



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 01:43 am BST

PDB ID : 3GV8
Title : Human DNA polymerase iota in complex with T template DNA and incoming dGTP
Authors : Kirouac, K.N.; Ling, H.
Deposited on : 2009-03-30
Resolution : 2.00 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

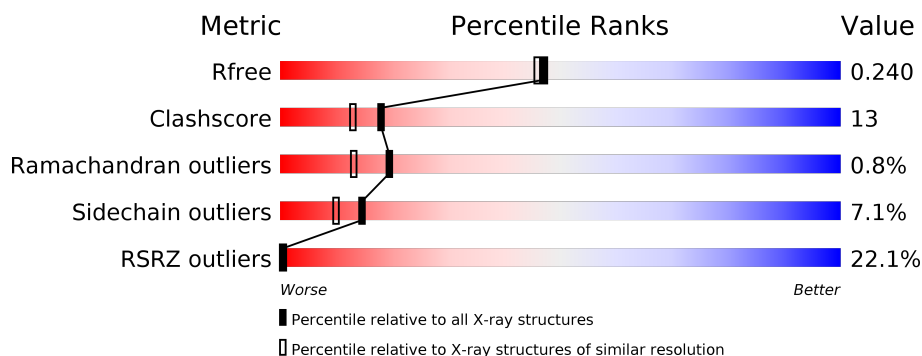
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	420	<div> <div>20%</div> <div> <div>70%</div> <div>15%</div> <div>• • 11%</div> </div> </div>
2	T	9	<div> <div>11%</div> <div> <div>78%</div> <div>22%</div> </div> </div>
3	P	7	<div> <div>29%</div> <div> <div>29%</div> <div>43%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DGT	B	421	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3496 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	B	374	Total	C	N	O	S	0	1	0
			2903	1845	504	533	21			

- Molecule 2 is a DNA chain called 5'-D(*AP*TP*GP*GP*GP*TP*CP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	9	Total	C	N	O	P	0	0	0
			181	88	32	53	8			

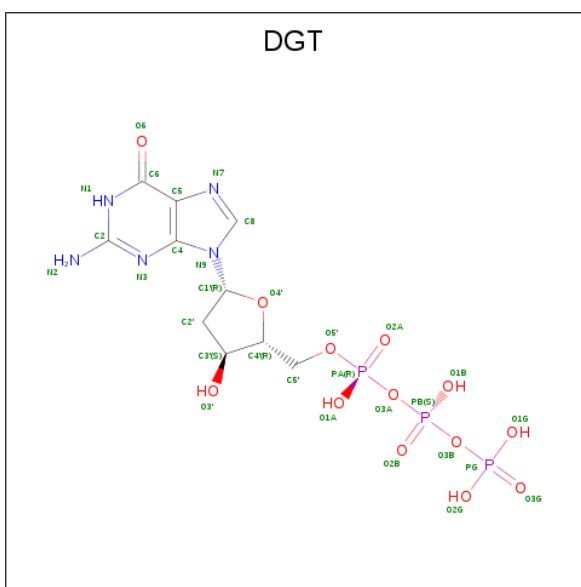
- Molecule 3 is a DNA chain called 5'-D(*AP*GP*GP*AP*CP*CP*C)-3'.

