



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:31 PM UTC

PDB ID : 3GV8 / pdb_00003gv8
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

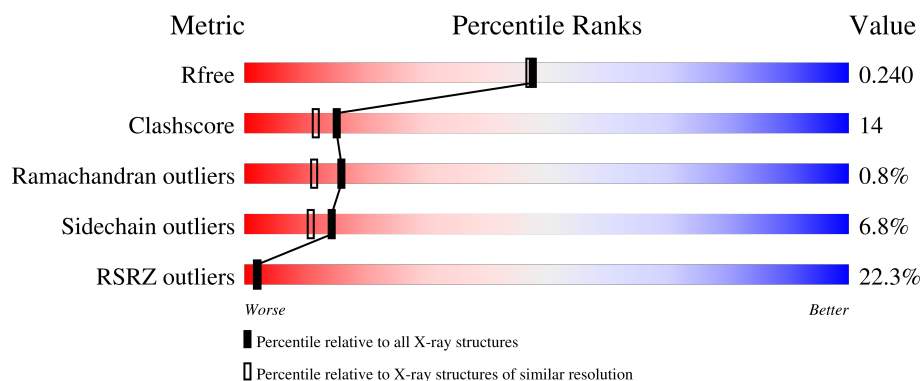
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of 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	20% 69% 17% • 11%
2	T	9	11% 33% 56% 11%
3	P	7	43% 57%

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			

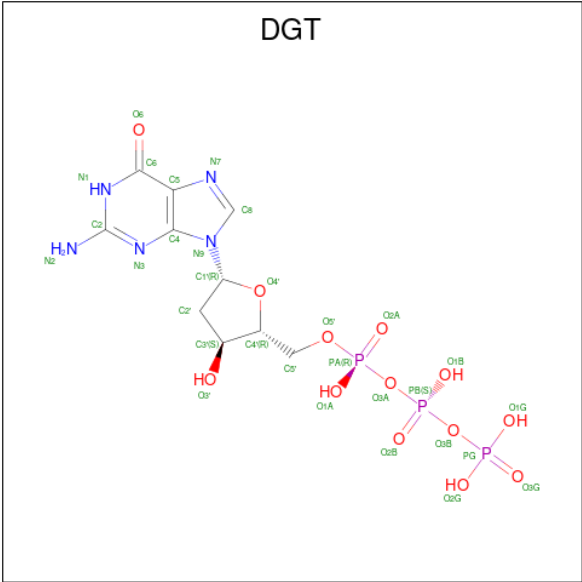
- Molecule 3 is a DNA chain called 5'-D(*AP*GP*GP*AP*CP*CP*C)-3'.

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 (CCD ID: 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 (CCD ID: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

