



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:33 AM GMT

PDB ID : 2R8H  
Title : Selectivity of Nucleoside Triphosphate Incorporation Opposite 1,N2-Propano deoxyguanosine (PdG) by the Sulfolobus solfataricus DNA Polymerase Dpo4 Polymerase  
Authors : Wang, Y.; Saleh, S.; Marnette, L.J.; Egli, M.; Stone, M.P.  
Deposited on : 2007-09-10  
Resolution : 2.48 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.

---

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

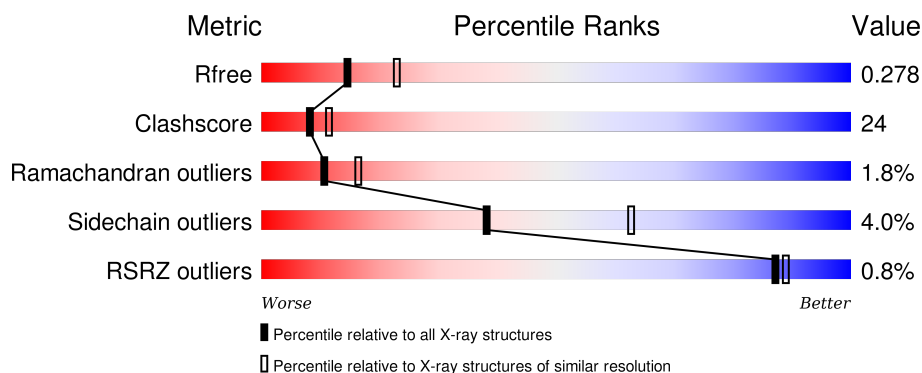
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


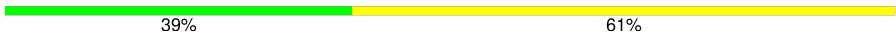

The reported resolution of this entry is 2.48 Å.

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	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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	P	13	
2	T	18	
3	A	352	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3490 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 DNA (5'-D(\*DGP\*DGP\*DGP\*DGP\*DGP\*DAP\*DAP\*DGP\*DGP\*DAP\*DTP\*DTP\*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	13	Total	C	N	O	P	0	0	0
			273	129	57	75	12			

- Molecule 2 is a DNA chain called DNA (5'-D(\*DTP\*DCP\*DAP\*DCP\*(P)P\*DGP\*DAP\*DAP\*DTP\*DCP\*DCP\*DTP\*DTP\*DCP\*DCP\*DCP\*DCP\*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	18	Total	C	N	O	P	0	0	1
			342	164	58	103	17			

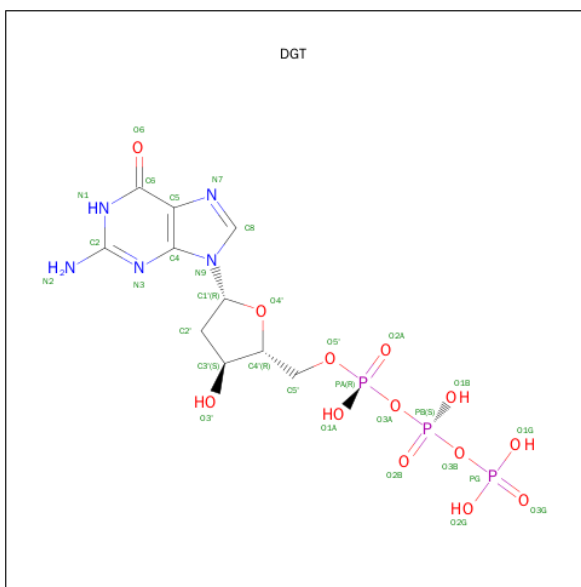
- Molecule 3 is a protein called DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	341	Total	C	N	O	S	0	0	0
			2743	1760	472	504	7			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		

- Molecule 5 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	61	Total O 61 61	0	0
6	P	22	Total O 22 22	0	0
6	T	15	Total O 15 15	0	0



- Molecule 1: DNA (5'-D(\*DGP\*DGP\*DGP\*DGP\*DGP\*DAP\*DAP\*DGP\*DGP\*DAP\*DTP\*DT\*DC)-3')

Diagram of a 1D lattice with 13 sites. Sites 1-5 are green, 6-8 are orange, 9 is yellow, 10 is green, 11 is yellow, 12 is orange, and 13 is green. Sites 1, 6, 9, 11, and 13 are occupied by particles (black dots).

