



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:13 PM UTC

PDB ID : 3GV7 / pdb_00003gv7
Title : Human DNA polymerase iota in complex with T template DNA and incoming dTTP
Authors : Kirouac, K.N.; Ling, H.
Deposited on : 2009-03-30
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

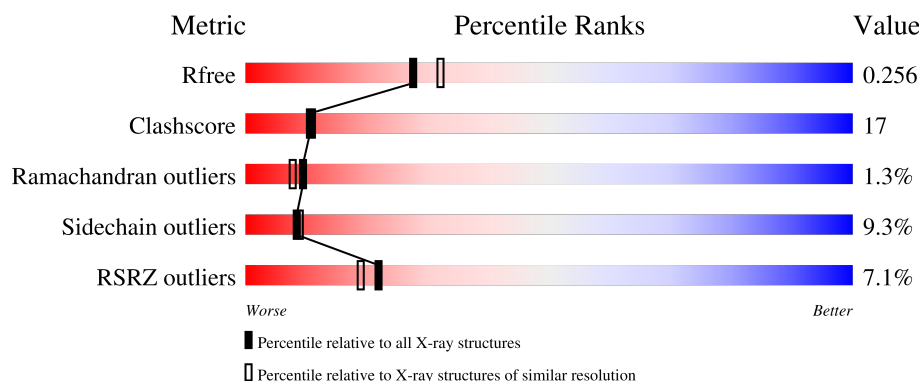
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	6% 64% 20% 5% 10%
2	T	9	11% 89% 11%
3	P	7	57% 14% 29%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3596 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	377	Total	C	N	O	S	0	0	0
			2978	1883	519	554	22			

- Molecule 2 is a DNA chain called 5'-D(P*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
			183	88	32	54	9			

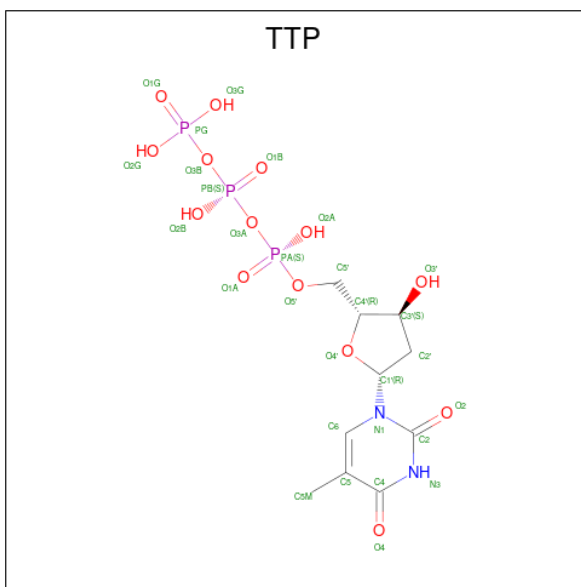
- Molecule 3 is a DNA chain called 5'-D(*AP*GP*GP*AP*CP*CP*C)-3'.

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 THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	240	Total O 240 240	0	0
6	T	16	Total O 16 16	0	0
6	P	9	Total O 9 9	0	0

- Molecule 1: DNA polymerase iota



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	97.19Å 97.19Å 201.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.04 – 2.20 27.04 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (27.04-2.20) 99.7 (27.04-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.209 , 0.258 0.205 , 0.256	Depositor DCC
R_{free} test set	604 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3596	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% 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, TTP

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	0.77	2/3021 (0.1%)	0.96	8/4071 (0.2%)
2	T	0.53	0/204	1.23	1/313 (0.3%)
3	P	0.58	0/156	1.42	2/238 (0.8%)
All	All	0.75	2/3381 (0.1%)	1.01	11/4622 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	381	THR	CA-C	10.02	1.65	1.52
1	B	383	MET	CG-SD	6.14	1.96	1.80