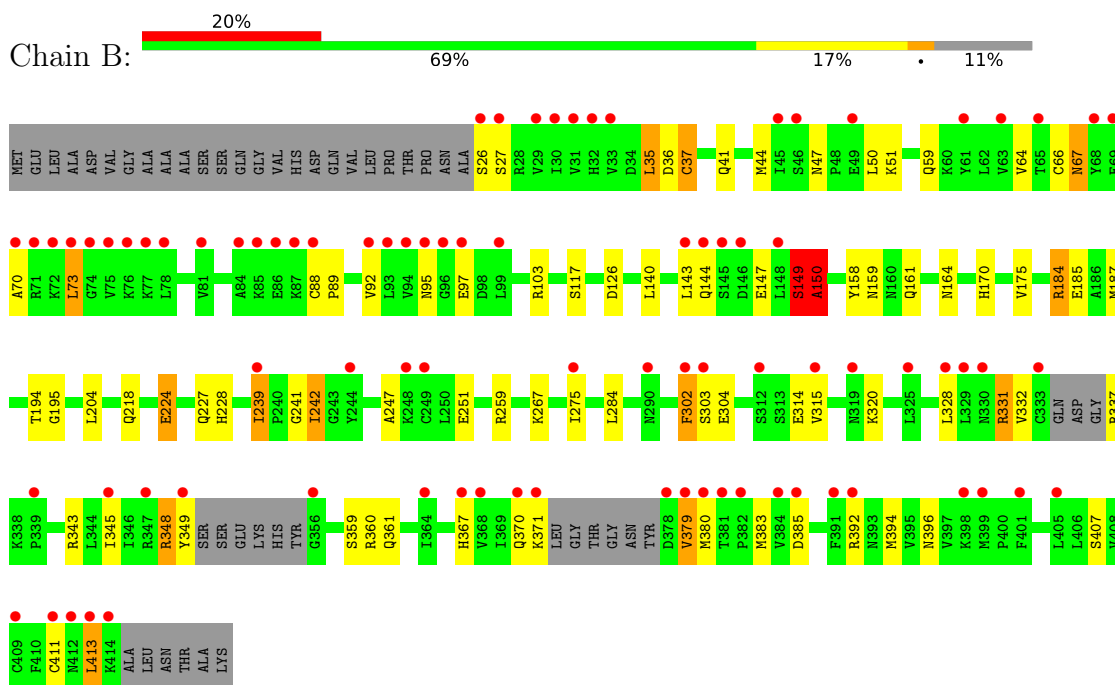
- Molecule 6 is water.

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

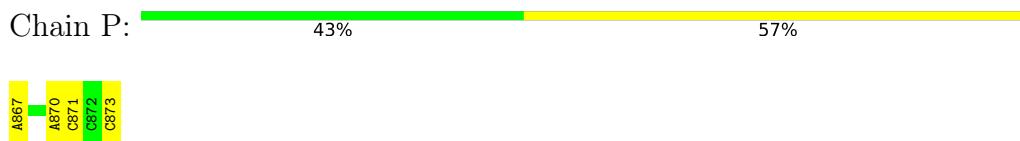
- Molecule 1: DNA polymerase iota



- 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 23.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (23.84-2.00) 99.4 (23.84-2.00)	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)	0.35 , 51.4	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	0.93	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: DGT, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	1.13	10/2946 (0.3%)	1.10	15/3981 (0.4%)
2	T	0.66	0/202	1.44	2/311 (0.6%)
3	P	0.62	0/156	1.13	0/238
All	All	1.08	10/3304 (0.3%)	1.12	17/4530 (0.4%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	379	VAL	CA-CB	17.44	1.76	1.54
1	B	367	HIS	CE1-NE2	10.42	1.43	1.32
1	B	383	MET	CG-SD	7.40	1.99	1.80
1	B	367	HIS	CG-ND1	6.99	1.46	1.38
1	B	89	PRO	C-O	6.12	1.32	1.24
1	B	367	HIS	CG-CD2	5.87	1.42	1.35
1	B	89	PRO	C-N	5.75	1.41	1.33
1	B	184	ARG	CD-NE	-5.67	1.38	1.46
1	B	242	ILE	CA-CB	5.17	1.60	1.53
1	B	385	ASP	C-N	5.11	1.40	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	ARG	NE-CZ-NH1	-9.46	112.04	121.50
1	B	184	ARG	NE-CZ-NH2	9.22	127.50	119.20
1	B	259	ARG	NE-CZ-NH2	9.16	127.45	119.20
1	B	184	ARG	NE-CZ-NH1	-8.84	112.66	121.50
1	B	149	SER	N-CA-C	7.78	125.48	113.19
1	B	315	VAL	CA-C-O	7.68	128.94	120.95
1	B	315	VAL	O-C-N	-7.54	114.56	121.87
1	B	150	ALA	N-CA-C	6.96	125.63	110.80
1	B	259	ARG	CD-NE-CZ	6.30	133.22	124.40
1	B	89	PRO	CA-C-O	5.85	127.72	118.89
2	T	843	DG	P-O5'-C5'	5.20	127.80	120.00
1	B	259	ARG	CG-CD-NE	-5.16	100.65	112.00
1	B	241	GLY	N-CA-C	-5.13	108.37	114.48
2	T	847	DT	O4'-C1'-N1	-5.06	100.81	108.40
1	B	149	SER	CA-C-N	5.04	131.16	121.54
1	B	149	SER	C-N-CA	5.04	131.16	121.54
1	B	331	ARG	NE-CZ-NH2	-5.02	114.68	119.20

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	68	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	87	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 14.