T601	C602	A603	C604	G605	G606		T609	C610	C611	T612	T613	C614		C618
------	------	------	------	------	------	--	------	------	------	------	------	------	--	------

M1	I2	V3	F8	D9	Y10	F11	Q14	C31	V32	R36	F37	S40	V43	A44	T45	R51	V55	K56	A57	G58	I59	I61	V62	E63	K66	I67	L68	A71	V72	Y73	E79	V80	Q83	V84	M89	E97	K98	L109	D110	K114	V115	P116
----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------

D117	R118	R119	E120	A121	Y122	N123		I127	I128	K129	H130	K131	I132	I133		K137	I138	I139	V140		I144	S145		D156		K159	P160	N161		V165		E170		L173	L174	I175	R176	K177	D178	I179	I180		I186	G187		A191	E192		K195		I199	N200	K201		T205	L206	S207	I208
------	------	------	------	------	------	------	--	------	------	------	------	------	------	------	--	------	------	------	------	--	------	------	--	------	--	------	------	------	--	------	--	------	--	------	------	------	------	------	------	------	------	--	------	------	--	------	------	--	------	--	------	------	------	--	------	------	------	------

D211	M216	I217	K221	D231	E232	Y233	N234	E235	P236	L237	R238	T239	R240	V241	R242	S244	I245	T248	N254	S255	R256	N257	L258	K262	F266	E270	Y273	L276	D277	K278	R279	L280	V286	V287	A288	E291	D292	L293	D294	I295	V296	S297	R298	H304	G305
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

K308	A311	Y312	S313	V316	K317	L318	Q320	K321	E325	D326	K329	G334	I341	GLU	ALA	ILE	GLY	LEU	ASP	LYS	PHE	ASP	THR
------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.40 Å 103.00 Å 52.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.48 45.96 – 2.29	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.48) 65.5 (45.96-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.96 (at 2.29 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.215 , 0.279 0.218 , 0.278	Depositor DCC
$R_{free}$ test set	738 reflections (5.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.6	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 37.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 15421 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3490	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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: P, CA, DGT

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	P	0.69	0/308	0.77	0/476
2	T	0.80	1/351 (0.3%)	0.82	0/535
3	A	0.40	0/2782	0.61	0/3736
All	All	0.49	1/3441 (0.0%)	0.66	0/4747

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	2	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	601	DT	O3'-P	-6.92	1.52	1.61

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	P	502	DG	C4',C3'

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	P	273	0	147	9	0
2	T	342	0	195	14	0
3	A	2743	0	2889	137	0
4	A	3	0	0	0	0
5	A	31	0	12	3	0
6	A	61	0	0	40	0
6	P	22	0	0	5	0
6	T	15	0	0	2	0
All	All	3490	0	3243	162	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 24.