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	SER	N-CA-C	9.99	124.81	112.23
3	P	867	DA	O5'-C5'-C4'	9.90	125.64	110.80
3	P	870	DA	C5'-C4'-C3'	-8.19	102.61	114.90
1	B	153	VAL	CB-CA-C	-7.54	100.88	111.28
1	B	149	SER	CA-C-N	7.19	134.65	121.70
1	B	149	SER	C-N-CA	7.19	134.65	121.70
1	B	332	VAL	N-CA-C	6.13	122.10	109.34
1	B	219	THR	CB-CA-C	5.83	121.22	109.38
2	T	847	DT	N1-C1'-C2'	5.79	122.18	113.50
1	B	332	VAL	CA-C-N	5.04	130.76	121.70
1	B	332	VAL	C-N-CA	5.04	130.76	121.70

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	B	2978	0	3073	108	0
2	T	183	0	103	0	1
3	P	139	0	77	2	1
4	B	2	0	0	0	0
5	B	29	0	13	2	0
6	B	240	0	0	15	0
6	P	9	0	0	1	0
6	T	16	0	0	0	0
All	All	3596	0	3266	111	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 17.

All (111) 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:131:ASP:OD2	1:B:133:THR:HG23	1.54	1.06
1:B:226:CYS:SG	6:B:616:HOH:O	2.12	1.04
1:B:29:VAL:H	1:B:133:THR:HG22	1.16	1.03
5:B:421:TTP:O2A	6:B:496:HOH:O	1.78	1.01
1:B:153:VAL:HG13	1:B:174:LEU:HD22	1.44	0.99
1:B:36:ASP:OD2	1:B:194:THR:HG22	1.61	0.98
1:B:149:SER:N	1:B:150:ALA:HB3	1.80	0.95
1:B:358:GLU:HB3	1:B:394:MET:HE1	1.49	0.94
1:B:358:GLU:HB3	1:B:394:MET:CE	2.00	0.91
1:B:358:GLU:CB	1:B:394:MET:HE1	1.99	0.91
1:B:41:GLN:HE22	1:B:194:THR:H	1.15	0.89
1:B:311:CYS:SG	6:B:659:HOH:O	2.31	0.88
1:B:394:MET:SD	6:B:631:HOH:O	2.31	0.87
1:B:164:ASN:H	1:B:170:HIS:HD2	1.25	0.85
1:B:36:ASP:OD2	1:B:194:THR:CG2	2.27	0.81
1:B:332:VAL:HG12	1:B:333:CYS:HB2	1.65	0.79
1:B:110:THR:CG2	1:B:122:ARG:HH11	1.96	0.79
1:B:348:ARG:O	1:B:349:TYR:HB2	1.83	0.78
1:B:90:GLN:H	1:B:90:GLN:HE21	1.29	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ARG:HE	1:B:404:THR:HG23	1.49	0.77
1:B:325:LEU:HD21	1:B:387:LEU:HD13	1.67	0.76
1:B:110:THR:HG21	1:B:122:ARG:HH11	1.52	0.74
3:P:869:DG:H1'	6:P:197:HOH:O	1.87	0.74
1:B:332:VAL:N	1:B:333:CYS:CB	2.52	0.71
5:B:421:TTP:O1A	6:B:661:HOH:O	2.08	0.71
1:B:341:THR:HG23	1:B:412:ASN:HB3	1.72	0.70
1:B:381:THR:O	1:B:385:ASP:OD2	2.10	0.70
1:B:325:LEU:HD21	1:B:387:LEU:CD1	2.23	0.68
1:B:332:VAL:CA	1:B:333:CYS:HB2	2.24	0.67
1:B:332:VAL:N	1:B:333:CYS:HB3	2.12	0.65
1:B:332:VAL:N	1:B:333:CYS:HB2	2.11	0.65
1:B:242:ILE:O	6:B:425:HOH:O	2.15	0.64
1:B:388:MET:HB3	1:B:392:ARG:NH1	2.13	0.64
1:B:156:HIS:HB2	1:B:219:THR:HB	1.79	0.64
1:B:304:GLU:OE2	6:B:486:HOH:O	2.15	0.63
1:B:29:VAL:N	1:B:133:THR:HG22	2.01	0.63
1:B:331:ARG:C	1:B:333:CYS:HB3	2.24	0.63
1:B:267:LYS:HE3	6:B:630:HOH:O	1.99	0.62
1:B:29:VAL:H	1:B:133:THR:CG2	2.04	0.62
1:B:112:LEU:HD23	1:B:112:LEU:C	2.24	0.62
1:B:44:MET:HE2	1:B:51:LYS:HA	1.83	0.61
1:B:345:ILE:HB	1:B:407:SER:HB3	1.83	0.61
1:B:267:LYS:HG2	6:B:471:HOH:O	2.02	0.60
1:B:332:VAL:HG12	1:B:333:CYS:CB	2.31	0.59
1:B:67:ASN:HD22	1:B:67:ASN:C	2.11	0.59
1:B:149:SER:N	1:B:150:ALA:CB	2.59	0.59
1:B:332:VAL:CG1	1:B:333:CYS:HB2	2.32	0.58