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mg	0	0
			2	2		

- Molecule 5 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

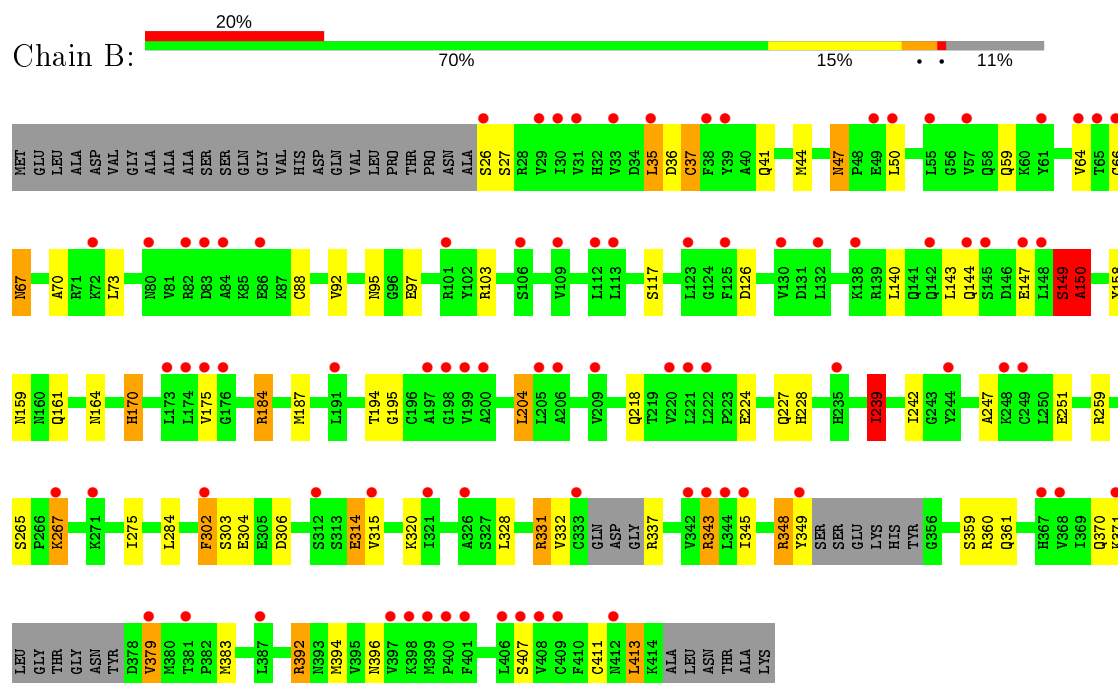
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	210	Total O 210 210	0	0
6	T	19	Total O 19 19	0	0
6	P	11	Total O 11 11	0	0

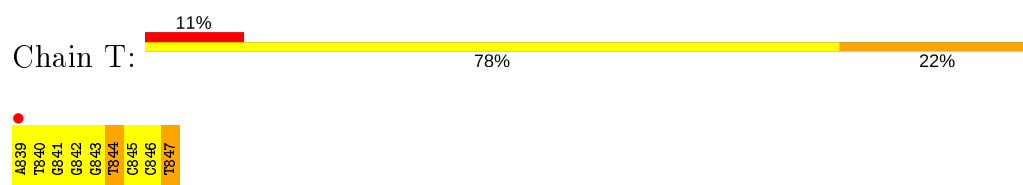
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

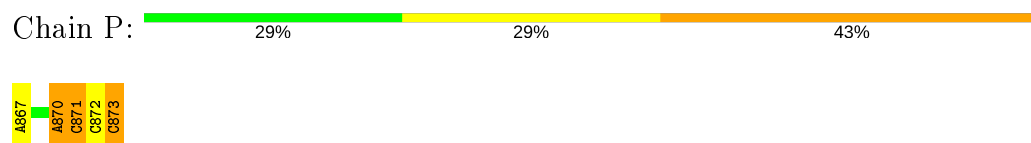
- Molecule 1: DNA polymerase iota



- Molecule 2: 5'-D(*AP*TP*GP*GP*GP*TP*CP*CP*T)-3'



- Molecule 3: 5'-D(*AP*GP*GP*AP*CP*CP*C)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.07Å 98.07Å 203.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.84 – 2.00 23.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (23.84-2.00) 99.6 (23.83-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.56 (at 1.99Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.218 , 0.248 0.215 , 0.240	Depositor DCC
R_{free} test set	826 reflections (2.08%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3496	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, 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	B	0.88	4/2946 (0.1%)	0.98	16/3981 (0.4%)
2	T	1.42	0/202	2.24	14/311 (4.5%)
3	P	1.29	0/156	1.72	4/238 (1.7%)
All	All	0.94	4/3304 (0.1%)	1.16	34/4530 (0.8%)

