



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 12:09 am GMT

PDB ID : 1X9N  
Title : Crystal Structure of Human DNA Ligase I bound to 5'-adenylated, nicked DNA  
Authors : Pascal, J.M.; O'Brien, P.J.; Tomkinson, A.E.; Ellenberger, T.  
Deposited on : 2004-08-23  
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

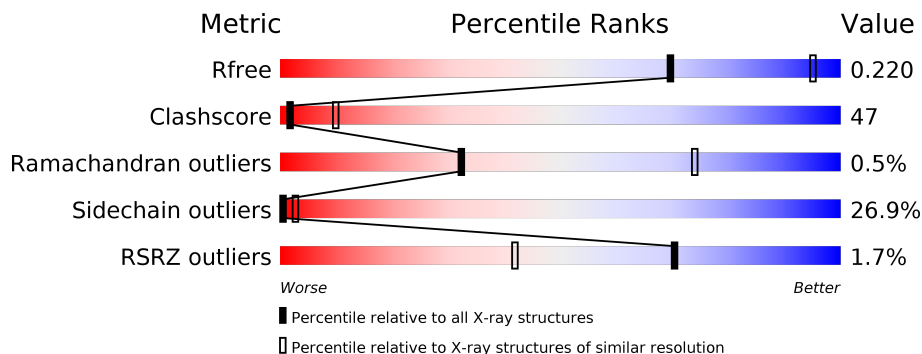
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	B	13	<div> <div>8%</div> <div>46%</div> <div>38%</div> <div>15%</div> </div>
2	C	15	<div> <div>7%</div> <div>7%</div> <div>13%</div> <div>40%</div> <div>40%</div> </div>
3	D	28	<div> <div>7%</div> <div>43%</div> <div>29%</div> <div>29%</div> </div>
4	A	688	<div> <div>%</div> <div>31%</div> <div>47%</div> <div>14%</div> <div>8%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5730 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 DNA chain called dideoxy terminated DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	11	Total	C	N	O	P	0	0	0
			222	107	40	65	10			

- Molecule 2 is a DNA chain called 5'-phosphorylated DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	P	0	0	0
			187	88	35	55	9			

- Molecule 3 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	20	Total	C	N	O	P	0	0	0
			404	192	78	115	19			

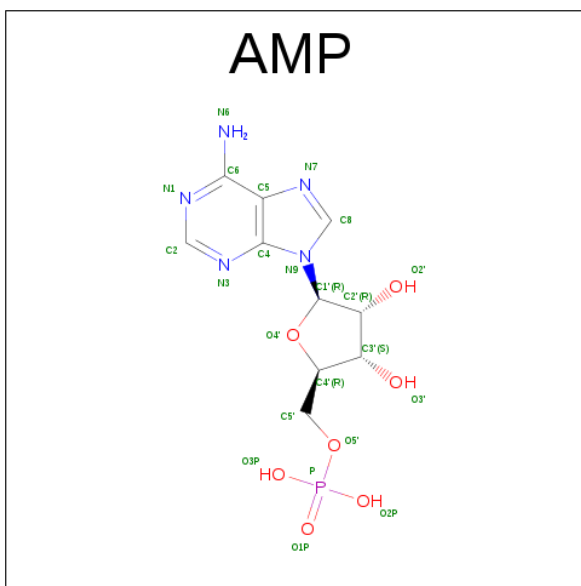
- Molecule 4 is a protein called DNA ligase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	A	632	Total	C	N	O	S	Se	0	0	0
			4894	3109	849	920	10	6			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	MET	-	INITIATING METHIONINE	UNP P18858
A	308	MSE	MET	MODIFIED RESIDUE	UNP P18858
A	393	MSE	MET	MODIFIED RESIDUE	UNP P18858
A	480	MSE	MET	MODIFIED RESIDUE	UNP P18858
A	501	MSE	MET	MODIFIED RESIDUE	UNP P18858
A	543	MSE	MET	MODIFIED RESIDUE	UNP P18858
A	723	MSE	MET	MODIFIED RESIDUE	UNP P18858

- Molecule 5 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).

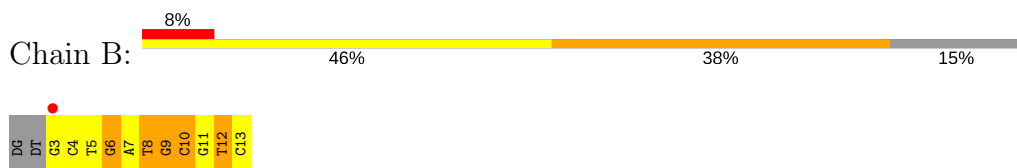


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

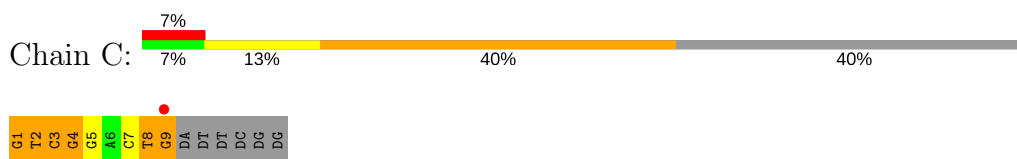
### 3 Residue-property plots

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.