1:B:358:GLU:HB2	1:B:394:MET:HE1	1.84	0.58
1:B:35:LEU:HD11	1:B:187:MET:CE	2.34	0.58
1:B:67:ASN:ND2	1:B:70:ALA:H	2.02	0.58
1:B:219:THR:CG2	6:B:443:HOH:O	2.51	0.58
1:B:164:ASN:H	1:B:170:HIS:CD2	2.15	0.57
1:B:90:GLN:H	1:B:90:GLN:NE2	2.00	0.57
1:B:322:GLU:HG2	1:B:384:VAL:HG11	1.86	0.57
1:B:322:GLU:O	1:B:380:MET:HE1	2.05	0.57
1:B:103:ARG:NH2	6:B:602:HOH:O	2.38	0.56
1:B:184:ARG:HE	1:B:218:GLN:HE21	1.53	0.56
1:B:332:VAL:CA	1:B:333:CYS:CB	2.84	0.56
1:B:149:SER:H	1:B:150:ALA:HB3	1.66	0.55
1:B:44:MET:HE3	1:B:67:ASN:OD1	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ARG:NE	1:B:404:THR:HG23	2.22	0.55
1:B:388:MET:HB3	1:B:392:ARG:HH12	1.72	0.54
1:B:343:ARG:NH2	1:B:361:GLN:HE22	2.04	0.54
1:B:358:GLU:HB3	1:B:394:MET:HE3	1.88	0.54
1:B:35:LEU:HD11	1:B:187:MET:HE1	1.90	0.53
1:B:245:LYS:HG3	3:P:870:DA:H5'	1.90	0.52
1:B:184:ARG:HH11	1:B:218:GLN:HE21	1.57	0.52
1:B:348:ARG:O	1:B:349:TYR:CB	2.57	0.51
1:B:219:THR:HG22	6:B:443:HOH:O	2.11	0.51
1:B:158:TYR:OH	1:B:228:HIS:HD2	1.94	0.50
1:B:326:ALA:HB2	1:B:380:MET:HE2	1.94	0.50
1:B:360:ARG:HG2	1:B:394:MET:CG	2.41	0.50
1:B:148:LEU:C	1:B:150:ALA:HB3	2.36	0.49
1:B:344:LEU:HB2	1:B:387:LEU:HD23	1.95	0.49
1:B:35:LEU:CD1	1:B:187:MET:HE1	2.43	0.49
1:B:144:GLN:HB2	1:B:147:GLU:HG3	1.94	0.49
1:B:35:LEU:HD23	1:B:38:PHE:CD1	2.48	0.48
1:B:110:THR:HG21	1:B:122:ARG:HG2	1.95	0.48
1:B:95:ASN:HD21	1:B:97:GLU:HB2	1.79	0.48
1:B:332:VAL:CB	1:B:333:CYS:HB2	2.43	0.48
1:B:413:LEU:HD12	1:B:413:LEU:N	2.29	0.47
1:B:48:PRO:O	1:B:51:LYS:HG2	2.14	0.47
1:B:231:HIS:HE1	6:B:452:HOH:O	1.97	0.47
1:B:253:LEU:HD11	1:B:272:GLU:HG2	1.95	0.47
1:B:325:LEU:CD2	1:B:387:LEU:HD13	2.40	0.47
1:B:47:ASN:C	1:B:49:GLU:H	2.22	0.46
1:B:110:THR:CG2	1:B:122:ARG:NH1	2.75	0.46
1:B:110:THR:HB	1:B:128:ASN:OD1	2.16	0.45
1:B:267:LYS:HD3	1:B:267:LYS:HA	1.64	0.45
1:B:35:LEU:HD21	1:B:109:VAL:HG21	1.98	0.45
1:B:83:ASP:O	1:B:87:LYS:HB2	2.16	0.45
1:B:394:MET:HE2	1:B:394:MET:HB3	1.71	0.45
1:B:231:HIS:HD2	6:B:439:HOH:O	2.00	0.45
1:B:227:GLN:NE2	6:B:616:HOH:O	2.49	0.45
1:B:44:MET:CE	1:B:67:ASN:OD1	2.66	0.44
1:B:380:MET:O	1:B:384:VAL:HG22	2.18	0.44
1:B:76:LYS:HB2	1:B:79:MET:HE3	2.00	0.44
1:B:35:LEU:HD23	1:B:38:PHE:CE1	2.54	0.43
1:B:36:ASP:O	1:B:37:CYS:C	2.61	0.43
1:B:41:GLN:HE22	1:B:194:THR:N	1.98	0.43
1:B:358:GLU:CB	1:B:394:MET:CE	2.72	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:SER:O	1:B:172:ARG:NH2	2.53	0.42
1:B:41:GLN:NE2	1:B:194:THR:H	1.98	0.42
1:B:184:ARG:HH11	1:B:218:GLN:NE2	2.18	0.42
1:B:67:ASN:C	1:B:67:ASN:ND2	2.78	0.41
1:B:59:GLN:OE1	1:B:64:VAL:HG11	2.21	0.41
1:B:47:ASN:HD21	1:B:49:GLU:HB2	1.86	0.41
1:B:47:ASN:ND2	1:B:49:GLU:HB2	2.36	0.40
1:B:47:ASN:C	1:B:47:ASN:HD22	2.29	0.40
1:B:379:VAL:O	1:B:382:PRO:HG2	2.20	0.40
1:B:345:ILE:N	1:B:345:ILE:HD12	2.37	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'	3:P:867:DA:O5'[12_544]	1.83	0.37

