



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:55 AM GMT

PDB ID : 3K5M  
Title : Crystal structure of E.coli Pol II-abasic DNA-ddGTP Lt(-2, 2) ternary complex  
Authors : Yang, W.; Wang, F.  
Deposited on : 2009-10-07  
Resolution : 2.04 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

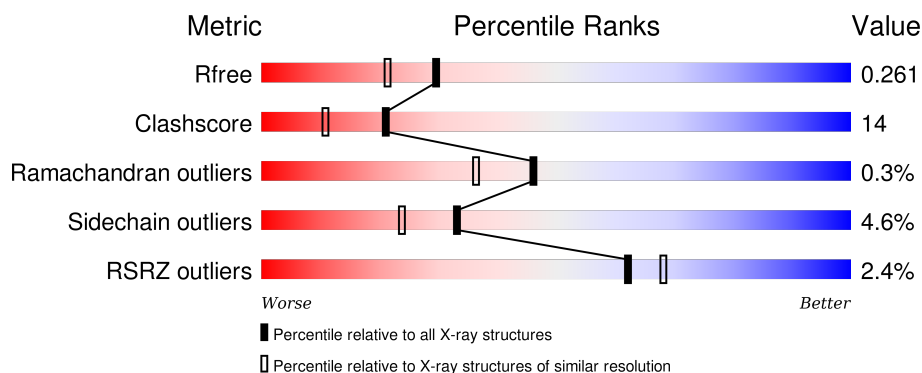
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.04 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	786	<div> <div>2%</div> <div>71%</div> <div>25%</div> <div>••</div> </div>
2	T	20	<div> <div>40%</div> <div>50%</div> <div>10%</div> </div>
3	P	13	<div> <div>46%</div> <div>38%</div> <div>15%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7390 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 II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	768	Total	C	N	O	S	0	0	0
			6204	3951	1109	1120	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P21189
A	-1	PRO	-	EXPRESSION TAG	UNP P21189
A	0	HIS	-	EXPRESSION TAG	UNP P21189
A	335	ASN	ASP	ENGINEERED	UNP P21189

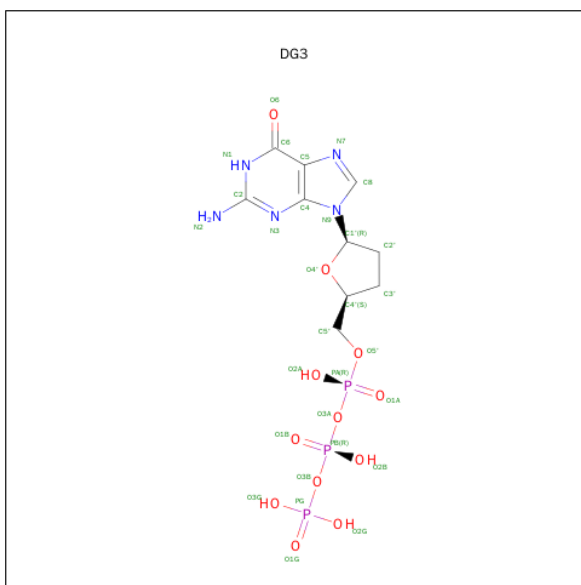
- Molecule 2 is a DNA chain called DNA (5'-D(\*AP\*GP\*TP\*CP\*CP\*TP\*GP\*(3DR)P\*AP\*CP\*GP\*CP\*TP\*AP\*GP\*GP\*CP\*AP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	20	Total	C	N	O	P	0	0	0
			397	189	74	115	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	P	0	0	0
			266	127	50	77	12			

- Molecule 4 is 2'-3'-DIDEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DG3) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