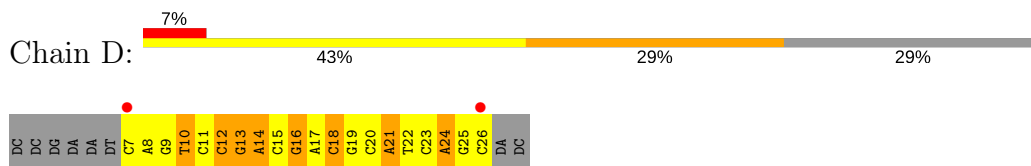
- Molecule 1: dideoxy terminated DNA



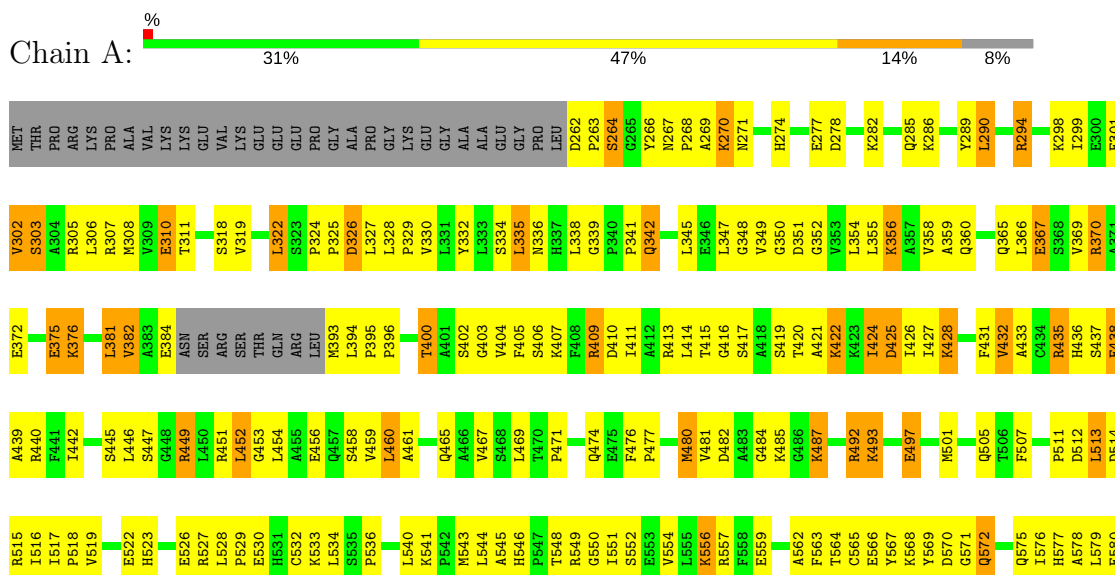
- Molecule 2: 5'-phosphorylated DNA

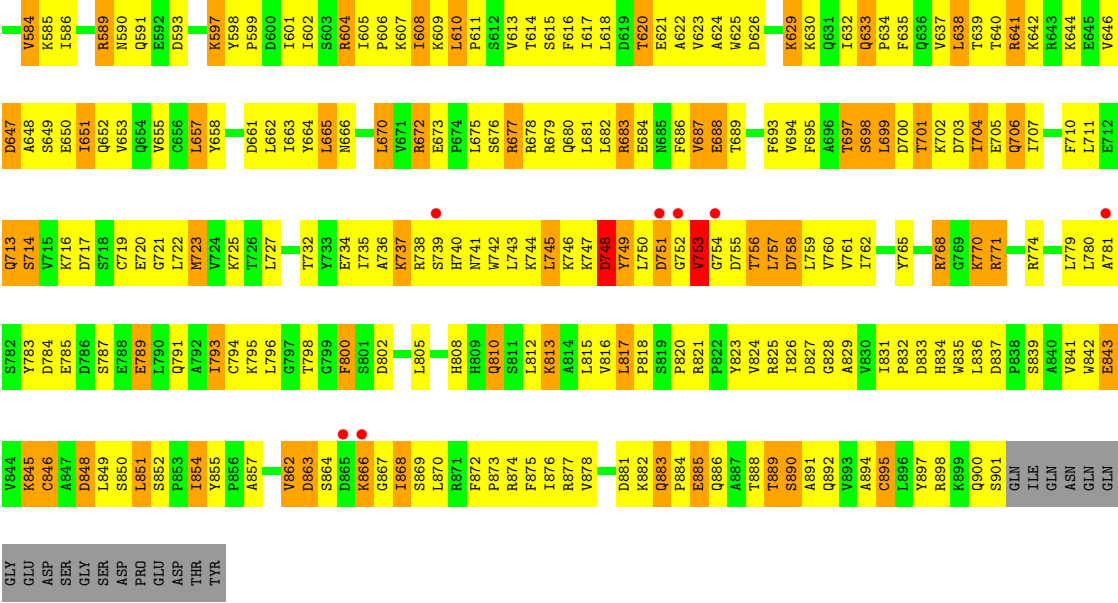


- Molecule 3: template DNA



- Molecule 4: DNA ligase I





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.89Å 161.89Å 88.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 19.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	50.0 (20.00-3.00) 99.0 (19.99-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.60 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.1.80	Depositor
R, $R_{free}$	0.235 , 0.268 0.215 , 0.220	Depositor DCC
$R_{free}$ test set	1287 reflections (5.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.1	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 79.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5730	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DOC, AMP

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	B	1.01	0/228	2.16	12/351 (3.4%)
2	C	1.40	3/209 (1.4%)	2.04	9/321 (2.8%)
3	D	1.15	0/453	1.95	19/696 (2.7%)
4	A	0.58	0/4987	0.82	15/6753 (0.2%)
All	All	0.71	3/5877 (0.1%)	1.12	55/8121 (0.7%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	DG	C3'-O3'	-7.01	1.34	1.44
2	C	3	DC	C3'-O3'	-5.51	1.36	1.44
2	C	4	DG	C3'-O3'	-5.22	1.37	1.44

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	DT	O4'-C1'-N1	18.87	121.21	108.00
3	D	16	DG	O4'-C4'-C3'	-9.17	100.50	106.00
3	D	15	DC	O4'-C4'-C3'	-8.89	100.67	106.00
3	D	11	DC	O4'-C1'-N1	-7.93	102.45	108.00
3	D	21	DA	O4'-C1'-N9	-7.78	102.56	108.00

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	B	222	0	126	18	0
2	C	187	0	102	15	0
3	D	404	0	224	30	0
4	A	4894	0	4925	468	0
5	C	23	0	12	3	0
All	All	5730	0	5389	520	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 47.

The worst 5 of 520 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)
4:A:480:MSE:CE	4:A:480:MSE:SE	2.15	1.44
4:A:548:THR:CG2	4:A:745:LEU:HD13	1.72	1.19
2:C:7:DC:H2"	2:C:8:DT:H5"	1.24	1.15
4:A:400:THR:HG22	4:A:403:GLY:H	1.08	1.14
4:A:551:ILE:CD1	4:A:707:ILE:HG22	1.79	1.13

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
4	A	628/688 (91%)	559 (89%)	66 (10%)	3 (0%)	32 74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	748	ASP
