.07	-0.96	14,18,22,23	0
4	GDP	A	1003	28/28	0.07	-1.29	17,21,26,30	0
6	CL	A	1005	1/1	0.03	-4.73	23,23,23,23	1

6.5 Other polymers ⓘ

There are no such residues in this entry.