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

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

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

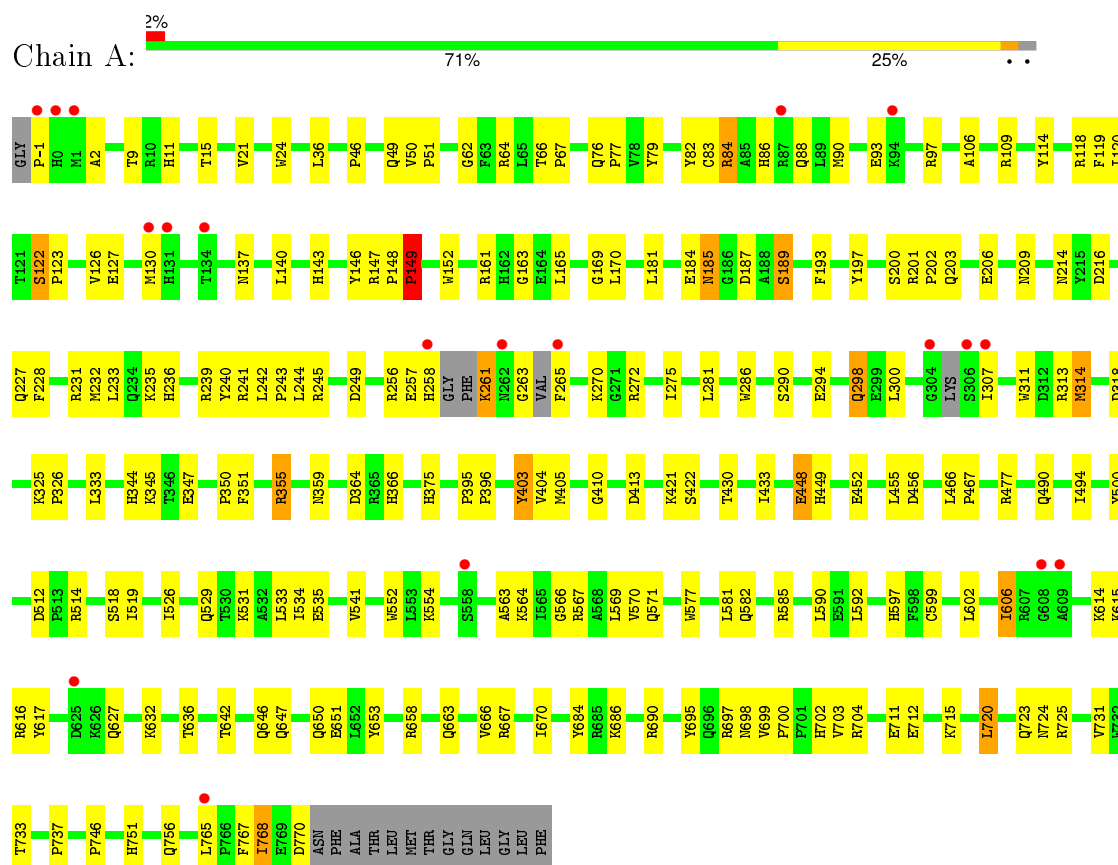
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	441	Total O 441 441	0	0
6	T	36	Total O 36 36	0	0
6	P	14	Total O 14 14	0	0

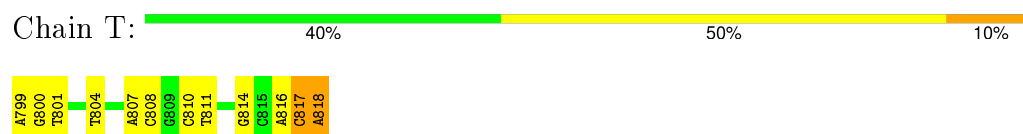
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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 II



