



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 02:08 pm GMT

PDB ID : 3UIQ  
Title : RB69 DNA Polymerase Ternary Complex containing dUpNpp  
Authors : Xia, S.; Konigsberg, W.H.; Wang, J.  
Deposited on : 2011-11-05  
Resolution : 1.88 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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
Xtriage (Phenix)	:	1.13
EDS	:	trunk31020
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk31020

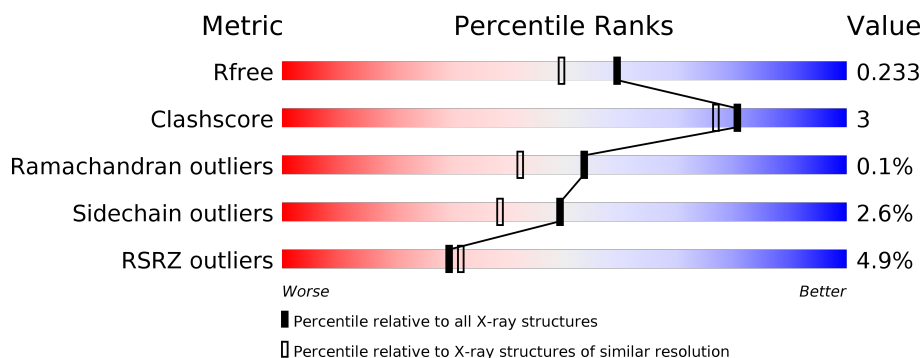
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.88 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))
$R_{free}$	111664	8255 (1.90-1.86)
Clashscore	122126	9028 (1.90-1.86)
Ramachandran outliers	120053	8930 (1.90-1.86)
Sidechain outliers	120020	8930 (1.90-1.86)
RSRZ outliers	108989	8087 (1.90-1.86)

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. 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  $\leq 5\%$ . 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	903	<div> <div>5%</div> <div>91%</div> <div>8%</div> </div>
2	T	18	<div> <div>11%</div> <div>61%</div> <div>39%</div> </div>
3	P	13	<div> <div>46%</div> <div>46%</div> <div>8%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8610 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 protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	901	Total	C	N	O	S	0	5	0
			7390	4746	1235	1376	33			

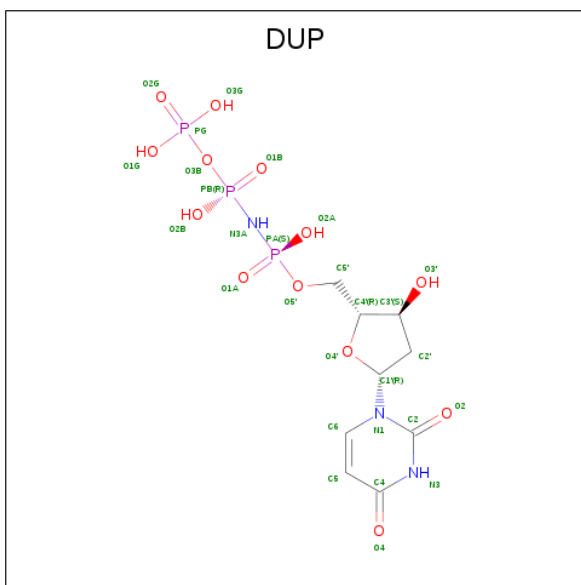
- Molecule 2 is a DNA chain called 5'-D(\*TP\*CP\*GP\*AP\*GP\*TP\*AP\*AP\*GP\*CP\*AP\*GP\*TP\*CP\*CP\*GP\*CP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	18	Total	C	N	O	P	0	0	0
			368	175	71	105	17			

- Molecule 3 is a DNA chain called 5'-D(\*GP\*CP\*GP\*GP\*AP\*CP\*TP\*GP\*CP\*TP\*TP\*AP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	P	0	0	0
			263	126	48	77	12			

