



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:49 AM GMT

PDB ID : 3G6V  
Title : DNA synthesis across an abasic lesion by human DNA polymerase- $\iota$   
Authors : Nair, D.T.; Aggarwal, A.K.  
Deposited on : 2009-02-09  
Resolution : 2.20 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  
<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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

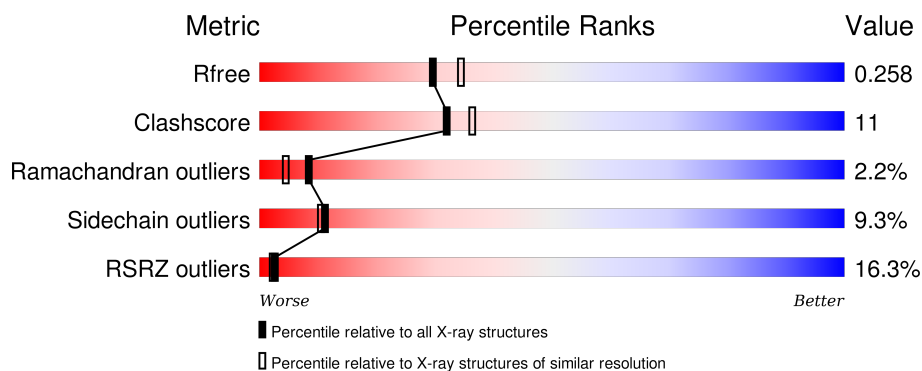
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	420	<div> <div>15%</div> <div>65%</div> <div>20%</div> <div>•</div> <div>11%</div> </div>
2	P	7	<div> <div>71%</div> <div>29%</div> </div>
3	T	12	<div> <div>8%</div> <div>8%</div> <div>50%</div> <div>17%</div> <div>25%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3390 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 iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2876	1809	504	542	21			

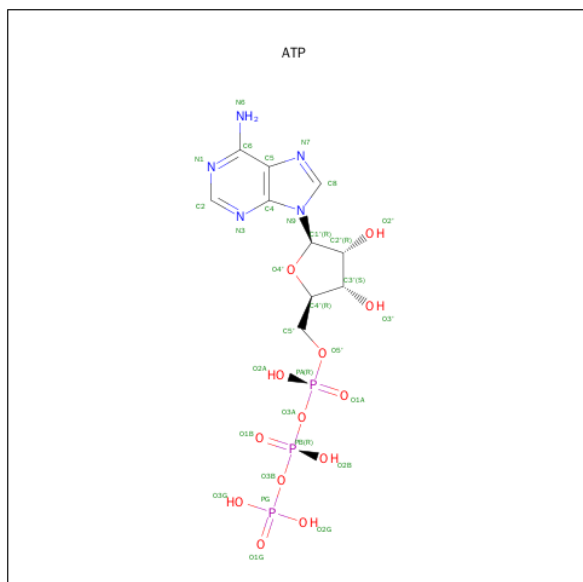
- Molecule 2 is a DNA chain called Primer DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	P	0	0	0
			139	67	29	37	6			

- Molecule 3 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	9	Total	C	N	O	P	0	0	0
			172	83	27	54	8			