#### • Molecule 2: DNA (5'-D(\*AP\*GP\*TP\*CP\*CP\*TP\*GP\*(3DR)P\*AP\*CP\*GP\*CP\*TP\*AP\*GP\*GP\*CP\*AP\*CP\*A)-3')



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



6901	6902	6903	6904	6905	6906	6913
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.11Å 95.23Å 144.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.43 – 2.04 45.25 – 2.04	Depositor EDS
% Data completeness (in resolution range)	88.7 (28.43-2.04) 88.5 (45.25-2.04)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 2.03Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.243 , 0.260 0.243 , 0.261	Depositor DCC
$R_{free}$ test set	1450 reflections (2.51%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 62368 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7390	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 4.09% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DG3, CA, 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	0.61	0/6369	0.78	1/8638 (0.0%)
2	T	1.49	12/432 (2.8%)	1.61	5/662 (0.8%)
3	P	0.95	0/298	1.35	3/459 (0.7%)
All	All	0.71	12/7099 (0.2%)	0.90	9/9759 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	818	DA	C5-C6	-9.81	1.32	1.41
2	T	818	DA	N9-C4	-8.19	1.32	1.37
2	T	818	DA	C1'-N9	-7.77	1.36	1.47
2	T	818	DA	C4'-O4'	-6.97	1.38	1.45
2	T	818	DA	P-O5'	-6.82	1.52	1.59
2	T	818	DA	N3-C4	-6.59	1.30	1.34
2	T	818	DA	C5-C4	-6.41	1.34	1.38
2	T	818	DA	C2-N3	-6.19	1.27	1.33
2	T	818	DA	C8-N7	-6.11	1.27	1.31
2	T	818	DA	C6-N6	-5.70	1.29	1.33
2	T	818	DA	O4'-C1'	-5.02	1.36	1.42
2	T	817	DC	O3'-P	-5.00	1.55	1.61

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	818	DA	O4'-C1'-N9	-23.78	91.36	108.00
3	P	903	DG	O5'-P-OP2	-8.09	98.42	105.70
3	P	904	DC	O4'-C1'-N1	6.48	112.53	108.00
2	T	817	DC	OP2-P-O3'	5.86	118.08	105.20
2	T	818	DA	O5'-P-OP2	-5.47	100.77	105.70
3	P	913	DG	C1'-O4'-C4'	-5.37	104.73	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	818	DA	N1-C2-N3	-5.33	126.64	129.30
2	T	817	DC	C1'-O4'-C4'	-5.14	104.96	110.10
1	A	149	PRO	N-CA-C	-5.09	98.87	112.10

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	6204	0	6048	172	0
2	T	397	0	220	12	0
3	P	266	0	148	9	0
4	A	30	0	11	1	0
5	A	2	0	0	0	0
6	A	441	0	0	10	0
6	P	14	0	0	0	0
6	T	36	0	0	0	0
All	All	7390	0	6427	191	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 14.