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	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	379	VAL	CA-CB	10.38	1.76	1.54
1	B	383	MET	CG-SD	6.96	1.99	1.81
1	B	314	GLU	CD-OE2	6.93	1.33	1.25
1	B	392	ARG	CG-CD	5.10	1.64	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	ARG	NE-CZ-NH1	-16.52	112.04	120.30
1	B	184	ARG	NE-CZ-NH1	-15.29	112.66	120.30
1	B	184	ARG	NE-CZ-NH2	14.39	127.50	120.30
1	B	259	ARG	NE-CZ-NH2	14.30	127.45	120.30
1	B	331	ARG	NE-CZ-NH2	-11.24	114.68	120.30
2	T	847	DT	O4'-C1'-N1	-10.26	100.81	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	392	ARG	NE-CZ-NH2	-8.84	115.88	120.30
2	T	846	DC	O4'-C1'-N1	-7.08	103.04	108.00
2	T	842	DG	C4-C5-N7	-6.88	108.05	110.80
1	B	259	ARG	CD-NE-CZ	6.87	133.22	123.60
1	B	204	LEU	CB-CG-CD2	6.86	122.66	111.00
3	P	870	DA	O4'-C1'-N9	6.85	112.79	108.00
1	B	331	ARG	NE-CZ-NH1	6.39	123.49	120.30
3	P	872	DC	O4'-C4'-C3'	-6.07	102.07	104.50
3	P	871	DC	O4'-C4'-C3'	-5.90	102.14	104.50
3	P	873	DC	O4'-C1'-N1	5.88	112.11	108.00
2	T	842	DG	O5'-P-OP2	-5.84	100.44	105.70
2	T	842	DG	N1-C6-O6	-5.82	116.41	119.90
2	T	844	DT	O4'-C1'-N1	5.68	111.97	108.00
1	B	184	ARG	CD-NE-CZ	5.55	131.37	123.60
1	B	306	ASP	CB-CG-OD1	5.54	123.28	118.30
1	B	239	ILE	CG1-CB-CG2	5.53	123.56	111.40
2	T	841	DG	O4'-C1'-N9	5.51	111.86	108.00
2	T	844	DT	N3-C4-O4	-5.51	116.59	119.90
2	T	842	DG	O5'-P-OP1	5.45	117.24	110.70
1	B	150	ALA	N-CA-C	5.42	125.63	111.00
1	B	149	SER	N-CA-C	5.36	125.48	111.00
1	B	259	ARG	CG-CD-NE	-5.31	100.65	111.80
2	T	842	DG	C5-C6-O6	5.30	131.78	128.60
2	T	841	DG	P-O3'-C3'	5.12	125.85	119.70
1	B	315	VAL	O-C-N	-5.09	114.56	122.70
2	T	843	DG	C3'-C2'-C1'	-5.05	96.44	102.50
2	T	842	DG	O4'-C1'-C2'	5.05	109.94	105.90
2	T	844	DT	O4'-C1'-C2'	5.01	109.91	105.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	149	SER	Peptide

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	2903	0	2942	67	0
2	T	181	0	101	8	1
3	P	139	0	77	4	0
4	B	2	0	0	0	0
5	B	31	0	12	13	0
6	B	210	0	0	12	0
6	P	11	0	0	1	1
6	T	19	0	0	0	0
All	All	3496	0	3132	86	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 13.