All (87) 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:CA	1:B:379:VAL:CB	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:HD2	1:B:267:LYS:H	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:184:ARG:HA	1:B:187:MET:HE3	1.71	0.72
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:CA	1:B:379:VAL:CG1	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:67:ASN:HD22	1:B:67:ASN:C	2.04	0.63
1:B:302[A]:PHE:HD1	1:B:302[A]:PHE:N	1.97	0.62
1:B:302[A]:PHE:N	1:B:302[A]:PHE:CD1	2.69	0.61
1:B:379:VAL:CA	1:B:379:VAL:CG2	2.73	0.60
1:B:379:VAL:CB	1:B:379:VAL:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:44:MET:HE3	1:B:67:ASN:OD1	2.04	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:379:VAL:CB	1:B:379:VAL:C	2.74	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:47:ASN:HD22	1:B:47:ASN:C	2.19	0.50
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:36:ASP:O	1:B:37:CYS:C	2.55	0.50
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
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:67:ASN:C	1:B:67:ASN:ND2	2.73	0.46
1:B:44:MET:HE2	1:B:51:LYS:HA	1.97	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
5:B:421:DGT:C8	5:B:421:DGT:C5'	2.68	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:HG2	1:B:147:GLU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LEU:N	1:B:73:LEU:HD23	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
1:B:184:ARG:HA	1:B:187:MET:CE	2.46	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

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%)	16 11

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%)	301 (93%)	23 (7%)	13	10

All (23) 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	67	ASN
1	B	73	LEU
1	B	126	ASP
1	B	143	LEU
1	B	185	GLU
1	B	204	LEU
1	B	224	GLU
1	B	227	GLN
1	B	239	ILE
1	B	275	ILE
1	B	302[A]	PHE
1	B	302[B]	PHE
1	B	320	LYS
1	B	348	ARG
1	B	371	LYS
1	B	380	MET
1	B	394	MET
1	B	396	ASN
1	B	411	CYS
1	B	413	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	41	GLN
1	B	47	ASN

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Mol	Chain	Res	Type
1	B	95	ASN
1	B	128	ASN
1	B	156	HIS
1	B	161	GLN
1	B	170	HIS
1	B	218	GLN
1	B	228	HIS
1	B	282	GLN
1	B	361	GLN
1	B	393	ASN
1	B	396	ASN
1	B	402	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
5	DGT	B	421	4	32,33,33	1.16	3 (9%)	48,52,52	1.73	12 (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
5	DGT	B	421	4	-	9/22/34/34	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	421	DGT	PB-O3B	3.66	1.63	1.59
5	B	421	DGT	C5-N7	-2.36	1.34	1.39
5	B	421	DGT	C2-N3	2.15	1.38	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	421	DGT	C5-C4-N3	-4.62	121.04	128.39
5	B	421	DGT	C2-N3-C4	3.87	118.97	112.30
5	B	421	DGT	O1B-PB-O3B	3.72	117.31	107.27
5	B	421	DGT	O3'-C3'-C2'	3.52	123.12	110.88
5	B	421	DGT	O1B-PB-O3A	2.69	114.55	107.27
5	B	421	DGT	O2G-PG-O3B	2.50	113.01	104.64
5	B	421	DGT	C2-N1-C6	-2.46	120.65	125.11
5	B	421	DGT	N9-C4-N3	2.46	130.87	125.95
5	B	421	DGT	O3A-PB-O2B	-2.34	103.67	110.70
5	B	421	DGT	O4'-C4'-C3'	2.33	110.97	105.65
5	B	421	DGT	O6-C6-C5	-2.25	120.60	126.53
5	B	421	DGT	C5'-C4'-C3'	-2.20	102.34	114.64

There are no chirality outliers.