All (191) 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:123:PRO:HB2	1:A:143:HIS:O	1.58	1.02
3:P:901:DG:H8	3:P:901:DG:H5'	1.24	1.00
1:A:62:GLY:HA3	1:A:84:ARG:HD3	1.49	0.95
1:A:534:ILE:HD13	1:A:569:LEU:HD22	1.52	0.91
1:A:2:ALA:HB2	1:A:127:GLU:HG2	1.57	0.87
3:P:901:DG:H2''	3:P:902:DT:H5'	1.55	0.86
1:A:185:ASN:HD21	1:A:325:LYS:H	1.24	0.85
3:P:905:DC:H2''	3:P:906:DT:OP2	1.77	0.82
3:P:901:DG:H5'	3:P:901:DG:C8	2.13	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:HIS:HB3	1:A:261:LYS:HG2	1.67	0.77
1:A:300:LEU:HD12	1:A:300:LEU:O	1.86	0.76
1:A:698:ASN:OD1	2:T:814:DG:H5'	1.86	0.75
1:A:582:GLN:HG3	6:A:1119:HOH:O	1.87	0.75
1:A:261:LYS:HD2	1:A:263:GLY:N	2.01	0.73
1:A:209:ASN:ND2	1:A:245:ARG:H	1.86	0.73
1:A:62:GLY:CA	1:A:84:ARG:HD3	2.19	0.73
1:A:200:SER:H	1:A:203:GLN:HE21	1.35	0.72
3:P:901:DG:H2''	3:P:902:DT:C5'	2.19	0.72
1:A:257:GLU:HB2	1:A:265:PHE:CE1	2.25	0.71
1:A:627:GLN:HE22	1:A:658:ARG:HD2	1.56	0.71
1:A:227:GLN:O	1:A:231:ARG:HD3	1.92	0.70
1:A:185:ASN:HD22	1:A:185:ASN:C	1.94	0.70
1:A:235:LYS:HG3	6:A:1082:HOH:O	1.90	0.70
1:A:765:LEU:HD23	1:A:768:ILE:HD11	1.74	0.68
1:A:209:ASN:HD21	1:A:245:ARG:H	1.38	0.68
1:A:552:TRP:CE2	1:A:554:LYS:HA	2.28	0.68
2:T:807:DA:H2''	2:T:808:DC:H5'	1.77	0.67
1:A:169:GLY:O	1:A:170:LEU:HD23	1.94	0.67
2:T:799:DA:H4'	2:T:800:DG:OP1	1.95	0.66
1:A:566:GLY:O	1:A:570:VAL:HG22	1.95	0.66
1:A:261:LYS:HD2	1:A:263:GLY:H	1.61	0.66
1:A:375:HIS:HD2	6:A:1032:HOH:O	1.78	0.65
1:A:410:GLY:HA2	1:A:767:PHE:CE1	2.32	0.64
1:A:404:VAL:HG11	1:A:614:LYS:HD2	1.78	0.64
1:A:529:GLN:O	1:A:533:LEU:HG	1.98	0.63
1:A:355:ARG:NH1	1:A:359:ASN:HD21	1.96	0.63
2:T:810:DC:H2'	2:T:811:DT:H71	1.81	0.63
1:A:161:ARG:NE	1:A:314:MET:HE2	2.15	0.62
1:A:704:ARG:CZ	1:A:737:PRO:HD2	2.29	0.62
1:A:161:ARG:HB3	1:A:314:MET:CE	2.29	0.62
1:A:366:HIS:HE1	6:A:941:HOH:O	1.82	0.61
1:A:765:LEU:O	1:A:768:ILE:HG13	2.01	0.61
1:A:62:GLY:HA3	1:A:84:ARG:CD	2.27	0.61
1:A:161:ARG:NE	1:A:314:MET:CE	2.64	0.61
1:A:83:CYS:HB3	1:A:88:GLN:OE1	2.02	0.60
1:A:602:LEU:HD23	1:A:653:TYR:CE2	2.37	0.60
1:A:216:ASP:HA	1:A:272:ARG:NH2	2.17	0.60