All (86) 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:B:379:VAL:CB	1:B:379:VAL:CA	1.76	1.56
5:B:421:DGT:H5'A	5:B:421:DGT:H8	1.25	1.16
5:B:421:DGT:H5'A	5:B:421:DGT:C8	1.76	1.16
5:B:421:DGT:O2A	6:B:632:HOH:O	1.68	1.10
5:B:421:DGT:H4'	6:B:631:HOH:O	1.60	0.99
3:P:867:DA:O5'	6:P:115:HOH:O	1.61	0.91
1:B:164:ASN:H	1:B:170:HIS:HD2	1.17	0.91
5:B:421:DGT:H8	5:B:421:DGT:C5'	2.04	0.86
1:B:41:GLN:HE22	1:B:194:THR:H	1.25	0.82
1:B:239:ILE:CD1	1:B:284:LEU:HB3	2.10	0.81
5:B:421:DGT:N2	2:T:840:DT:O2	2.14	0.81
5:B:421:DGT:C4'	6:B:631:HOH:O	2.23	0.77
1:B:239:ILE:HD12	1:B:284:LEU:HB3	1.68	0.76
1:B:267:LYS:H	1:B:267:LYS:HD2	1.49	0.76
1:B:117:SER:OG	6:B:626:HOH:O	2.05	0.75
1:B:161:GLN:NE2	1:B:224:GLU:HG2	2.03	0.73
1:B:331:ARG:CD	6:B:544:HOH:O	2.39	0.71
1:B:247:ALA:O	1:B:251:GLU:HG3	1.94	0.68
1:B:379:VAL:CG1	1:B:379:VAL:CA	2.72	0.67
1:B:164:ASN:H	1:B:170:HIS:CD2	2.08	0.67
1:B:331:ARG:HD2	6:B:544:HOH:O	1.96	0.66
1:B:304:GLU:OE2	6:B:457:HOH:O	2.12	0.66
1:B:343:ARG:HH21	1:B:361:GLN:HE22	1.46	0.64
1:B:302[A]:PHE:N	1:B:302[A]:PHE:HD1	1.97	0.62
1:B:302[A]:PHE:CD1	1:B:302[A]:PHE:N	2.69	0.61
1:B:67:ASN:HD22	1:B:67:ASN:C	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:VAL:CG2	1:B:379:VAL:CA	2.73	0.60
1:B:379:VAL:N	1:B:379:VAL:CB	2.59	0.59
1:B:184:ARG:HH11	1:B:218:GLN:HE21	1.49	0.58
1:B:267:LYS:H	1:B:267:LYS:CD	2.16	0.58
5:B:421:DGT:C8	3:P:873:DC:H2'	2.33	0.58
2:T:839:DA:H3'	2:T:840:DT:H72	1.86	0.57
1:B:328:LEU:O	1:B:332:VAL:HG23	2.05	0.57
1:B:345:ILE:HB	1:B:407:SER:HB3	1.86	0.57
1:B:239:ILE:CD1	1:B:284:LEU:CB	2.83	0.57
1:B:239:ILE:HD11	1:B:284:LEU:CB	2.35	0.57
1:B:348:ARG:O	1:B:349:TYR:HB2	2.05	0.57
1:B:159:ASN:OD1	6:B:497:HOH:O	2.17	0.56
1:B:239:ILE:HD11	1:B:284:LEU:HB3	1.87	0.56
1:B:144:GLN:O	1:B:147:GLU:HG2	2.06	0.55
1:B:170:HIS:HE1	1:B:224:GLU:OE2	1.91	0.54
1:B:337:ARG:NH2	1:B:413:LEU:HD23	2.23	0.53
5:B:421:DGT:H8	3:P:873:DC:H2'	1.89	0.53