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

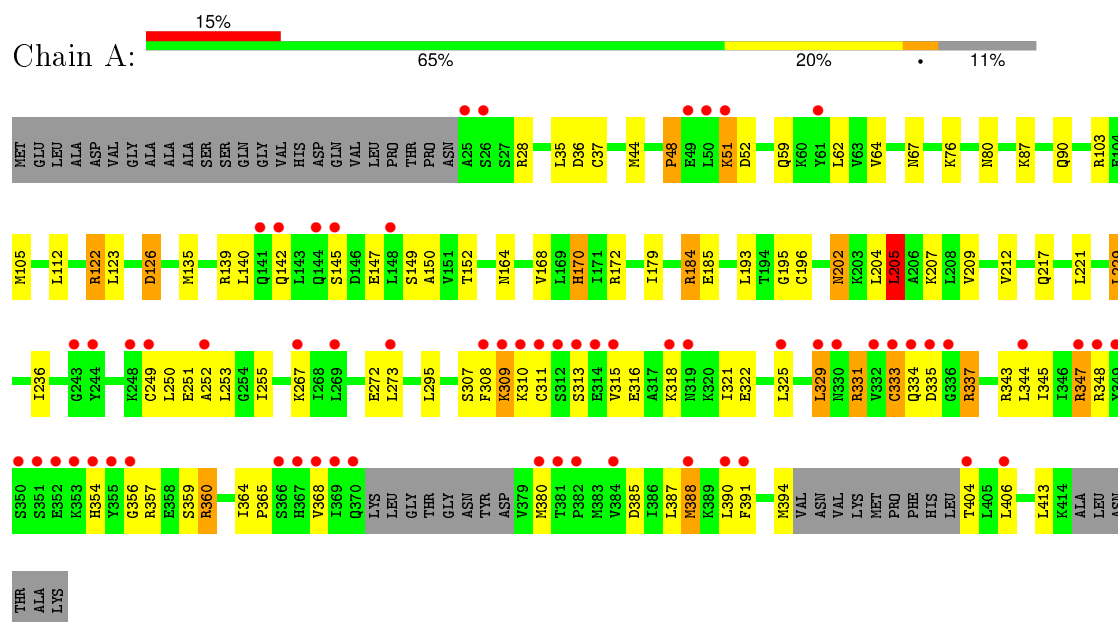
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	156	Total	O	0	0
			156	156		
6	P	3	Total	O	0	0
			3	3		
6	T	12	Total	O	0	0
			12	12		

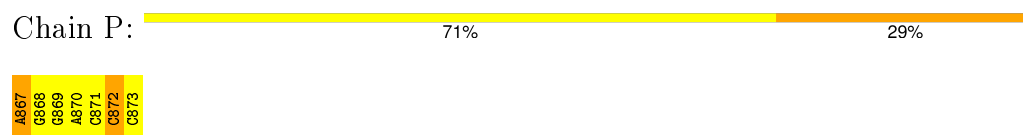
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

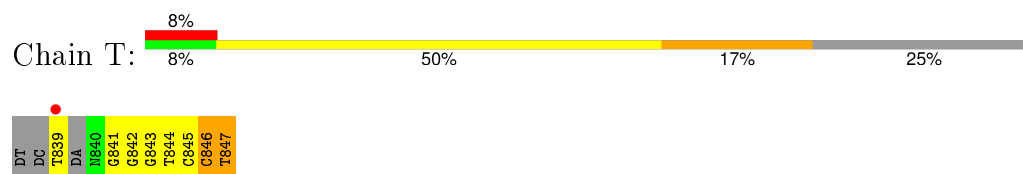
- Molecule 1: DNA polymerase iota



- Molecule 2: Primer DNA strand



- Molecule 3: Template DNA strand



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.15Å 98.15Å 203.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.22 – 2.20 39.21 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.0 (39.22-2.20) 97.0 (39.21-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.46 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.211 , 0.251 0.217 , 0.258	Depositor DCC
$R_{free}$ test set	2417 reflections (8.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 30025 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3390	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, MG, ATP, 3DR

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	1.10	5/2914 (0.2%)	1.18	15/3934 (0.4%)
2	P	1.81	0/136	3.27	20/208 (9.6%)
3	T	1.92	2/178 (1.1%)	2.92	24/271 (8.9%)
All	All	1.20	7/3228 (0.2%)	1.51	59/4413 (1.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	842	DG	C3'-O3'	-6.86	1.35	1.44
1	A	212	VAL	CB-CG1	6.83	1.67	1.52
3	T	839	DT	C1'-N1	6.72	1.57	1.49
1	A	122	ARG	CD-NE	-6.54	1.35	1.46
1	A	207	LYS	CE-NZ	-6.45	1.32	1.49
1	A	185	GLU	CB-CG	-5.73	1.41	1.52
1	A	122	ARG	CG-CD	5.04	1.64	1.51