1:A:200:SER:H	1:A:203:GLN:NE2	2.00	0.58
1:A:314:MET:HE3	1:A:318:ASP:OD2	2.04	0.58
1:A:404:VAL:HG11	1:A:614:LYS:CD	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PHE:O	1:A:232:MET:HG2	2.04	0.57
1:A:67:PRO:HD3	1:A:79:TYR:CE2	2.40	0.56
1:A:300:LEU:HD11	1:A:345:LYS:HG2	1.86	0.56
1:A:46:PRO:HB2	1:A:49:GLN:HG3	1.86	0.56
1:A:711:GLU:O	1:A:715:LYS:HE2	2.06	0.56
1:A:704:ARG:NH1	1:A:737:PRO:HD2	2.21	0.55
1:A:366:HIS:HD2	6:A:805:HOH:O	1.88	0.55
3:P:901:DG:H2'	3:P:902:DT:C6	2.42	0.55
1:A:203:GLN:HA	1:A:206:GLU:HG3	1.89	0.55
1:A:616:ARG:HA	1:A:632:LYS:O	2.07	0.55
1:A:403:TYR:CD2	1:A:403:TYR:C	2.80	0.55
1:A:161:ARG:HB3	1:A:314:MET:HE2	1.89	0.55
1:A:185:ASN:ND2	1:A:325:LYS:H	2.02	0.54
1:A:187:ASP:OD1	1:A:189:SER:HB2	2.08	0.53
1:A:193:PHE:CG	1:A:333:LEU:HD22	2.43	0.53
1:A:64:ARG:HG2	1:A:82:TYR:HB2	1.90	0.53
1:A:684:TYR:OH	1:A:751:HIS:HE1	1.92	0.53
1:A:700:PRO:HD2	1:A:703:VAL:HB	1.91	0.53
1:A:-1:PRO:O	1:A:130:MET:HG3	2.07	0.53
1:A:216:ASP:HA	1:A:272:ARG:HH21	1.72	0.53
1:A:146:TYR:O	1:A:147:ARG:HD3	2.09	0.52
1:A:690:ARG:HB2	1:A:695:TYR:CZ	2.44	0.52
1:A:642:THR:H	1:A:756:GLN:NE2	2.07	0.52
4:A:914:DG3:H5'1	3:P:913:DG:H2''	1.92	0.52
2:T:807:DA:H2'	2:T:808:DC:C6	2.44	0.52
1:A:300:LEU:HD11	1:A:345:LYS:HD3	1.92	0.52
1:A:404:VAL:HG12	1:A:405:MET:N	2.25	0.52
1:A:667:ARG:HH11	1:A:667:ARG:HG2	1.76	0.51
1:A:209:ASN:HD21	1:A:245:ARG:N	2.08	0.51
1:A:258:HIS:HB3	1:A:261:LYS:CG	2.39	0.51
2:T:810:DC:H2'	2:T:811:DT:C7	2.39	0.51
1:A:325:LYS:N	1:A:326:PRO:CD	2.73	0.51
1:A:765:LEU:CD2	1:A:768:ILE:HD11	2.41	0.51
1:A:512:ASP:OD2	1:A:514:ARG:HB2	2.11	0.51
1:A:232:MET:HE3	1:A:232:MET:HA	1.93	0.51
1:A:181:LEU:HD22	1:A:201:ARG:HD3	1.93	0.51
2:T:818:DA:H5'	2:T:818:DA:C8	2.45	0.51
1:A:200:SER:OG	1:A:203:GLN:HG3	2.11	0.50
1:A:240:TYR:HB2	1:A:242:LEU:CD2	2.42	0.50
1:A:209:ASN:ND2	1:A:245:ARG:N	2.58	0.49
1:A:161:ARG:CZ	1:A:314:MET:HE2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:TRP:CH2	1:A:344:HIS:CE1	3.01	0.49
1:A:724:ASN:O	1:A:725:ARG:HB2	2.13	0.49
1:A:240:TYR:HB2	1:A:242:LEU:HD23	1.93	0.49