1:B:239:ILE:HG12	1:B:242:ILE:HD12	1.91	0.53
1:B:161:GLN:HE22	1:B:224:GLU:HG2	1.71	0.53
1:B:348:ARG:O	1:B:349:TYR:CB	2.56	0.53
5:B:421:DGT:C2	2:T:840:DT:O2	2.58	0.52
1:B:50:LEU:HD22	1:B:92:VAL:HG11	1.92	0.52
1:B:343:ARG:HH21	1:B:361:GLN:NE2	2.06	0.51
5:B:421:DGT:H16	2:T:840:DT:H3	1.59	0.51
1:B:331:ARG:HD3	6:B:544:HOH:O	2.06	0.51
1:B:158:TYR:OH	1:B:228:HIS:HD2	1.94	0.50
1:B:35:LEU:HD23	6:B:442:HOH:O	2.12	0.50
1:B:184:ARG:HA	1:B:187:MET:HE3	1.94	0.49
1:B:149:SER:HB3	6:B:598:HOH:O	2.11	0.49
1:B:184:ARG:HD2	1:B:195:GLY:O	2.13	0.49
1:B:95:ASN:HD21	1:B:97:GLU:HB2	1.77	0.49
1:B:379:VAL:C	1:B:379:VAL:CB	2.74	0.48
5:B:421:DGT:N1	2:T:840:DT:O2	2.47	0.48
2:T:839:DA:H2'	2:T:840:DT:C6	2.49	0.48
1:B:73:LEU:HD12	1:B:88:CYS:SG	2.54	0.47
1:B:67:ASN:ND2	1:B:70:ALA:H	2.13	0.47
1:B:44:MET:HE1	1:B:67:ASN:OD1	2.14	0.46
1:B:303:SER:O	1:B:331:ARG:NH2	2.48	0.46
1:B:59:GLN:OE1	1:B:64:VAL:HG11	2.16	0.46
3:P:870:DA:H2'	3:P:871:DC:C6	2.51	0.46
1:B:47:ASN:HD22	1:B:47:ASN:C	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ASP:O	1:B:37:CYS:C	2.55	0.45
5:B:421:DGT:C5'	5:B:421:DGT:C8	2.68	0.45
1:B:184:ARG:HA	1:B:187:MET:CE	2.46	0.45
2:T:844:DT:H2''	2:T:845:DC:H5'	1.98	0.45
1:B:103:ARG:CZ	1:B:331:ARG:HD3	2.48	0.44
1:B:147:GLU:H	1:B:147:GLU:HG2	1.68	0.44
1:B:66:CYS:HB2	1:B:70:ALA:HB3	2.00	0.43
1:B:95:ASN:ND2	1:B:97:GLU:H	2.16	0.43
1:B:314:GLU:OE1	1:B:392:ARG:NH1	2.52	0.43
1:B:302[B]:PHE:CE2	1:B:413:LEU:HD21	2.53	0.42
1:B:73:LEU:HD23	1:B:73:LEU:N	2.35	0.42
1:B:147:GLU:O	1:B:150:ALA:HB3	2.20	0.41
1:B:359:SER:O	1:B:360:ARG:HD3	2.20	0.41
1:B:44:MET:CE	1:B:67:ASN:OD1	2.68	0.41
2:T:844:DT:H2'	2:T:845:DC:C6	2.56	0.41
1:B:140:LEU:HD21	1:B:175:VAL:HG21	2.02	0.41
1:B:35:LEU:CD2	6:B:442:HOH:O	2.69	0.40
1:B:302[B]:PHE:HE2	1:B:413:LEU:HD21	1.87	0.40
1:B:67:ASN:ND2	1:B:67:ASN:C	2.73	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:T:847:DT:O3'	6:P:115:HOH:O[12_544]	1.80	0.40