All (9) torsion outliers are listed below:

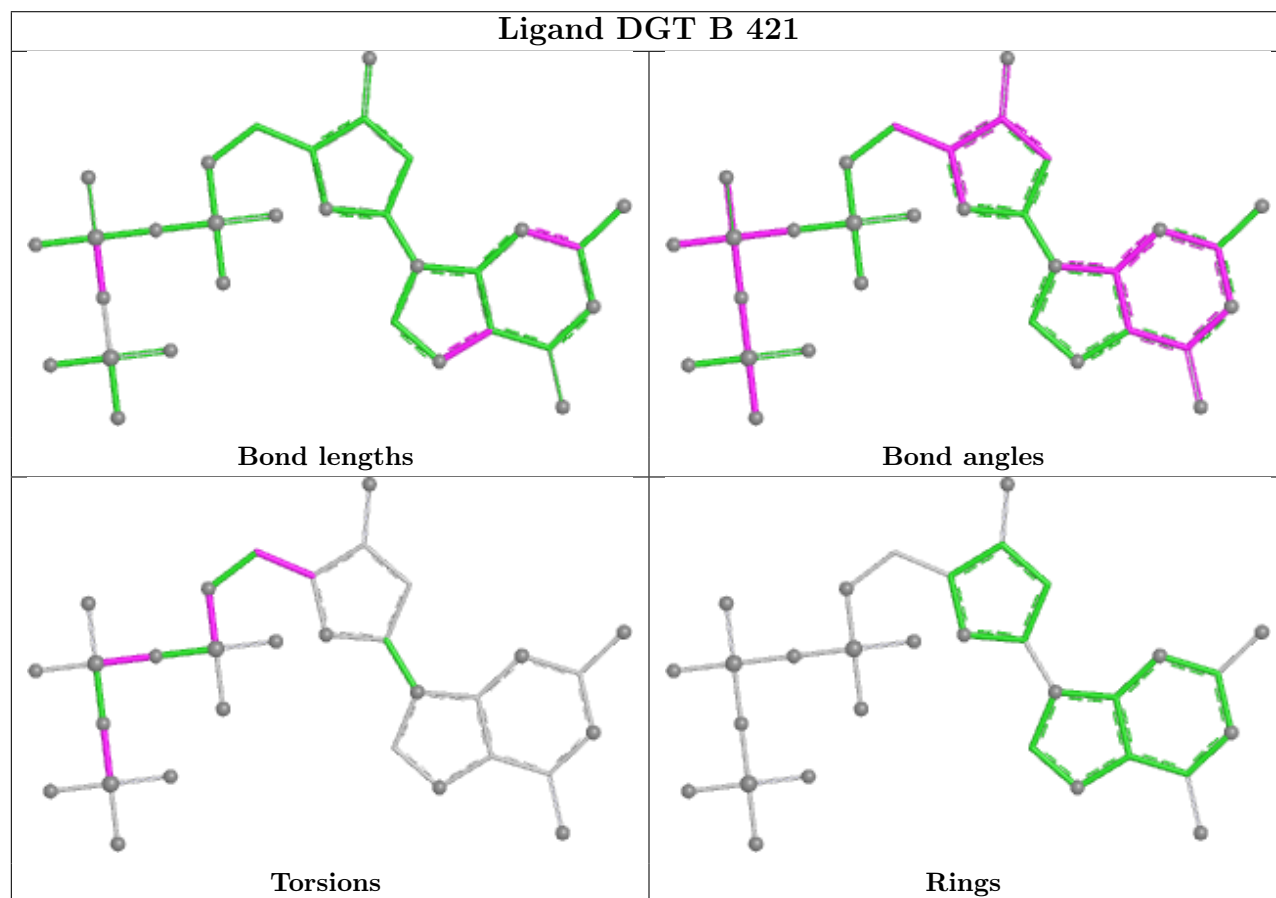
Mol	Chain	Res	Type	Atoms
5	B	421	DGT	PB-O3B-PG-O2G
5	B	421	DGT	C5'-O5'-PA-O1A
5	B	421	DGT	C3'-C4'-C5'-O5'
5	B	421	DGT	PA-O3A-PB-O1B
5	B	421	DGT	C5'-O5'-PA-O3A
5	B	421	DGT	C5'-O5'-PA-O2A
5	B	421	DGT	O4'-C4'-C5'-O5'
5	B	421	DGT	PA-O3A-PB-O2B
5	B	421	DGT	PB-O3B-PG-O3G