All (162) 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)
3:A:114:LYS:H	3:A:114:LYS:HD2	1.21	1.02
3:A:14:GLN:HB3	6:A:9327:HOH:O	1.64	0.97
3:A:144:ILE:HA	6:A:9059:HOH:O	1.67	0.92
3:A:63:GLU:HB3	6:A:9215:HOH:O	1.71	0.91
3:A:296:VAL:HB	6:A:9122:HOH:O	1.71	0.90
3:A:341:ILE:HB	6:A:9212:HOH:O	1.74	0.88
3:A:14:GLN:HE22	3:A:139:THR:H	1.23	0.86
1:P:503:DG:H2''	1:P:504:DG:H5'	1.58	0.85
3:A:291:GLU:HA	6:A:9226:HOH:O	1.77	0.84
3:A:59:ILE:HB	6:A:9215:HOH:O	1.79	0.81
2:T:602:DC:N4	6:T:9323:HOH:O	2.13	0.80
3:A:288:ALA:HB3	6:A:9122:HOH:O	1.83	0.78
3:A:83:GLN:N	3:A:83:GLN:HE21	1.84	0.75
3:A:109:LEU:HD22	6:A:9317:HOH:O	1.86	0.74
3:A:45:THR:HG21	6:A:9052:HOH:O	1.89	0.72
3:A:145:SER:O	6:A:9222:HOH:O	2.08	0.72
3:A:14:GLN:NE2	3:A:139:THR:H	1.87	0.72
1:P:509:DG:N3	6:P:9309:HOH:O	2.22	0.71
3:A:3:VAL:O	6:A:9059:HOH:O	2.08	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:266:PHE:O	3:A:270:GLU:HG2	1.92	0.70
3:A:110:ASP:HB2	3:A:237:ILE:HD12	1.74	0.69
3:A:14:GLN:HE22	3:A:139:THR:N	1.90	0.68
3:A:137:LYS:HA	3:A:137:LYS:HE2	1.74	0.68
1:P:504:DG:H2''	1:P:505:DG:OP2	1.94	0.68
3:A:55:VAL:HG21	3:A:68:LEU:HD12	1.76	0.67
3:A:118:TYR:HB3	3:A:165:VAL:HG11	1.75	0.67
3:A:109:LEU:HA	6:A:9317:HOH:O	1.94	0.67
3:A:123:ASN:HB2	6:A:9058:HOH:O	1.96	0.66
3:A:187:GLY:HA2	6:A:9311:HOH:O	1.96	0.66
3:A:273:TYR:HE1	6:A:9062:HOH:O	1.79	0.66
3:A:114:LYS:H	3:A:114:LYS:CD	1.98	0.65
2:T:603:DA:H2'	2:T:603:DA:N3	2.12	0.64
1:P:503:DG:C2'	1:P:504:DG:H5'	2.28	0.64
3:A:83:GLN:HE21	3:A:83:GLN:H	1.46	0.63
3:A:14:GLN:NE2	3:A:138:ILE:HA	2.14	0.63
2:T:602:DC:H2''	2:T:603:DA:H5'	1.80	0.63
3:A:138:ILE:HD12	6:A:9327:HOH:O	1.99	0.63
3:A:280:ILE:HD12	3:A:280:ILE:N	2.14	0.63
3:A:133:LEU:O	3:A:137:LYS:HE2	2.00	0.61
3:A:31:CYS:HB3	3:A:61:ILE:HD11	1.84	0.59
1:P:502:DG:H2''	1:P:503:DG:C8	2.37	0.59
3:A:258:LEU:O	3:A:262:LYS:HG3	2.02	0.59
3:A:116:ARG:HH11	3:A:116:ARG:HG2	1.67	0.59
3:A:238:ARG:HG2	3:A:239:THR:N	2.19	0.58
3:A:131:LYS:N	6:A:9066:HOH:O	2.37	0.58
3:A:280:ILE:HD12	3:A:280:ILE:H	1.67	0.57
1:P:509:DG:H1'	6:P:9309:HOH:O	2.02	0.57
3:A:2:ILE:HA	6:A:9222:HOH:O	2.04	0.57
3:A:291:GLU:OE1	3:A:329:LYS:HB2	2.04	0.57
3:A:120:GLU:C	6:A:9058:HOH:O	2.43	0.57
3:A:156:ASP:HA	3:A:159:LYS:HE3	1.86	0.57
2:T:610:DC:H5'	2:T:610:DC:H6	1.71	0.56
2:T:606:DG:OP2	2:T:606:DG:H2'	2.06	0.56
3:A:116:ARG:HB2	3:A:120:GLU:OE2	2.06	0.56