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	B	371/420 (88%)	359 (97%)	7 (2%)	5 (1%)	9 8

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	150	ALA
1	B	333	CYS
1	B	370	GLN
1	B	37	CYS
1	B	48	PRO

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	344/376 (92%)	312 (91%)	32 (9%)	8 9

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	35	LEU
1	B	62	LEU
1	B	67	ASN
1	B	76	LYS
1	B	85	LYS
1	B	87	LYS
1	B	90	GLN
1	B	110	THR
1	B	126	ASP
1	B	133	THR
1	B	142	GLN
1	B	143	LEU
1	B	153	VAL
1	B	160	ASN
1	B	166	LEU
1	B	194	THR
1	B	204	LEU
1	B	219	THR
1	B	221	LEU
1	B	267	LYS
1	B	275	ILE
1	B	309	LYS
1	B	320	LYS
1	B	325	LEU
1	B	332	VAL
1	B	337	ARG
1	B	341	THR
1	B	357	ARG
1	B	371	LYS
1	B	380	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	387	LEU
1	B	405	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	41	GLN
1	B	47	ASN
1	B	58	GLN
1	B	90	GLN
1	B	95	ASN
1	B	156	HIS
1	B	170	HIS
1	B	218	GLN
1	B	228	HIS
1	B	231	HIS
1	B	279	GLN
1	B	282	GLN
1	B	319	ASN
1	B	330	ASN
1	B	340	HIS
1	B	361	GLN
1	B	393	ASN

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	TTP	B	421	4	29,30,30	1.49	4 (13%)	43,47,47	2.08	8 (18%)

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	TTP	B	421	4	-	5/22/34/34	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	421	TTP	PB-O3B	4.10	1.63	1.59
5	B	421	TTP	C6-C5	3.28	1.40	1.34
5	B	421	TTP	C2-N1	3.11	1.43	1.38
5	B	421	TTP	C4-C5	2.24	1.48	1.44

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	421	TTP	C4-N3-C2	-6.17	119.25	127.34
5	B	421	TTP	N3-C2-N1	5.95	122.64	114.89
5	B	421	TTP	C5-C4-N3	5.22	119.86	115.32
5	B	421	TTP	O4-C4-C5	-4.95	119.25	124.92
5	B	421	TTP	C5-C6-N1	-3.23	119.81	123.31
5	B	421	TTP	O4'-C1'-N1	2.93	113.07	107.86
5	B	421	TTP	O2-C2-N1	-2.66	119.33	122.80
5	B	421	TTP	O3A-PB-O1B	2.46	118.11	110.70

There are no chirality outliers.