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%)	1.21	86 (22%) 2 2	20, 42, 60, 65	1 (0%)
2	T	9/9 (100%)	0.48	1 (11%) 10 9	33, 39, 62, 84	0
3	P	7/7 (100%)	0.23	0 100 100	34, 39, 50, 54	0
All	All	390/436 (89%)	1.17	87 (22%) 2 2	20, 42, 60, 84	1 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	ALA	7.0
1	B	94	VAL	5.9
1	B	96	GLY	5.8
1	B	97	GLU	5.4
1	B	73	LEU	5.3
1	B	381	THR	4.7
1	B	75	VAL	4.6
1	B	95	ASN	4.1
1	B	29	VAL	4.1
1	B	302[A]	PHE	3.9
1	B	68	TYR	3.9
1	B	413	LEU	3.8
1	B	61	TYR	3.7
1	B	74	GLY	3.7
1	B	86	GLU	3.7
1	B	78	LEU	3.7
1	B	93	LEU	3.6
1	B	46	SER	3.6
1	B	401	PHE	3.6
1	B	72	LYS	3.6
1	B	315	VAL	3.5
1	B	30	ILE	3.4
1	B	330	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	382	PRO	3.4
1	B	77	LYS	3.3
1	B	385	ASP	3.3
1	B	303	SER	3.3
1	B	249	CYS	3.3
1	B	92	VAL	3.3
1	B	398	LYS	3.3
1	B	69	GLU	3.2
1	B	88	CYS	3.2
1	B	312	SER	3.2
1	B	71	ARG	3.1
1	B	384	VAL	3.1
1	B	84	ALA	3.1
1	B	368	VAL	3.1
1	B	380	MET	3.1
1	B	333	CYS	3.1
1	B	31	VAL	3.1
1	B	414	LYS	3.0
1	B	329	LEU	3.0
1	B	379	VAL	3.0
1	B	244	TYR	3.0
1	B	371	LYS	3.0
1	B	33	VAL	2.9
1	B	87	LYS	2.9
1	B	145	SER	2.9
1	B	349	TYR	2.9
2	T	839	DA	2.8
1	B	144	GLN	2.8
1	B	399	MET	2.7
1	B	370	GLN	2.7
1	B	392	ARG	2.7
1	B	412	ASN	2.6
1	B	81	VAL	2.6
1	B	319	ASN	2.6
1	B	239	ILE	2.6
1	B	378	ASP	2.5
1	B	49	GLU	2.5
1	B	356	GLY	2.5
1	B	99	LEU	2.5
1	B	275	ILE	2.5
1	B	63	VAL	2.4
1	B	409	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	45	ILE	2.4
1	B	339	PRO	2.4
1	B	391	PHE	2.3
1	B	27	SER	2.3
1	B	290	ASN	2.3
1	B	248	LYS	2.3
1	B	32	HIS	2.3
1	B	85	LYS	2.3
1	B	328	LEU	2.3
1	B	143	LEU	2.2
1	B	148	LEU	2.2
1	B	367	HIS	2.2
1	B	65	THR	2.2
1	B	146	ASP	2.1
1	B	345	ILE	2.1
1	B	364	ILE	2.1
1	B	411	CYS	2.1
1	B	26	SER	2.1
1	B	405	LEU	2.0
1	B	347	ARG	2.0
1	B	76	LYS	2.0
1	B	325	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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.