- Molecule 4 is 2'-DEOXYURIDINE 5'-ALPHA,BETA-IMIDO-TRIPHOSPHATE (three-letter code: DUP) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	6	Total Ca 6 6	0	0

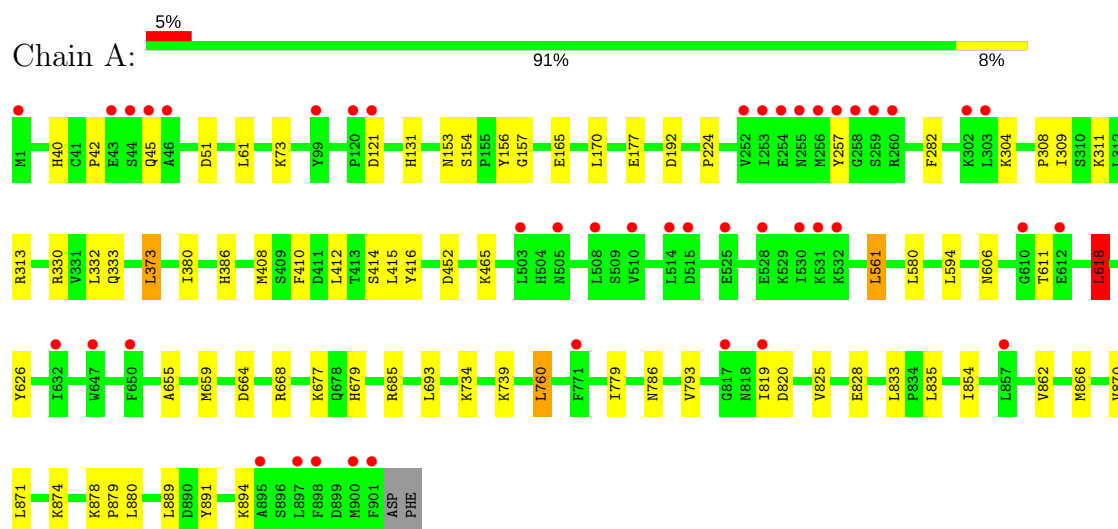
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	503	Total O 506 506	0	3
6	T	34	Total O 34 34	0	0
6	P	15	Total O 15 15	0	0

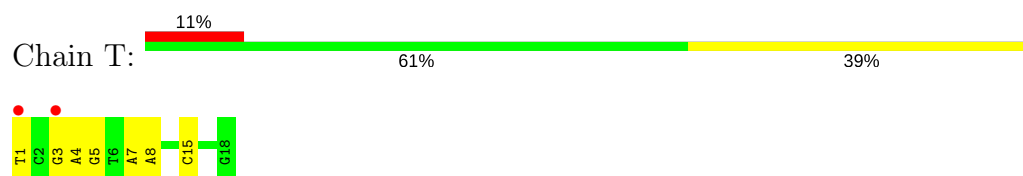
### 3 Residue-property plots [i](#)

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.

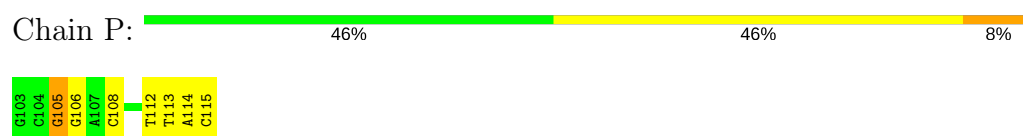
#### • Molecule 1: DNA polymerase



#### • Molecule 2: 5'-D(\*TP\*CP\*GP\*AP\*GP\*TP\*AP\*AP\*GP\*CP\*AP\*GP\*TP\*CP\*CP\*GP\*CP\*G)-3'



#### • Molecule 3: 5'-D(\*GP\*CP\*GP\*GP\*AP\*CP\*TP\*GP\*CP\*TP\*TP\*AP\*C)-3'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.24Å 120.20Å 130.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.23 – 1.88 49.23 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.23-1.88) 99.0 (49.23-1.88)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.189 , 0.220 0.199 , 0.233	Depositor DCC
$R_{free}$ test set	4804 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8610	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: DUP, CA