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ARG	NE-CZ-NH2	-27.27	106.66	120.30
1	A	184	ARG	NE-CZ-NH2	-15.63	112.48	120.30
2	P	870	DA	O4'-C1'-N9	15.62	118.94	108.00
1	A	122	ARG	NE-CZ-NH1	15.31	127.95	120.30
2	P	867	DA	O4'-C1'-N9	13.79	117.65	108.00
1	A	184	ARG	NE-CZ-NH1	13.74	127.17	120.30
2	P	867	DA	O4'-C4'-C3'	-11.62	99.03	106.00
2	P	870	DA	O5'-P-OP2	-11.56	95.30	105.70
3	T	841	DG	C2-N3-C4	11.46	117.63	111.90
2	P	869	DG	O4'-C1'-N9	11.15	115.80	108.00
3	T	841	DG	C5-C6-N1	10.96	116.98	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	871	DC	O5'-P-OP2	-10.54	96.21	105.70
1	A	126	ASP	CB-CG-OD1	-10.16	109.16	118.30
1	A	122	ARG	CD-NE-CZ	9.80	137.31	123.60
3	T	841	DG	O4'-C1'-N9	9.23	114.46	108.00
3	T	845	DC	P-O5'-C5'	8.87	135.10	120.90
2	P	870	DA	O4'-C4'-C3'	8.73	111.24	106.00
3	T	839	DT	O4'-C1'-N1	8.57	114.00	108.00
3	T	845	DC	P-O3'-C3'	8.49	129.89	119.70
3	T	841	DG	C5-C6-O6	-8.45	123.53	128.60
3	T	842	DG	O4'-C1'-C2'	8.08	112.37	105.90
2	P	868	DG	N1-C6-O6	7.83	124.60	119.90
2	P	869	DG	N9-C4-C5	7.46	108.39	105.40
3	T	846	DC	N1-C2-O2	7.36	123.31	118.90
3	T	842	DG	N1-C6-O6	-7.16	115.61	119.90
2	P	869	DG	C8-N9-C4	-7.06	103.58	106.40
1	A	122	ARG	CG-CD-NE	-7.05	96.98	111.80
3	T	842	DG	O4'-C1'-N9	-6.96	103.13	108.00
2	P	872	DC	O4'-C4'-C3'	-6.83	101.77	104.50
3	T	847	DT	C6-C5-C7	-6.83	118.80	122.90
3	T	847	DT	C4-C5-C7	6.64	122.98	119.00
3	T	843	DG	O4'-C4'-C3'	-6.43	101.93	104.50
2	P	871	DC	O4'-C4'-C3'	-6.32	101.97	104.50
3	T	841	DG	C6-N1-C2	-6.26	121.34	125.10
2	P	872	DC	C6-N1-C2	6.25	122.80	120.30
3	T	843	DG	O5'-P-OP2	-6.25	100.08	105.70
3	T	842	DG	N1-C2-N2	-6.20	110.62	116.20
2	P	869	DG	P-O3'-C3'	-6.15	112.32	119.70
1	A	331	ARG	NE-CZ-NH1	6.06	123.33	120.30
3	T	844	DT	C6-C5-C7	-5.99	119.30	122.90
2	P	871	DC	C4'-C3'-C2'	-5.99	97.71	103.10
3	T	847	DT	O4'-C1'-N1	-5.94	103.84	108.00
1	A	205	LEU	CB-CG-CD1	5.72	120.72	111.00
1	A	28	ARG	NE-CZ-NH2	-5.62	117.49	120.30
3	T	846	DC	N3-C4-N4	-5.50	114.15	118.00
2	P	868	DG	C5-C6-O6	-5.44	125.34	128.60
2	P	869	DG	C4-C5-N7	-5.38	108.65	110.80
2	P	871	DC	N1-C2-O2	-5.37	115.68	118.90
2	P	870	DA	C3'-C2'-C1'	5.32	108.89	102.50
1	A	337	ARG	NE-CZ-NH1	5.23	122.92	120.30
3	T	846	DC	C5-C4-N4	5.21	123.84	120.20
3	T	839	DT	C6-N1-C2	-5.18	118.71	121.30
3	T	842	DG	C5-C6-O6	5.13	131.68	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	869	DG	N1-C6-O6	-5.13	116.83	119.90
1	A	135	MET	CG-SD-CE	-5.12	92.01	100.20
3	T	844	DT	N1-C2-N3	5.11	117.67	114.60
1	A	347	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	103	ARG	NE-CZ-NH1	-5.03	117.79	120.30
1	A	140	LEU	CB-CG-CD1	-5.03	102.46	111.00

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	A	2876	0	2899	65	0
2	P	139	0	79	1	1
3	T	172	0	102	1	1
4	A	30	0	10	0	0
5	A	2	0	0	0	0
6	A	156	0	0	3	0
6	P	3	0	0	0	0
6	T	12	0	0	0	0
All	All	3390	0	3090	67	1

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 11.