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	B	367/420 (87%)	357 (97%)	7 (2%)	3 (1%)	19 13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	150	ALA
1	B	370	GLN
1	B	37	CYS

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	B	324/376 (86%)	300 (93%)	24 (7%)	13 9

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	26	SER
1	B	27	SER
1	B	35	LEU
1	B	47	ASN
1	B	67	ASN
1	B	126	ASP
1	B	143	LEU
1	B	170	HIS
1	B	204	LEU
1	B	227	GLN
1	B	239	ILE
1	B	265	SER
1	B	267	LYS
1	B	275	ILE
1	B	302[A]	PHE
1	B	302[B]	PHE
1	B	320	LYS
1	B	343	ARG
1	B	348	ARG
1	B	371	LYS
1	B	394	MET
1	B	396	ASN

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Mol	Chain	Res	Type
1	B	411	CYS
1	B	413	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	41	GLN
1	B	47	ASN
1	B	95	ASN
1	B	156	HIS
1	B	170	HIS
1	B	189	ASN
1	B	217	GLN
1	B	218	GLN
1	B	228	HIS
1	B	361	GLN
1	B	396	ASN
1	B	402	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
5	DGT	B	421	4	26,33,33	1.10	2 (7%)	32,52,52	1.81	9 (28%)

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	B	421	4	-	9/18/34/34	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	421	DGT	C6-N1	3.41	1.39	1.33
5	B	421	DGT	C2-N1	2.59	1.40	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	421	DGT	N3-C2-N1	-4.65	121.03	127.22
5	B	421	DGT	C5-C6-N1	-3.85	118.17	123.43
5	B	421	DGT	O3'-C3'-C2'	3.42	123.12	110.90
5	B	421	DGT	C2-N3-C4	3.16	118.97	115.36
5	B	421	DGT	C6-N1-C2	2.97	120.65	115.93
5	B	421	DGT	O2G-PG-O3B	2.50	113.01	104.64
5	B	421	DGT	PB-O3B-PG	-2.34	124.81	132.83
5	B	421	DGT	O4'-C4'-C3'	2.27	110.97	105.67
5	B	421	DGT	C5'-C4'-C3'	-2.11	102.34	114.74

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	421	DGT	PB-O3B-PG-O2G
5	B	421	DGT	C5'-O5'-PA-O3A
5	B	421	DGT	C3'-C4'-C5'-O5'
5	B	421	DGT	PA-O3A-PB-O1B

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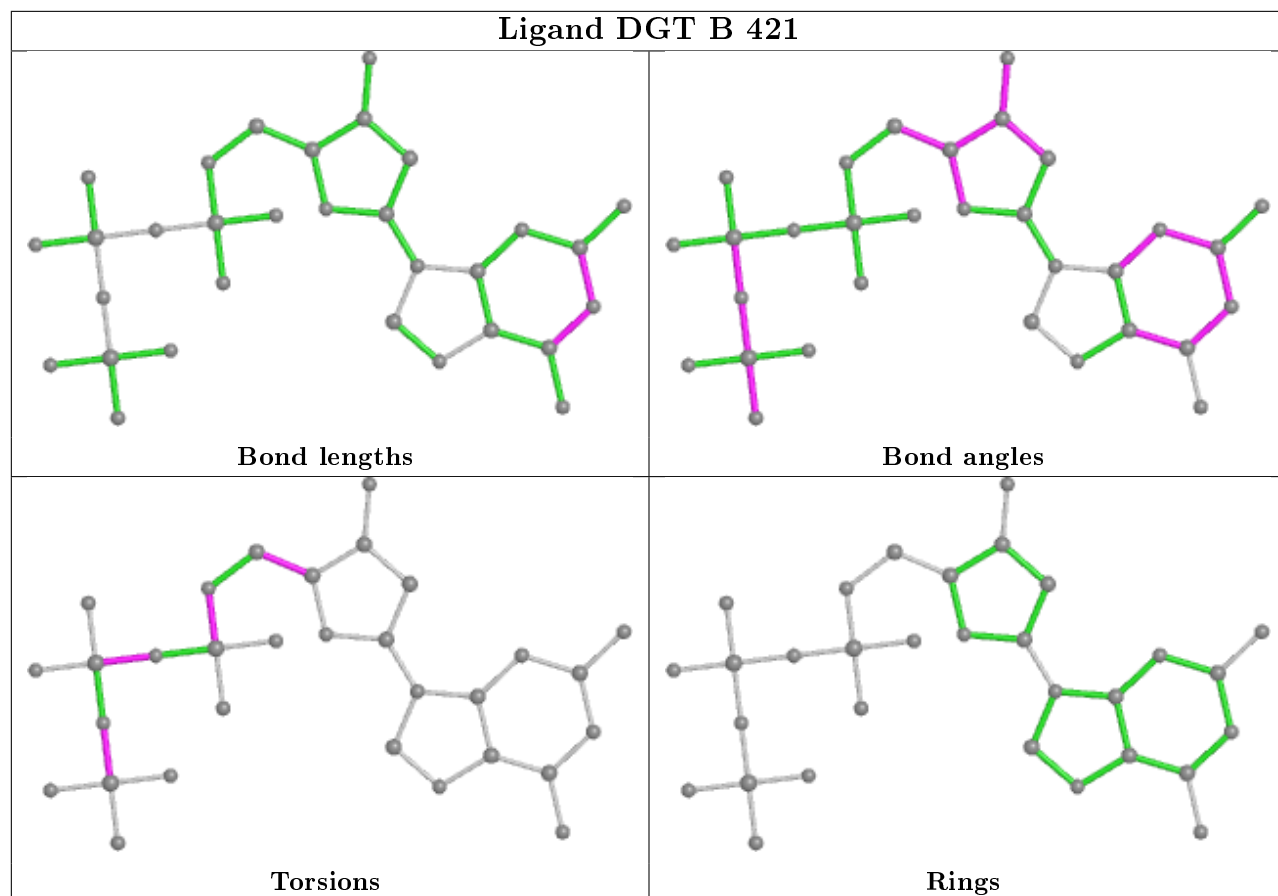
Mol	Chain	Res	Type	Atoms
5	B	421	DGT	C5'-O5'-PA-O1A
5	B	421	DGT	C5'-O5'-PA-O2A
5	B	421	DGT	O4'-C4'-C5'-O5'
5	B	421	DGT	PA-O3A-PB-O2B
5	B	421	DGT	PB-O3B-PG-O3G