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	0.43	0/7585	0.54	1/10247 (0.0%)
2	T	0.78	0/413	1.40	6/636 (0.9%)
3	P	0.75	0/294	1.47	5/452 (1.1%)
All	All	0.47	0/8292	0.68	12/11335 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	8	DA	O4'-C1'-N9	9.02	114.31	108.00
2	T	7	DA	O4'-C1'-N9	-7.29	102.90	108.00
3	P	115	DC	O4'-C1'-N1	6.87	112.81	108.00
3	P	105	DG	P-O3'-C3'	6.59	127.61	119.70
2	T	15	DC	O4'-C1'-N1	6.56	112.59	108.00
3	P	115	DC	C1'-O4'-C4'	-6.37	103.73	110.10
1	A	618	LEU	CA-CB-CG	6.13	129.39	115.30
2	T	3	DG	P-O3'-C3'	5.48	126.28	119.70
3	P	112	DT	O4'-C1'-N1	5.46	111.82	108.00
3	P	108	DC	O4'-C1'-N1	5.29	111.71	108.00
2	T	5	DG	O4'-C4'-C3'	-5.18	102.43	104.50
2	T	4	DA	C4'-C3'-C2'	-5.09	98.52	103.10

There are no chirality outliers.

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	7390	0	7301	39	0
2	T	368	0	203	2	0
3	P	263	0	148	6	0
4	A	28	0	12	2	0
5	A	6	0	0	0	0
6	A	506	0	0	3	0
6	P	15	0	0	0	0
6	T	34	0	0	0	0
All	All	8610	0	7664	45	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 3.

All (45) 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:786:ASN:HD21	2:T:1:DT:H3	1.15	0.90
1:A:330[B]:ARG:HH11	1:A:333:GLN:HE22	1.26	0.82
1:A:825:VAL:HB	1:A:828:GLU:HG3	1.66	0.78
1:A:685:ARG:HD3	6:A:1058:HOH:O	1.85	0.74
3:P:105:DG:H2'	3:P:106:DG:C8	2.26	0.70
1:A:786:ASN:ND2	2:T:1:DT:H3	1.90	0.65
3:P:105:DG:H2''	3:P:106:DG:O5'	1.98	0.64
1:A:42:PRO:O	1:A:45:GLN:HG2	2.01	0.61
1:A:170:LEU:HA	1:A:177:GLU:HG3	1.84	0.59
1:A:878:LYS:HB2	1:A:879:PRO:HD3	1.84	0.58
1:A:131:HIS:HD2	1:A:156:TYR:OH	1.88	0.56
1:A:308:PRO:HG2	1:A:311:LYS:HG3	1.87	0.56
1:A:282:PHE:HZ	1:A:561:LEU:HG	1.70	0.55
3:P:105:DG:C2'	3:P:106:DG:C8	2.90	0.54
1:A:870:VAL:HG13	1:A:874:LYS:HD3	1.90	0.53
1:A:121:ASP:HA	1:A:819:ILE:HD12	1.91	0.52
1:A:410:PHE:HZ	1:A:659:MET:HE3	1.74	0.51
1:A:154:SER:HB3	1:A:313:ARG:NH2	2.26	0.50
1:A:664:ASP:O	1:A:668[A]:ARG:HG3	2.13	0.49
4:A:904:DUP:N3A	4:A:904:DUP:O1G	2.44	0.48
1:A:779:ILE:HB	1:A:871:LEU:HD21	1.94	0.48
1:A:734:LYS:HG2	3:P:113:DT:H5'	1.96	0.47
1:A:408:MET:HE1	1:A:655:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:105:DG:H2'	3:P:106:DG:H8	1.76	0.46
1:A:408:MET:CE	1:A:655:ALA:HB2	2.46	0.45
1:A:373:LEU:HD23	1:A:380:ILE:HG22	1.98	0.45
1:A:793:VAL:HG23	1:A:793:VAL:O	2.17	0.45
1:A:330[B]:ARG:NH1	1:A:333:GLN:HE22	2.04	0.45
1:A:386:HIS:HE1	6:A:948:HOH:O	2.00	0.44
3:P:113:DT:H2''	3:P:114:DA:H5'	1.98	0.44
1:A:157:GLY:O	1:A:313:ARG:NH2	2.44	0.44
1:A:760:LEU:HD13	1:A:891:TYR:HA	2.00	0.43
1:A:416:TYR:CD2	4:A:904:DUP:H2'2	2.54	0.43
1:A:330[B]:ARG:HH11	1:A:333:GLN:NE2	2.05	0.43
1:A:412:LEU:HD13	1:A:415:LEU:HD13	2.02	0.42
1:A:606:ASN:OD1	1:A:611:THR:HG23	2.20	0.42
1:A:862:VAL:O	1:A:866:MET:HG3	2.20	0.42
1:A:618:LEU:HD13	1:A:626:TYR:O	2.20	0.41
1:A:854:ILE:HD13	1:A:862:VAL:HG21	2.02	0.41
1:A:679:HIS:HD2	6:A:922:HOH:O	2.03	0.41
1:A:833:LEU:HD13	1:A:866:MET:HG2	2.03	0.41
1:A:165:GLU:CD	1:A:165:GLU:H	2.23	0.41
1:A:40:HIS:HE1	1:A:51:ASP:OD2	2.04	0.40
1:A:153:ASN:HB2	1:A:192:ASP:O	2.21	0.40
1:A:465:LYS:HE3	1:A:677:LYS:HA	2.04	0.40