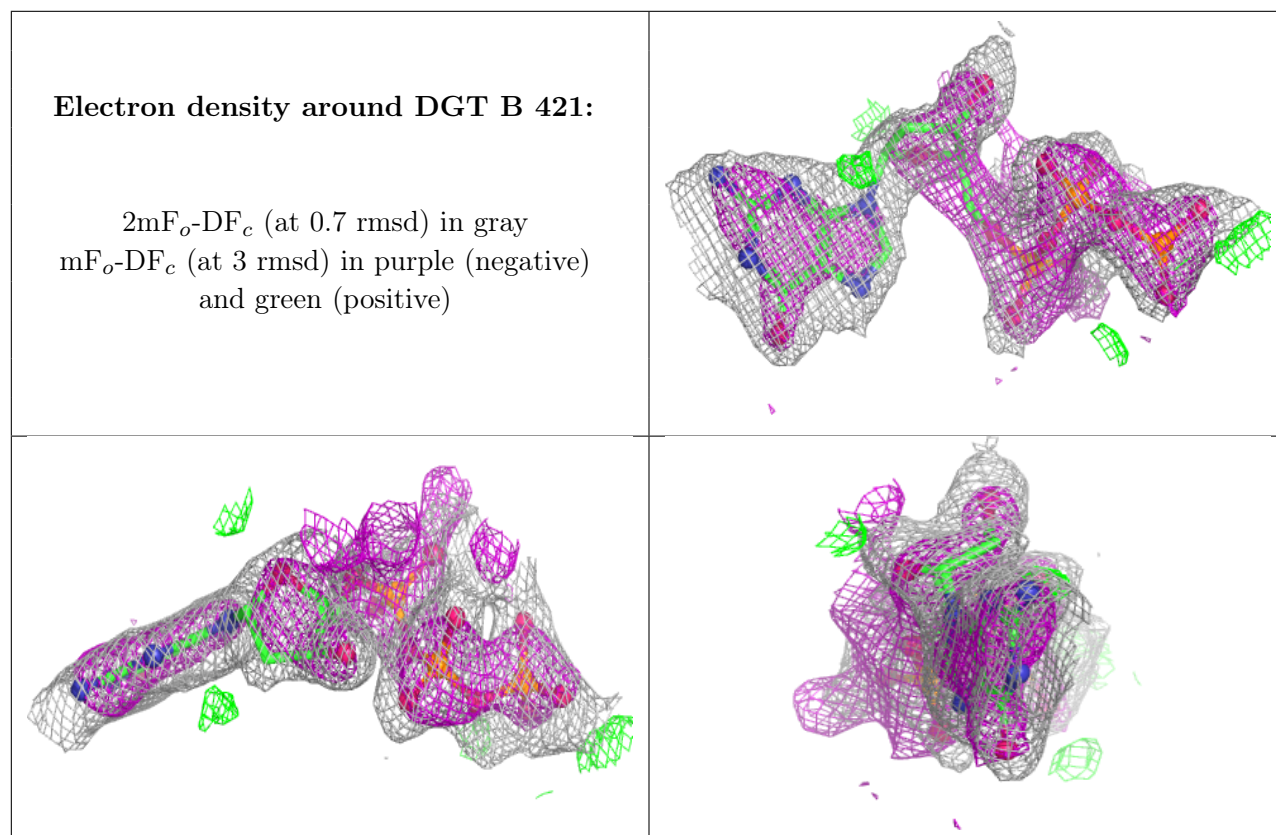
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	B	422	1/1	0.83	0.36	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DGT	B	421	31/31	0.84	0.16	37,49,51,53	0
4	MG	B	871	1/1	0.95	0.14	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 ⓘ

There are no such residues in this entry.