All (5) torsion outliers are listed below:

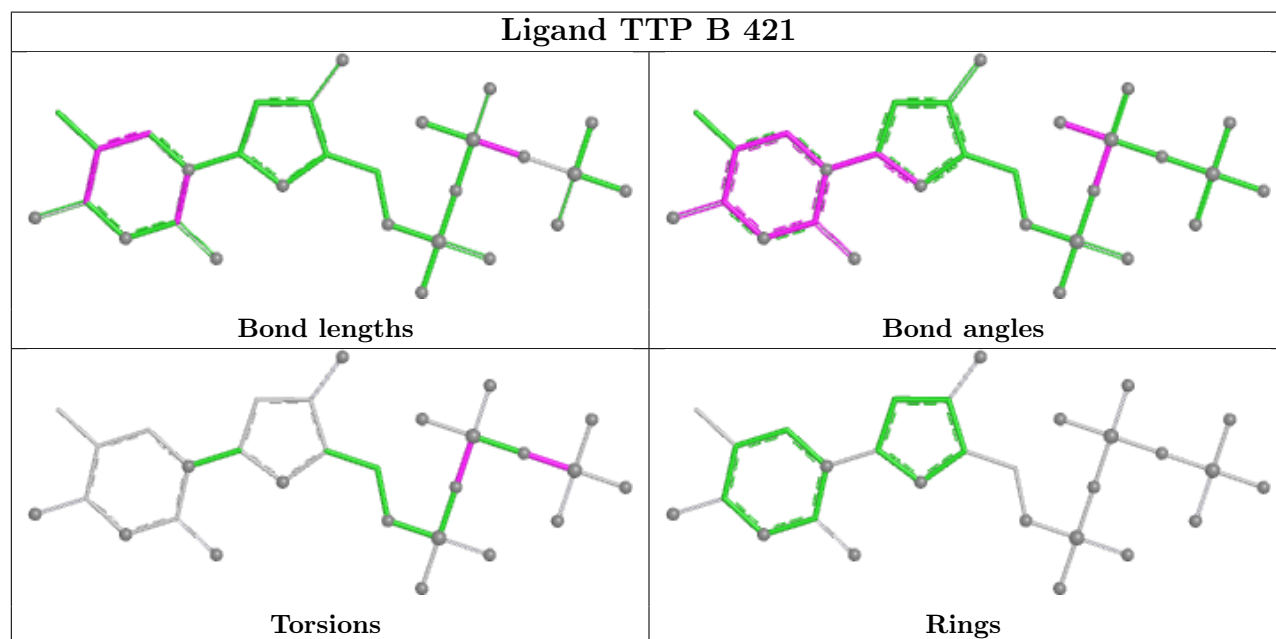
Mol	Chain	Res	Type	Atoms
5	B	421	TTP	PB-O3B-PG-O1G
5	B	421	TTP	PB-O3B-PG-O2G
5	B	421	TTP	PB-O3B-PG-O3G
5	B	421	TTP	PA-O3A-PB-O1B
5	B	421	TTP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	421	TTP	2	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	377/420 (89%)	0.73	27 (7%) 21 18	31, 49, 66, 72	0
2	T	9/9 (100%)	0.55	1 (11%) 10 8	39, 42, 57, 79	0
3	P	7/7 (100%)	0.13	0 100 100	41, 43, 48, 52	0
All	All	393/436 (90%)	0.72	28 (7%) 22 19	31, 48, 66, 79	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	VAL	5.8
1	B	30	ILE	5.5
1	B	27	SER	5.4
1	B	33	VAL	4.2
1	B	26	SER	4.2
1	B	332	VAL	4.1
1	B	31	VAL	4.0
2	T	839	DA	3.7
1	B	385	ASP	3.5
1	B	28	ARG	3.4
1	B	32	HIS	3.2
1	B	335	ASP	2.9
1	B	303	SER	2.8
1	B	75	VAL	2.7
1	B	381	THR	2.5
1	B	148	LEU	2.5
1	B	73	LEU	2.5
1	B	382	PRO	2.4
1	B	249	CYS	2.4
1	B	61	TYR	2.3
1	B	300	GLN	2.3
1	B	349	TYR	2.2
1	B	302	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	153	VAL	2.1
1	B	143	LEU	2.1
1	B	244	TYR	2.1
1	B	413	LEU	2.0
1	B	146	ASP	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](#)