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 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	904/903 (100%)	884 (98%)	19 (2%)	1 (0%)	53 42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	414	SER

### 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 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	803/802 (100%)	782 (97%)	21 (3%)	49 38

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	73	LYS
1	A	224	PRO
1	A	257	TYR
1	A	304	LYS
1	A	309	ILE
1	A	332	LEU
1	A	373	LEU
1	A	452	ASP
1	A	561	LEU
1	A	580	LEU
1	A	594	LEU
1	A	618	LEU
1	A	693	LEU
1	A	739	LYS
1	A	760	LEU
1	A	820	ASP
1	A	835	LEU
1	A	880	LEU
1	A	889	LEU
1	A	894	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	98	ASN
1	A	112	ASN
1	A	131	HIS
1	A	203	ASN
1	A	333	GLN
1	A	339	GLN
1	A	354	GLN
1	A	386	HIS
1	A	539	ASN
1	A	546	GLN
1	A	564	ASN
1	A	679	HIS
1	A	761	GLN
1	A	773	GLN
1	A	786	ASN
1	A	823	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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
4	DUP	A	904	5	29,29,29	3.71	13 (44%)	37,45,45	3.05	14 (37%)

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
4	DUP	A	904	5	-	0/18/34/34	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	904	DUP	C6-N1	-13.11	1.30	1.47
4	A	904	DUP	C6-C5	-7.63	1.38	1.52
4	A	904	DUP	PA-O2A	-5.79	1.40	1.56
4	A	904	DUP	C5-C4	-5.53	1.37	1.50
4	A	904	DUP	C4-N3	-3.70	1.31	1.37
4	A	904	DUP	PG-O3B	-3.34	1.55	1.60
4	A	904	DUP	PB-O2B	-2.71	1.49	1.56
4	A	904	DUP	C2-N3	-2.56	1.33	1.38
4	A	904	DUP	O4'-C4'	-2.12	1.40	1.45
4	A	904	DUP	PG-O3G	-2.11	1.46	1.54
4	A	904	DUP	C2-N1	2.66	1.39	1.35
4	A	904	DUP	O2-C2	3.80	1.30	1.23
4	A	904	DUP	O4-C4	4.45	1.32	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	904	DUP	C4-N3-C2	-7.46	119.42	125.81
4	A	904	DUP	C2'-C1'-N1	-6.26	107.96	115.61
4	A	904	DUP	O1A-PA-N3A	-4.00	105.81	111.79
4	A	904	DUP	PG-O3B-PB	-3.44	120.34	132.40
4	A	904	DUP	O3B-PB-N3A	-3.38	97.22	106.59