3:A:51:ARG:HD3	6:A:9214:HOH:O	2.04	0.56
3:A:255:SER:OG	3:A:256:ARG:N	2.38	0.56
3:A:127:GLU:O	3:A:131:LYS:HB2	2.06	0.55
3:A:258:LEU:CD2	3:A:320:GLN:HE21	2.18	0.55
3:A:258:LEU:HD21	3:A:320:GLN:HE21	1.71	0.55
3:A:313:SER:O	3:A:316:VAL:HG12	2.06	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3:VAL:N	6:A:9222:HOH:O	2.40	0.54
3:A:238:ARG:NH1	3:A:240:ARG:HA	2.21	0.54
3:A:123:ASN:N	6:A:9058:HOH:O	2.39	0.54
3:A:131:LYS:HG3	6:A:9119:HOH:O	2.07	0.54
3:A:14:GLN:CB	6:A:9327:HOH:O	2.39	0.54
3:A:36:ARG:O	3:A:37:PHE:HB3	2.06	0.54
3:A:1:MET:N	6:A:9219:HOH:O	2.41	0.54
3:A:207:SER:C	3:A:208:ILE:HD12	2.28	0.54
3:A:37:PHE:CD1	3:A:40:SER:HB3	2.43	0.53
3:A:14:GLN:HE22	3:A:138:ILE:HA	1.74	0.53
1:P:503:DG:C2'	6:P:9301:HOH:O	2.56	0.53
2:T:605:P:H5'	3:A:32:VAL:HG11	1.91	0.53
3:A:179:ASP:HB3	6:A:9217:HOH:O	2.09	0.52
3:A:316:VAL:O	3:A:320:GLN:HG3	2.10	0.52
3:A:286:VAL:HG21	3:A:318:LEU:HB2	1.91	0.52
3:A:119:ARG:C	3:A:119:ARG:HD3	2.29	0.52
3:A:270:GLU:OE2	3:A:312:TYR:OH	2.27	0.51
3:A:98:LYS:HB2	3:A:110:ASP:HB3	1.92	0.51
3:A:60:PRO:HD2	6:A:9215:HOH:O	2.10	0.51
3:A:129:LYS:NZ	3:A:161:ASN:OD1	2.40	0.51
6:T:9034:HOH:O	3:A:248:ILE:HB	2.10	0.51
3:A:144:ILE:HG23	6:A:9059:HOH:O	2.09	0.51
3:A:276:LEU:O	3:A:279:ARG:HB2	2.11	0.50
3:A:178:LEU:HD12	6:A:9217:HOH:O	2.10	0.50
2:T:609:DT:H2''	2:T:610:DC:C5'	2.41	0.50
2:T:605:P:H2'	2:T:606:DG:OP2	2.12	0.50
2:T:611:DC:H2'	2:T:612:DT:H71	1.93	0.50
3:A:195:LYS:HE2	6:A:9216:HOH:O	2.12	0.50
3:A:8:PHE:N	3:A:8:PHE:CD1	2.79	0.49
3:A:192:GLU:OE1	3:A:192:GLU:HA	2.10	0.49
5:A:7000:DGT:O1A	5:A:7000:DGT:H8	2.13	0.49
3:A:89:MET:HB2	6:A:9316:HOH:O	2.12	0.49
3:A:10:TYR:CE1	3:A:14:GLN:HB2	2.48	0.48
3:A:115:VAL:HG11	3:A:121:ALA:HB2	1.95	0.48
3:A:238:ARG:CZ	3:A:240:ARG:HA	2.43	0.48
3:A:9:ASP:O	3:A:10:TYR:C	2.51	0.48
3:A:217:ILE:HD12	3:A:221:LYS:HG2	1.95	0.48
3:A:14:GLN:OE1	3:A:139:THR:HG23	2.13	0.48
3:A:8:PHE:HA	3:A:140:VAL:HG12	1.95	0.48
3:A:137:LYS:CA	3:A:137:LYS:HE2	2.41	0.48
3:A:10:TYR:CD1	3:A:14:GLN:HB2	2.49	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:14:GLN:CD	3:A:139:THR:HG23	2.35	0.47
5:A:7000:DGT:O3B	5:A:7000:DGT:O2A	2.33	0.47
2:T:613:DT:H1'	2:T:614:DC:H5'	1.96	0.47
1:P:512:DT:H73	6:P:9308:HOH:O	2.14	0.47
3:A:235:GLU:OE2	3:A:236:PRO:HD2	2.15	0.47
2:T:611:DC:C2'	2:T:612:DT:H71	2.46	0.46
3:A:98:LYS:CB	3:A:110:ASP:HB3	2.46	0.46
3:A:242:ARG:HG2	3:A:242:ARG:HH11	1.81	0.45