All (67) 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:344:LEU:CD1	1:A:387:LEU:HD13	1.81	1.10
1:A:309:LYS:H	1:A:309:LYS:CD	1.64	1.08
1:A:344:LEU:HD11	1:A:387:LEU:CD1	1.86	1.05
1:A:309:LYS:HD2	1:A:309:LYS:H	1.16	1.05
1:A:344:LEU:HD11	1:A:387:LEU:HD13	0.97	0.93
1:A:44:MET:CE	1:A:67:ASN:HD22	1.80	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ARG:HD2	6:A:1014:HOH:O	1.70	0.92
1:A:164:ASN:H	1:A:170:HIS:HD2	1.20	0.88
1:A:344:LEU:HD13	1:A:390:LEU:HD12	1.60	0.84
1:A:309:LYS:N	1:A:309:LYS:CD	2.45	0.79
1:A:249:CYS:SG	1:A:273:LEU:HD21	2.27	0.73
1:A:44:MET:HE3	1:A:67:ASN:HD22	1.53	0.73
1:A:335:ASP:OD2	1:A:337:ARG:HD3	1.88	0.72
1:A:347:ARG:HD2	1:A:404:THR:OG1	1.89	0.71
1:A:80:ASN:HB3	6:A:1018:HOH:O	1.94	0.68
1:A:164:ASN:H	1:A:170:HIS:CD2	2.09	0.66
1:A:44:MET:CE	1:A:67:ASN:ND2	2.58	0.66
1:A:44:MET:HE1	1:A:67:ASN:HD22	1.60	0.65
1:A:48:PRO:O	1:A:51:LYS:HB2	1.98	0.64
1:A:343:ARG:HD2	1:A:345:ILE:HD11	1.80	0.64
1:A:335:ASP:CG	1:A:337:ARG:HD3	2.21	0.61
1:A:202:ASN:ND2	1:A:205:LEU:H	1.99	0.60
1:A:321:ILE:HD11	1:A:406:LEU:HD22	1.84	0.59
1:A:309:LYS:HD2	1:A:309:LYS:N	2.01	0.59
1:A:44:MET:HE2	1:A:51:LYS:O	2.03	0.59
1:A:360:ARG:HG2	1:A:394:MET:HG3	1.86	0.57
1:A:335:ASP:OD1	1:A:337:ARG:HD3	2.05	0.56
1:A:333:CYS:O	1:A:335:ASP:N	2.40	0.55
1:A:44:MET:HE3	1:A:67:ASN:ND2	2.19	0.55
1:A:365:PRO:HB2	1:A:368:VAL:HG13	1.89	0.53
1:A:309:LYS:HD3	1:A:311:CYS:SG	2.50	0.52
1:A:44:MET:HE1	1:A:67:ASN:ND2	2.23	0.51
1:A:318:LYS:HB2	1:A:388:MET:SD	2.50	0.51
1:A:309:LYS:H	1:A:309:LYS:HD3	1.67	0.51
1:A:184:ARG:HD2	1:A:195:GLY:O	2.12	0.49
1:A:112:LEU:HD23	1:A:112:LEU:C	2.35	0.47
1:A:122:ARG:HD3	6:A:957:HOH:O	2.14	0.47
3:T:846:DC:H1'	3:T:847:DT:H5'	1.96	0.47
1:A:308:PHE:HD1	1:A:311:CYS:H	1.62	0.47
1:A:202:ASN:C	1:A:202:ASN:HD22	2.18	0.46
1:A:329:LEU:HD13	1:A:380:MET:HG3	1.97	0.46
1:A:253:LEU:HD11	1:A:272:GLU:HG2	1.98	0.46
1:A:36:ASP:O	1:A:37:CYS:C	2.55	0.46
1:A:168:VAL:HG22	1:A:172:ARG:HD2	1.97	0.45
1:A:139:ARG:CZ	1:A:179:ILE:CD1	2.94	0.45
1:A:388:MET:O	1:A:391:PHE:HB3	2.18	0.44
1:A:196:CYS:HA	1:A:217:GLN:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:HD22	1:A:229:LEU:HD12	1.99	0.44
1:A:44:MET:HE2	1:A:51:LYS:HA	2.00	0.43
1:A:105:MET:CG	1:A:193:LEU:HD11	2.48	0.43
1:A:59:GLN:OE1	1:A:64:VAL:HG11	2.19	0.43
1:A:251:GLU:O	1:A:252:ALA:C	2.57	0.42
1:A:325:LEU:O	1:A:329:LEU:HD12	2.19	0.42
1:A:164:ASN:N	1:A:170:HIS:HD2	2.02	0.42
1:A:345:ILE:HG13	1:A:359:SER:HB3	2.02	0.42
1:A:309:LYS:N	1:A:309:LYS:HD3	2.31	0.42
1:A:364:ILE:HG23	1:A:368:VAL:HG22	2.01	0.42
1:A:344:LEU:O	1:A:359:SER:HA	2.20	0.42
1:A:347:ARG:HD2	1:A:404:THR:HG1	1.83	0.41
1:A:147:GLU:HG2	1:A:147:GLU:H	1.56	0.41
1:A:250:LEU:HB3	1:A:255:ILE:HB	2.01	0.41
2:P:872:DC:H2'	2:P:873:DOC:H6	2.03	0.41
1:A:359:SER:O	1:A:360:ARG:HD3	2.21	0.40
1:A:76:LYS:HA	1:A:76:LYS:HD3	1.84	0.40
1:A:202:ASN:HD21	1:A:205:LEU:H	1.68	0.40
1:A:150:ALA:O	1:A:152:THR:HG23	2.20	0.40
1:A:322:GLU:HG3	1:A:322:GLU:H	1.73	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:867:DA:O5'	3:T:847:DT:O3'[10_665]	1.84	0.36