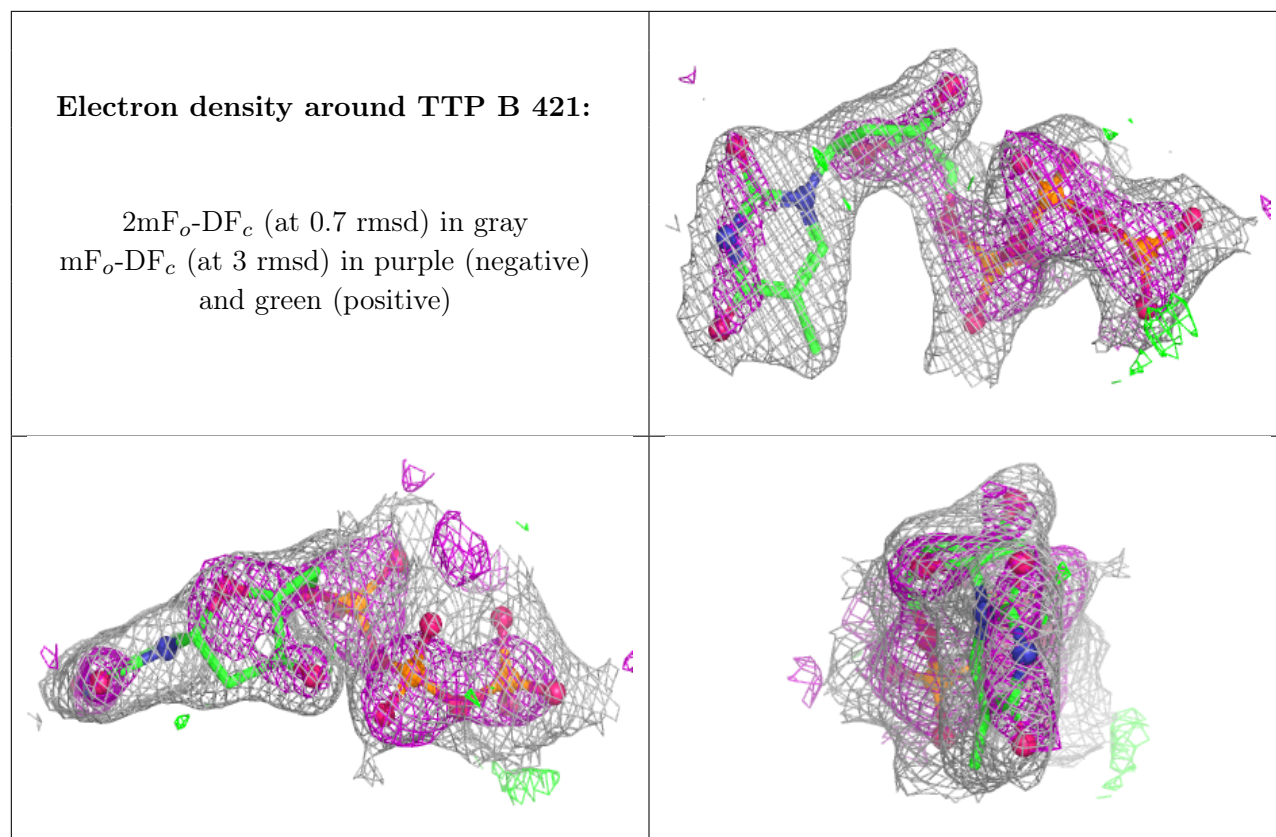
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
4	MG	B	422	1/1	0.87	0.24	59,59,59,59	0
5	TTP	B	421	29/29	0.93	0.13	38,44,47,50	0
4	MG	B	871	1/1	0.98	0.10	32,32,32,32	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.