4	A	904	DUP	O2-C2-N1	-2.66	119.84	123.12
4	A	904	DUP	O5'-PA-N3A	2.38	112.28	107.27
4	A	904	DUP	O3G-PG-O1G	2.92	119.16	107.59
4	A	904	DUP	C5-C4-N3	3.00	119.59	116.73
4	A	904	DUP	O4'-C1'-N1	4.00	113.51	108.41
4	A	904	DUP	O2A-PA-O1A	4.27	118.72	109.88
4	A	904	DUP	O2B-PB-O1B	5.14	120.50	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	904	DUP	N3-C2-N1	5.34	122.00	116.73
4	A	904	DUP	C5-C6-N1	8.03	118.99	110.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	904	DUP	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	901/903 (99%)	0.33	44 (4%) 29 31	18, 31, 59, 90	0
2	T	18/18 (100%)	0.11	2 (11%) 5 6	21, 32, 53, 62	0
3	P	13/13 (100%)	0.03	0 100 100	22, 30, 53, 53	0
All	All	932/934 (99%)	0.32	46 (4%) 29 31	18, 31, 59, 90	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	819	ILE	8.7
1	A	253	ILE	8.1
1	A	44	SER	7.7
1	A	252	VAL	6.3
1	A	257	TYR	6.1
1	A	256	MET	5.9
1	A	254	GLU	5.2
1	A	897	LEU	4.9
1	A	43	GLU	4.9
1	A	303	LEU	4.7
1	A	46	ALA	4.6
1	A	528	GLU	4.2
1	A	514	LEU	4.2
1	A	510	VAL	4.2
1	A	901	PHE	4.2
1	A	817	GLY	4.2
1	A	508	LEU	4.2
1	A	45	GLN	4.0
1	A	505	ASN	3.8
1	A	610	GLY	3.6
1	A	121	ASP	3.5
1	A	1	MET	3.5
1	A	612	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	259	SER	3.0
1	A	260	ARG	2.9
1	A	258	GLY	2.9
1	A	503	LEU	2.8
1	A	530	ILE	2.7
1	A	515	ASP	2.7
1	A	632	ILE	2.7
1	A	99	TYR	2.6
1	A	647	TRP	2.6
2	T	1	DT	2.6
1	A	898	PHE	2.6
1	A	857	LEU	2.5
1	A	255	ASN	2.5
1	A	532	LYS	2.5
1	A	900	MET	2.4
1	A	895	ALA	2.4
2	T	3	DG	2.3
1	A	302	LYS	2.3
1	A	120	PRO	2.2
1	A	531	LYS	2.2
1	A	525	GLU	2.2
1	A	650	PHE	2.1
1	A	771	PHE	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CA	A	908	1/1	0.78	0.22	90,90,90,90	0
5	CA	A	910	1/1	0.87	0.27	30,30,30,30	0
4	DUP	A	904	28/28	0.89	0.14	19,23,48,63	0
5	CA	A	907	1/1	0.90	0.10	49,49,49,49	0
5	CA	A	906	1/1	0.91	0.09	66,66,66,66	0
5	CA	A	905	1/1	0.94	0.07	51,51,51,51	0
5	CA	A	909	1/1	0.97	0.06	51,51,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.