## 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	367/420 (87%)	341 (93%)	18 (5%)	8 (2%)	<b>8</b> <b>4</b>

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	LYS
1	A	315	VAL
1	A	333	CYS
1	A	334	GLN
1	A	354	HIS
1	A	313	SER
1	A	316	GLU
1	A	356	GLY

### 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	321/376 (85%)	291 (91%)	30 (9%)	11	10

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	48	PRO
1	A	51	LYS
1	A	52	ASP
1	A	62	LEU
1	A	87	LYS
1	A	90	GLN
1	A	123	LEU
1	A	126	ASP
1	A	142	GLN
1	A	145	SER
1	A	149	SER
1	A	170	HIS
1	A	202	ASN
1	A	204	LEU
1	A	205	LEU
1	A	209	VAL

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Mol	Chain	Res	Type
1	A	229	LEU
1	A	236	ILE
1	A	267	LYS
1	A	295	LEU
1	A	307	SER
1	A	309	LYS
1	A	329	LEU
1	A	348	ARG
1	A	357	ARG
1	A	360	ARG
1	A	385	ASP
1	A	388	MET
1	A	413	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	67	ASN
1	A	170	HIS
1	A	202	ASN
1	A	262	GLN
1	A	300	GLN
1	A	412	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	DOC	P	873	3,2	11,19,20	0.99	0	14,26,29	2.81	7 (50%)
3	3DR	T	840	3	7,11,12	1.39	1 (14%)	8,14,17	2.48	3 (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
2	DOC	P	873	3,2	-	0/3/18/19	0/2/2/2
3	3DR	T	840	3	-	0/3/15/16	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	840	3DR	O4'-C4'	-3.08	1.38	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	873	DOC	C2'-C1'-N1	-5.72	100.91	112.49
3	T	840	3DR	O4'-C4'-C5'	-5.43	97.66	109.53
2	P	873	DOC	C3'-C4'-C5'	-3.13	103.29	116.05
3	T	840	3DR	O3'-C3'-C2'	-2.86	105.17	111.71
3	T	840	3DR	O4'-C1'-C2'	-2.42	101.66	106.64
2	P	873	DOC	O4'-C4'-C5'	2.29	112.92	109.54
2	P	873	DOC	O4'-C4'-C3'	3.01	109.73	104.69
2	P	873	DOC	O4'-C1'-N1	3.09	113.06	107.72
2	P	873	DOC	C2-N3-C4	3.97	121.21	115.61
2	P	873	DOC	C3'-C2'-C1'	5.10	108.40	102.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	873	DOC	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 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	ATP	A	875	5	24,32,33	1.81	7 (29%)	32,50,52	2.03	8 (25%)