3:A:199:ILE:HG21	3:A:205:THR:HG22	1.98	0.45
3:A:79:GLU:H	3:A:79:GLU:CD	2.19	0.45
3:A:176:ARG:O	3:A:201:LYS:HG2	2.16	0.45
3:A:116:ARG:N	3:A:120:GLU:OE2	2.50	0.45
3:A:123:ASN:O	3:A:127:GLU:HG3	2.16	0.45
3:A:308:LYS:HE2	3:A:312:TYR:CE2	2.52	0.45
3:A:233:TYR:CE1	3:A:235:GLU:HG2	2.51	0.45
3:A:14:GLN:NE2	3:A:138:ILE:HG23	2.32	0.45
3:A:31:CYS:HB3	3:A:61:ILE:CD1	2.47	0.45
5:A:7000:DGT:O3A	5:A:7000:DGT:H3'	2.17	0.44
3:A:114:LYS:O	3:A:115:VAL:HG23	2.17	0.44
3:A:187:GLY:CA	6:A:9311:HOH:O	2.60	0.44
3:A:14:GLN:HE22	3:A:138:ILE:CA	2.29	0.44
3:A:248:ILE:HA	3:A:334:GLY:HA3	2.00	0.44
1:P:505:DG:H5'	6:P:9045:HOH:O	2.17	0.44
3:A:114:LYS:N	3:A:114:LYS:HD2	2.06	0.44
3:A:308:LYS:O	3:A:311:ALA:HB3	2.18	0.44
2:T:602:DC:H2''	2:T:603:DA:C5'	2.48	0.43
3:A:133:LEU:O	3:A:137:LYS:HA	2.18	0.43
3:A:37:PHE:CE1	3:A:40:SER:HB3	2.52	0.43
3:A:43:VAL:O	3:A:57:ALA:HA	2.19	0.43
3:A:80:VAL:O	3:A:84:VAL:HG23	2.19	0.43
3:A:170:GLU:O	3:A:173:ARG:HG3	2.18	0.43
3:A:175:ILE:HG22	3:A:175:ILE:O	2.18	0.43
3:A:139:THR:OG1	3:A:161:ASN:HB2	2.19	0.43
2:T:609:DT:H2''	2:T:610:DC:H5''	1.99	0.42
3:A:180:ILE:CG2	6:A:9216:HOH:O	2.66	0.42
3:A:244:SER:O	3:A:245:ILE:HG13	2.19	0.42
3:A:60:PRO:N	6:A:9215:HOH:O	2.51	0.42
3:A:321:LYS:HG3	3:A:325:GLU:OE2	2.18	0.42
3:A:10:TYR:C	6:A:9052:HOH:O	2.56	0.42
3:A:60:PRO:CD	6:A:9215:HOH:O	2.67	0.42
3:A:71:ALA:HB3	3:A:73:TYR:CE2	2.55	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:44:ALA:O	3:A:45:THR:HB	2.20	0.42
3:A:292:ASP:OD1	3:A:294:ASP:HB2	2.19	0.41
3:A:296:VAL:HG13	3:A:298:ARG:HH12	1.84	0.41
3:A:36:ARG:HH12	3:A:254:ASN:ND2	2.19	0.41
3:A:195:LYS:NZ	3:A:200:ASN:ND2	2.68	0.41
3:A:115:VAL:HG12	3:A:116:ARG:N	2.35	0.41
3:A:9:ASP:O	3:A:11:PHE:N	2.54	0.41
3:A:116:ARG:NH1	3:A:116:ARG:HG2	2.35	0.41
3:A:3:VAL:HG22	3:A:237:ILE:HD11	2.02	0.41
3:A:109:LEU:CD2	6:A:9317:HOH:O	2.57	0.41
3:A:308:LYS:HE2	3:A:312:TYR:HE2	1.86	0.41
3:A:97:GLU:N	3:A:97:GLU:CD	2.74	0.41
3:A:304:HIS:CD2	3:A:305:GLY:O	2.74	0.41
3:A:308:LYS:HG2	3:A:312:TYR:CE2	2.56	0.41
3:A:270:GLU:CD	3:A:312:TYR:OH	2.60	0.40
3:A:62:VAL:HG12	3:A:66:LYS:HE3	2.02	0.40
3:A:133:LEU:HB3	6:A:9066:HOH:O	2.21	0.40
2:T:609:DT:C2'	2:T:610:DC:H5''	2.51	0.40
3:A:286:VAL:CG2	3:A:318:LEU:HB2	2.52	0.40
3:A:186:ILE:C	6:A:9042:HOH:O	2.59	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
3	A	339/352 (96%)	296 (87%)	37 (11%)	6 (2%)	11 16