1:A:120:ILE:O	1:A:375:HIS:HE1	1.94	0.49
1:A:201:ARG:N	1:A:202:PRO:HD2	2.28	0.49
1:A:490:GLN:O	1:A:494:ILE:HG12	2.13	0.49
1:A:185:ASN:C	1:A:185:ASN:ND2	2.65	0.48
1:A:712:GLU:HA	1:A:715:LYS:HE3	1.95	0.48
1:A:114:TYR:CE1	1:A:118:ARG:CZ	2.96	0.48
1:A:2:ALA:HA	1:A:126:VAL:O	2.13	0.48
1:A:122:SER:H	1:A:123:PRO:HD2	1.79	0.48
1:A:636:THR:HG21	1:A:650:GLN:HG3	1.96	0.48
1:A:50:VAL:HB	1:A:51:PRO:HD3	1.94	0.48
1:A:300:LEU:HD11	1:A:345:LYS:CG	2.44	0.48
1:A:118:ARG:O	1:A:119:PHE:HB2	2.14	0.48
1:A:433:ILE:HD12	1:A:518:SER:HB3	1.95	0.48
1:A:733:THR:HB	1:A:746:PRO:O	2.13	0.48
1:A:663:GLN:O	1:A:667:ARG:HG3	2.13	0.48
1:A:564:LYS:HB2	1:A:564:LYS:HE3	1.48	0.48
2:T:804:DT:H2''	2:T:807:DA:H5'	1.96	0.48
1:A:165:LEU:O	1:A:201:ARG:HD2	2.14	0.48
1:A:294:GLU:O	1:A:298:GLN:HB2	2.13	0.48
1:A:647:GLN:O	1:A:651:GLU:HG3	2.13	0.47
1:A:410:GLY:HA2	1:A:767:PHE:CD1	2.48	0.47
1:A:577:TRP:O	1:A:581:LEU:HD13	2.15	0.47
1:A:9:THR:OG1	1:A:11:HIS:CE1	2.67	0.47
1:A:249:ASP:HA	6:A:1176:HOH:O	2.15	0.47
1:A:577:TRP:HE3	1:A:581:LEU:HD11	1.80	0.47
1:A:581:LEU:N	1:A:581:LEU:HD12	2.30	0.47
1:A:21:VAL:HB	1:A:36:LEU:HD12	1.97	0.47
1:A:770:ASP:OD1	1:A:770:ASP:C	2.51	0.47
1:A:636:THR:CG2	1:A:650:GLN:HG3	2.45	0.47
1:A:233:LEU:HB3	1:A:244:LEU:HD21	1.97	0.46
1:A:711:GLU:O	1:A:715:LYS:CE	2.63	0.46
1:A:684:TYR:OH	1:A:751:HIS:CE1	2.68	0.46
1:A:699:VAL:HA	1:A:700:PRO:HD3	1.83	0.46
1:A:636:THR:HA	1:A:646:GLN:HG2	1.98	0.46
1:A:275:ILE:HD13	1:A:364:ASP:HB3	1.96	0.46
1:A:577:TRP:CG	1:A:590:LEU:HD12	2.50	0.46
1:A:50:VAL:N	1:A:51:PRO:CD	2.78	0.46
1:A:563:ALA:O	1:A:567:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:THR:OG1	1:A:11:HIS:HE1	2.00	0.45
1:A:90:MET:CE	1:A:109:ARG:NH2	2.79	0.45
1:A:666:VAL:O	1:A:670:ILE:HG13	2.16	0.45
1:A:615:LYS:HD2	2:T:808:DC:O4'	2.16	0.45
1:A:430:THR:CG2	1:A:581:LEU:HD23	2.46	0.45
1:A:617:TYR:CZ	1:A:632:LYS:HG3	2.51	0.45
1:A:126:VAL:HG23	1:A:140:LEU:HD23	1.98	0.45
1:A:300:LEU:CD1	1:A:345:LYS:HD3	2.47	0.45
1:A:686:LYS:HD2	1:A:702:HIS:CG	2.53	0.44
1:A:270:LYS:NZ	6:A:1172:HOH:O	2.47	0.44
1:A:410:GLY:CA	1:A:767:PHE:CE1	3.00	0.44