4	A	753	VAL
4	A	644	LYS

### 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
4	A	525/576 (91%)	384 (73%)	141 (27%)	<b>0</b> <b>3</b>

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	597	LYS
4	A	652	GLN
4	A	862	VAL
4	A	607	LYS
4	A	633	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
4	A	474	GLN
4	A	594	ASN
4	A	713	GLN
4	A	360	GLN
4	A	706	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](#)

1 non-standard protein/DNA/RNA residue is 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	DOC	B	13	1,3	13,19,20	1.15	2 (15%)	12,26,29	1.74	2 (16%)

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	DOC	B	13	1,3	-	0/3/18/19	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	13	DOC	C2-N3	-2.58	1.33	1.38
1	B	13	DOC	C6-C5	-2.43	1.32	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	DOC	C2'-C1'-N1	-3.90	105.04	112.47
1	B	13	DOC	C3'-C2'-C1'	-3.08	99.26	102.69

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
1	B	13	DOC	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
5	AMP	C	100	2	22,25,25	1.16	2 (9%)	24,38,38	2.14	2 (8%)

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
5	AMP	C	100	2	-	0/6/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	100	AMP	C2-N1	2.31	1.38	1.33
5	C	100	AMP	C2-N3	3.67	1.38	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	100	AMP	N3-C2-N1	-9.17	120.87	128.86
5	C	100	AMP	P-O5'-C5'	2.87	126.19	118.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	100	AMP	3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	B	10/13 (76%)	0.27	1 (10%) 8 3	44, 50, 65, 66	0
2	C	9/15 (60%)	-0.22	1 (11%) 6 2	40, 46, 55, 61	0
3	D	20/28 (71%)	-0.07	2 (10%) 8 3	38, 46, 58, 70	0
4	A	626/688 (90%)	-0.31	7 (1%) 80 55	26, 41, 50, 61	0
All	All	665/744 (89%)	-0.29	11 (1%) 70 42	26, 41, 52, 70	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	26	DC	3.3
1	B	3	DG	3.0
4	A	866	LYS	2.9
4	A	739	SER	2.7
4	A	781	ALA	2.6

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	DOC	B	13	18/19	0.97	0.16	-	35,37,42,42	0

### 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. 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, 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	AMP	C	100	23/23	0.98	0.14	-1.31	36,38,45,48	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.