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	10	TYR

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
3	A	114	LYS
3	A	231	ASP
3	A	37	PHE
3	A	131	LYS
3	A	161	ASN

### 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
3	A	300/309 (97%)	288 (96%)	12 (4%)	38 63

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	83	GLN
3	A	114	LYS
3	A	119	ARG
3	A	139	THR
3	A	177	GLU
3	A	192	GLU
3	A	211	ASP
3	A	216	MET
3	A	238	ARG
3	A	239	THR
3	A	278	LYS
3	A	326	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	14	GLN
3	A	70	ASN
3	A	83	GLN
3	A	123	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	A	130	ASN
3	A	188	ASN
3	A	200	ASN
3	A	254	ASN
3	A	320	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	P	T	605	2	19,28,29	2.16	2 (10%)	19,41,44	3.61	3 (15%)

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	P	T	605	2	-	0/3/28/29	0/3/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	605	P	C6A-N2	-6.29	1.38	1.45
2	T	605	P	C8A-N1	-6.27	1.39	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	605	P	C5-C6-N1	-13.89	112.34	120.52
2	T	605	P	C2-N3-C4	-2.23	112.40	115.09
2	T	605	P	C7A-C8A-N1	6.47	121.03	109.65

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
2	T	605	P	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 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	$\# Z  > 2$
5	DGT	A	7000	4	25,33,33	1.53	4 (16%)	35,52,52	2.17	11 (31%)

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	DGT	A	7000	4	-	0/18/34/34	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	7000	DGT	PA-O2A	2.80	1.61	1.51
5	A	7000	DGT	C2-N1	2.93	1.40	1.35
5	A	7000	DGT	PG-O3G	3.13	1.61	1.51
5	A	7000	DGT	C6-N1	4.03	1.40	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	7000	DGT	N3-C2-N1	-4.97	119.87	127.44
5	A	7000	DGT	PA-O3A-PB	-4.51	120.07	132.73
5	A	7000	DGT	O5'-PA-O2A	-3.92	94.40	109.62
5	A	7000	DGT	O3A-PA-O5'	-3.89	92.61	102.94
5	A	7000	DGT	C5-C6-N1	-3.35	119.01	123.59
5	A	7000	DGT	PB-O3B-PG	-2.86	123.07	132.67
5	A	7000	DGT	C2'-C3'-C4'	-2.47	97.65	102.77
5	A	7000	DGT	C4-C5-N7	-2.08	107.56	109.48
5	A	7000	DGT	O1G-PG-O3B	2.03	114.28	105.09
5	A	7000	DGT	C6-N1-C2	2.50	119.41	115.94
5	A	7000	DGT	O1A-PA-O3A	3.89	122.76	105.09

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	A	7000	DGT	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	P	13/13 (100%)	-0.67	0	100 100	40, 49, 66, 71	0
2	T	17/18 (94%)	-0.55	0	100 100	43, 59, 119, 122	0
3	A	341/352 (96%)	0.02	3 (0%)	85 88	33, 61, 83, 95	23 (6%)
All	All	371/383 (96%)	-0.03	3 (0%)	87 89	33, 61, 83, 122	23 (6%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	191	ALA	2.8
3	A	293	LEU	2.2
3	A	180	ILE	2.2

### 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	P	T	605	25/26	0.95	0.13	-	39,50,56,56	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	CA	A	8001	1/1	0.17	0.19	1.49	90,90,90,90	0
5	DGT	A	7000	31/31	0.92	0.16	0.12	24,42,48,49	20
4	CA	A	8003	1/1	0.95	0.12	-0.91	68,68,68,68	0
4	CA	A	8002	1/1	0.64	0.09	-	115,115,115,115	0

## 6.5 Other polymers

There are no such residues in this entry.