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	421	DGT	13	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 95th 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 ²)	Q<0.9
1	B	374/420 (89%)	1.09	85 (22%) 0 0	28, 42, 60, 65	0
2	T	9/9 (100%)	0.23	1 (11%) 5 4	33, 39, 62, 84	0
3	P	7/7 (100%)	-0.16	0 100 100	34, 39, 50, 54	0
All	All	390/436 (89%)	1.05	86 (22%) 0 0	28, 42, 60, 84	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	399	MET	7.6
1	B	333	CYS	5.8
1	B	199	VAL	5.6
1	B	244	TYR	5.6
1	B	349	TYR	5.4
1	B	398	LYS	5.3
1	B	401	PHE	5.1
1	B	173	LEU	4.6
1	B	33	VAL	4.5
1	B	86	GLU	4.4
1	B	221	LEU	4.4
1	B	387	LEU	4.4
1	B	26	SER	4.2
1	B	400	PRO	4.2
1	B	345	ILE	4.1
2	T	839	DA	4.0
1	B	83	ASP	4.0
1	B	61	TYR	4.0
1	B	31	VAL	3.9
1	B	82	ARG	3.8
1	B	109	VAL	3.7
1	B	220	VAL	3.7
1	B	367	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	148	LEU	3.6
1	B	397	VAL	3.5
1	B	381	THR	3.4
1	B	49	GLU	3.4
1	B	38	PHE	3.4
1	B	312	SER	3.3
1	B	147	GLU	3.2
1	B	408	VAL	3.2
1	B	409	CYS	3.1
1	B	176	GLY	3.0
1	B	344	LEU	3.0
1	B	84	ALA	3.0
1	B	342	VAL	3.0
1	B	200	ALA	3.0
1	B	406	LEU	2.9
1	B	29	VAL	2.9
1	B	39	TYR	2.9
1	B	145	SER	2.9
1	B	315	VAL	2.9
1	B	65	THR	2.9
1	B	175	VAL	2.8
1	B	138	LYS	2.8
1	B	50	LEU	2.8
1	B	371	LYS	2.7
1	B	209	VAL	2.7
1	B	66	CYS	2.6
1	B	249	CYS	2.6
1	B	222	LEU	2.6
1	B	407	SER	2.6
1	B	198	GLY	2.6
1	B	144	GLN	2.5
1	B	412	ASN	2.5
1	B	35	LEU	2.5
1	B	132	LEU	2.5
1	B	321	ILE	2.5
1	B	206	ALA	2.5
1	B	80	ASN	2.5
1	B	379	VAL	2.4
1	B	142	GLN	2.4
1	B	64	VAL	2.4
1	B	123	LEU	2.4
1	B	125	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	191	LEU	2.3
1	B	30	ILE	2.3
1	B	326	ALA	2.3
1	B	248	LYS	2.3
1	B	302[A]	PHE	2.3
1	B	113	LEU	2.2
1	B	267	LYS	2.2
1	B	343	ARG	2.2
1	B	106	SER	2.2
1	B	57	VAL	2.2
1	B	55	LEU	2.2
1	B	174	LEU	2.2
1	B	72	LYS	2.2
1	B	101	ARG	2.2
1	B	271	LYS	2.1
1	B	368	VAL	2.1
1	B	112	LEU	2.1
1	B	235	HIS	2.1
1	B	130	VAL	2.0
1	B	197	ALA	2.0
1	B	205	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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. The B-factors column lists the minimum, median, 95th 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.