1:A:355:ARG:NH1	1:A:359:ASN:ND2	2.64	0.44
1:A:636:THR:HG21	1:A:650:GLN:CG	2.47	0.44
1:A:731:VAL:O	1:A:737:PRO:HA	2.18	0.44
1:A:76:GLN:HA	1:A:77:PRO:HD3	1.85	0.44
1:A:286:TRP:HA	6:A:1163:HOH:O	2.18	0.44
1:A:161:ARG:HE	1:A:314:MET:CE	2.30	0.44
1:A:448:GLU:HG2	1:A:449:HIS:CE1	2.53	0.44
2:T:799:DA:C4'	2:T:800:DG:OP1	2.63	0.43
1:A:433:ILE:HG13	1:A:519:ILE:HG12	2.00	0.43
1:A:413:ASP:HA	1:A:599:CYS:O	2.19	0.43
1:A:455:LEU:O	1:A:456:ASP:HB2	2.19	0.43
1:A:606:ILE:HD13	1:A:606:ILE:HA	1.77	0.43
1:A:351:PHE:C	1:A:351:PHE:CD2	2.92	0.43
1:A:11:HIS:CE1	1:A:24:TRP:HD1	2.36	0.43
1:A:261:LYS:HD2	1:A:263:GLY:CA	2.48	0.43
1:A:421:LYS:O	1:A:422:SER:C	2.57	0.42
1:A:690:ARG:HB2	1:A:695:TYR:CE2	2.54	0.42
1:A:723:GLN:HB2	6:A:808:HOH:O	2.19	0.42
1:A:50:VAL:N	1:A:51:PRO:HD2	2.35	0.42
2:T:816:DA:H2''	2:T:817:DC:O5'	2.19	0.42
1:A:477:ARG:HG2	6:A:1046:HOH:O	2.20	0.42
1:A:720:LEU:HB3	1:A:723:GLN:HG2	2.01	0.42
1:A:570:VAL:HG12	1:A:592:LEU:HG	2.00	0.41
1:A:93:GLU:HG3	1:A:106:ALA:HB3	2.01	0.41
1:A:257:GLU:HB2	1:A:265:PHE:CD1	2.55	0.41
1:A:93:GLU:HG3	1:A:106:ALA:CB	2.50	0.41
1:A:697:ARG:O	1:A:698:ASN:C	2.56	0.41
1:A:355:ARG:HB3	1:A:355:ARG:HE	1.43	0.41
1:A:466:LEU:N	1:A:467:PRO:CD	2.84	0.41
3:P:902:DT:H2''	3:P:903:DG:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:TRP:CZ3	1:A:554:LYS:HG2	2.56	0.41
1:A:395:PRO:HA	1:A:396:PRO:HD3	1.74	0.41
3:P:905:DC:C2'	3:P:906:DT:OP2	2.51	0.41
1:A:765:LEU:HA	1:A:765:LEU:HD23	1.74	0.41
1:A:577:TRP:HE3	1:A:581:LEU:CD1	2.33	0.41
1:A:430:THR:HG21	1:A:581:LEU:HD23	2.03	0.41
1:A:581:LEU:CD1	1:A:581:LEU:N	2.83	0.41
1:A:86:HIS:NE2	1:A:109:ARG:HD3	2.36	0.41
1:A:90:MET:HE2	1:A:109:ARG:NH2	2.36	0.41
1:A:347:GLU:O	1:A:350:PRO:HD2	2.21	0.41
1:A:148:PRO:HA	1:A:149:PRO:HD3	1.97	0.40
1:A:531:LYS:HG3	1:A:541:VAL:HG11	2.04	0.40
1:A:184:GLU:HA	1:A:197:TYR:CE1	2.56	0.40
1:A:163:GLY:O	1:A:236:HIS:HE1	2.04	0.40
1:A:243:PRO:HG3	1:A:245:ARG:NH2	2.37	0.40
2:T:799:DA:C8	2:T:801:DT:O4'	2.74	0.40
1:A:526:ILE:HG23	1:A:577:TRP:CZ2	2.56	0.40
1:A:531:LYS:HE2	1:A:535:GLU:OE2	2.21	0.40