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	ATP	A	875	5	-	0/18/34/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	875	ATP	C5'-C4'	2.17	1.58	1.51
4	A	875	ATP	C2'-C1'	2.23	1.58	1.52
4	A	875	ATP	C2-N3	2.30	1.36	1.32
4	A	875	ATP	C8-N7	2.41	1.39	1.34
4	A	875	ATP	C4-N3	3.18	1.40	1.35
4	A	875	ATP	O3'-C3'	3.44	1.51	1.43
4	A	875	ATP	C5-C4	4.25	1.50	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	875	ATP	N3-C2-N1	-7.10	123.46	128.89
4	A	875	ATP	C1'-N9-C4	-2.44	123.02	127.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	875	ATP	PA-O3A-PB	-2.19	126.59	132.73
4	A	875	ATP	O3'-C3'-C2'	2.36	118.57	110.74
4	A	875	ATP	C4-C5-N7	2.63	111.90	109.48
4	A	875	ATP	C2-N1-C6	2.74	123.67	118.77
4	A	875	ATP	O2B-PB-O3A	3.10	119.17	105.09
4	A	875	ATP	N6-C6-N1	3.34	126.37	119.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	373/420 (88%)	0.84	62 (16%) <b>2</b> <b>2</b>	11, 25, 46, 62	0
2	P	6/7 (85%)	0.23	0 <b>100</b> <b>100</b>	22, 29, 32, 35	0
3	T	8/12 (66%)	1.06	1 (12%) <b>5</b> <b>5</b>	15, 18, 25, 162	0
All	All	387/439 (88%)	0.83	63 (16%) <b>2</b> <b>2</b>	11, 25, 46, 162	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	354	HIS	16.3
1	A	25	ALA	14.1
1	A	355	TYR	12.2
3	T	839	DT	8.8
1	A	353	LYS	8.0
1	A	311	CYS	7.6
1	A	244	TYR	7.5
1	A	352	GLU	7.4
1	A	312	SER	6.9
1	A	336	GLY	5.2
1	A	350	SER	4.9
1	A	333	CYS	4.8
1	A	368	VAL	4.6
1	A	26	SER	4.4
1	A	390	LEU	4.4
1	A	391	PHE	4.3
1	A	315	VAL	4.2
1	A	348	ARG	4.1
1	A	308	PHE	4.0
1	A	332	VAL	3.8
1	A	380	MET	3.7
1	A	144	GLN	3.7
1	A	334	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	319	ASN	3.6
1	A	384	VAL	3.5
1	A	351	SER	3.5
1	A	329	LEU	3.4
1	A	314	GLU	3.4
1	A	325	LEU	3.4
1	A	252	ALA	3.3
1	A	335	ASP	3.2
1	A	369	ILE	3.2
1	A	148	LEU	3.1
1	A	406	LEU	3.0
1	A	50	LEU	3.0
1	A	381	THR	3.0
1	A	142	GLN	2.8
1	A	388	MET	2.8
1	A	370	GLN	2.8
1	A	145	SER	2.7
1	A	356	GLY	2.7
1	A	141	GLN	2.7
1	A	366	SER	2.7
1	A	382	PRO	2.6
1	A	347	ARG	2.6
1	A	367	HIS	2.5
1	A	249	CYS	2.5
1	A	243	GLY	2.4
1	A	310	LYS	2.4
1	A	313	SER	2.4
1	A	248	LYS	2.4
1	A	309	LYS	2.4
1	A	349	TYR	2.4
1	A	61	TYR	2.3
1	A	330	ASN	2.3
1	A	51	LYS	2.3
1	A	49	GLU	2.2
1	A	273	LEU	2.2
1	A	404	THR	2.1
1	A	344	LEU	2.1
1	A	267	LYS	2.1
1	A	318	LYS	2.1
1	A	269	LEU	2.0

## 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
2	DOC	P	873	18/19	0.98	0.18	-	12,16,24,25	0
3	3DR	T	840	11/12	0.95	0.15	-	22,37,53,53	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(Å <sup>2</sup> )	Q<0.9
4	ATP	A	875	30/31	0.94	0.14	0.03	14,27,29,33	0
5	MG	A	871	1/1	0.94	0.07	-1.89	16,16,16,16	0
5	MG	A	872	1/1	0.63	0.38	-	58,58,58,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.