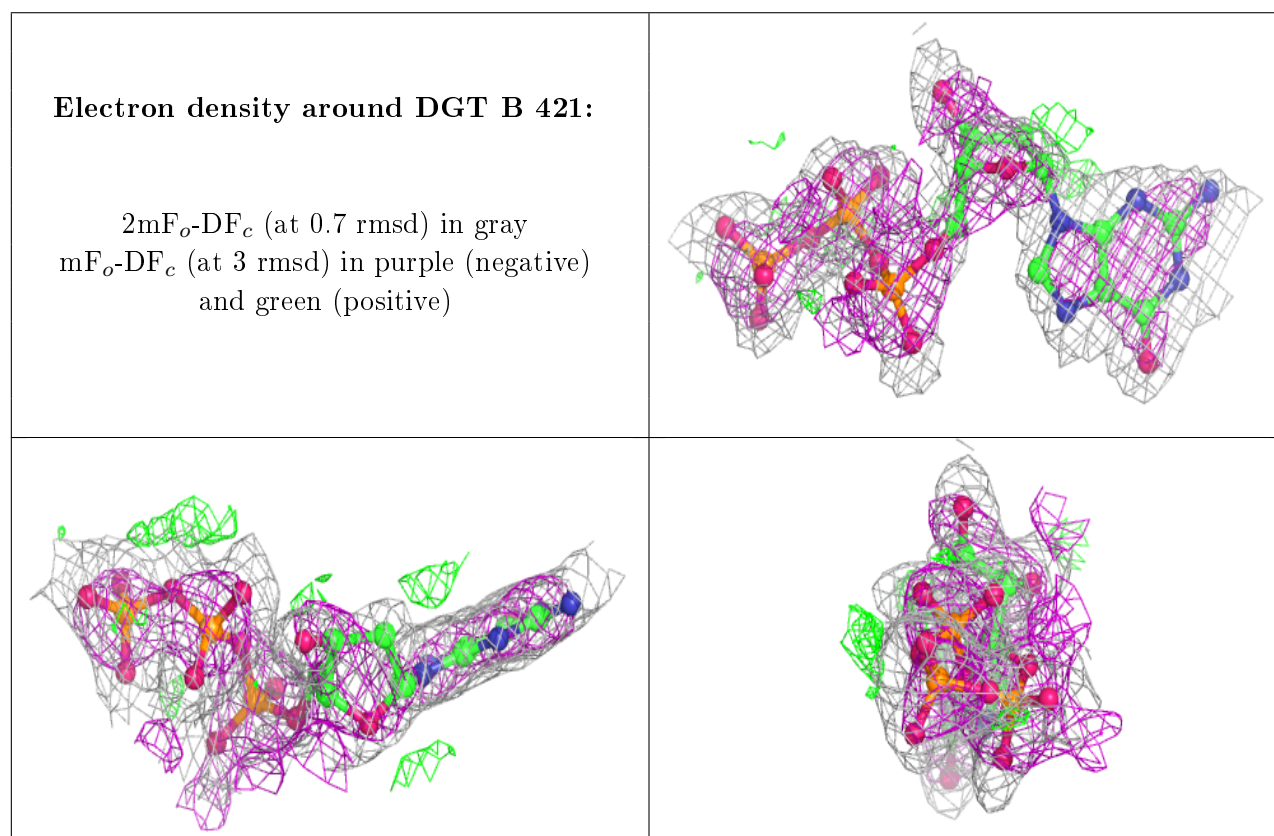
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	B	422	1/1	0.93	0.35	54,54,54,54	0
5	DGT	B	421	31/31	0.94	0.21	37,49,51,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	B	871	1/1	0.95	0.13	40,40,40,40	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.