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	760/786 (97%)	745 (98%)	13 (2%)	2 (0%)	46 36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	SER
1	A	307	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	648/672 (96%)	618 (95%)	30 (5%)	33	24

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

Mol	Chain	Res	Type
1	A	15	THR
1	A	66	THR
1	A	84	ARG
1	A	97	ARG
1	A	137	ASN
1	A	149	PRO
1	A	185	ASN
1	A	189	SER
1	A	214	ASN
1	A	239	ARG
1	A	241	ARG
1	A	256	ARG
1	A	261	LYS
1	A	281	LEU
1	A	290	SER
1	A	298	GLN
1	A	311	TRP
1	A	313	ARG
1	A	314	MET
1	A	355	ARG
1	A	403	TYR
1	A	448	GLU
1	A	452	GLU
1	A	500	TYR
1	A	571	GLN
1	A	585	ARG
1	A	597	HIS
1	A	606	ILE
1	A	720	LEU
1	A	768	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	17	GLN
1	A	61	GLN
1	A	185	ASN
1	A	203	GLN
1	A	209	ASN
1	A	214	ASN
1	A	298	GLN
1	A	366	HIS
1	A	375	HIS
1	A	397	HIS
1	A	472	ASN
1	A	475	HIS
1	A	571	GLN
1	A	597	HIS
1	A	627	GLN
1	A	713	ASN
1	A	735	ASN
1	A	751	HIS
1	A	756	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z  > 2$
2	3DR	T	806	2	7,11,12	0.39	0	8,14,17	0.69	0



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	3DR	T	806	2	-	0/3/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	DG3	A	914	5	24,32,32	1.43	3 (12%)	31,50,50	2.38	14 (45%)

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	DG3	A	914	5	-	0/18/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	914	DG3	PA-O2A	2.08	1.63	1.54
4	A	914	DG3	C2-N1	2.43	1.39	1.35
4	A	914	DG3	C6-N1	4.28	1.41	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	914	DG3	N3-C2-N1	-4.81	120.12	127.44
4	A	914	DG3	O3A-PA-O5'	-4.62	90.69	102.94
4	A	914	DG3	C2'-C1'-N9	-3.76	104.87	112.49
4	A	914	DG3	PB-O3B-PG	-3.68	120.34	132.67
4	A	914	DG3	C5-C6-N1	-3.59	118.68	123.59
4	A	914	DG3	O2A-PA-O3A	-3.17	90.72	105.09
4	A	914	DG3	C4-C5-N7	-2.27	107.39	109.48
4	A	914	DG3	C3'-C2'-C1'	-2.17	100.28	102.71
4	A	914	DG3	C2'-C3'-C4'	-2.05	98.59	102.59
4	A	914	DG3	C6-N1-C2	2.40	119.27	115.94
4	A	914	DG3	O4'-C4'-C5'	2.40	113.09	109.54
4	A	914	DG3	C3'-C4'-C5'	2.93	127.98	116.05
4	A	914	DG3	O4'-C1'-N9	3.26	113.37	107.72
4	A	914	DG3	O5'-PA-O1A	3.84	124.54	109.62

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
4	A	914	DG3	1	0

## 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, 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	768/786 (97%)	0.44	19 (2%) 61 67	22, 31, 45, 67	0
2	T	19/20 (95%)	0.37	0 100 100	26, 33, 64, 81	0
3	P	13/13 (100%)	0.25	0 100 100	25, 35, 56, 57	0
All	All	800/819 (97%)	0.44	19 (2%) 62 68	22, 31, 47, 81	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	ASN	6.2
1	A	307	ILE	5.3
1	A	304	GLY	3.7
1	A	94	LYS	3.2
1	A	1	MET	3.1
1	A	-1	PRO	2.8
1	A	131	HIS	2.7
1	A	87	ARG	2.7
1	A	130	MET	2.6
1	A	625	ASP	2.6
1	A	608	GLY	2.6
1	A	306	SER	2.5
1	A	258	HIS	2.5
1	A	765	LEU	2.4
1	A	558	SER	2.4
1	A	265	PHE	2.4
1	A	134	THR	2.1
1	A	609	ALA	2.1
1	A	0	HIS	2.1

## 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	3DR	T	806	11/12	0.94	0.13	-	29,32,32,33	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	DG3	A	914	30/30	0.90	0.16	0.34	23,33,43,44	0
5	CA	A	1001	1/1	0.99	0.10	-2.09	32,32,32,32	0
5	CA	A	1002	1/1	0.84	0.09	-	59,59,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.