Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 12:25 AM EDT

PDB ID	:	3G6Y
Title	:	Ternary complex of DNA Polymerase iota:DNA:dTTP with an abasic site at the templating position
Authors	:	Nair, D.T.; Aggarwal, A.K.
Deposited on	:	2009-02-09
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

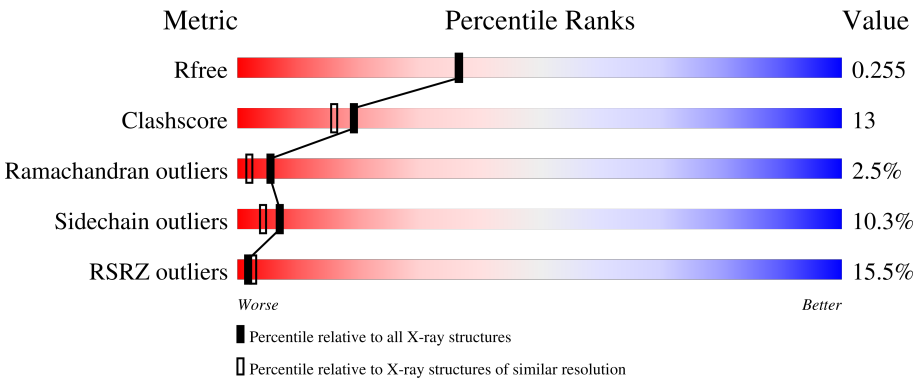
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	420	14% 63% 20% 5% • 11%
2	P	7	86% 14%
3	T	11	36% 36% 27%

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	MG	A	872	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3414 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
			Total	C	N	O	S			
1	A	373	2876	1809	504	542	21	0	0	0

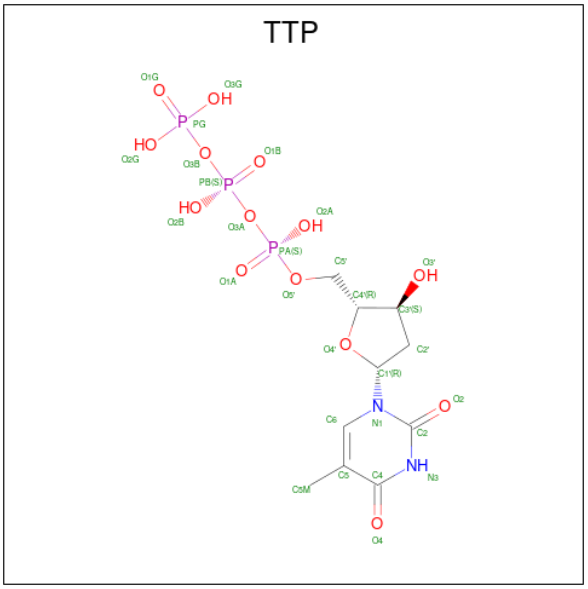
- Molecule 2 is a DNA chain called Primer DNA strand.

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

- Molecule 3 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	T	8	155	73	25	49	8	0	0	0

- Molecule 4 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is water.

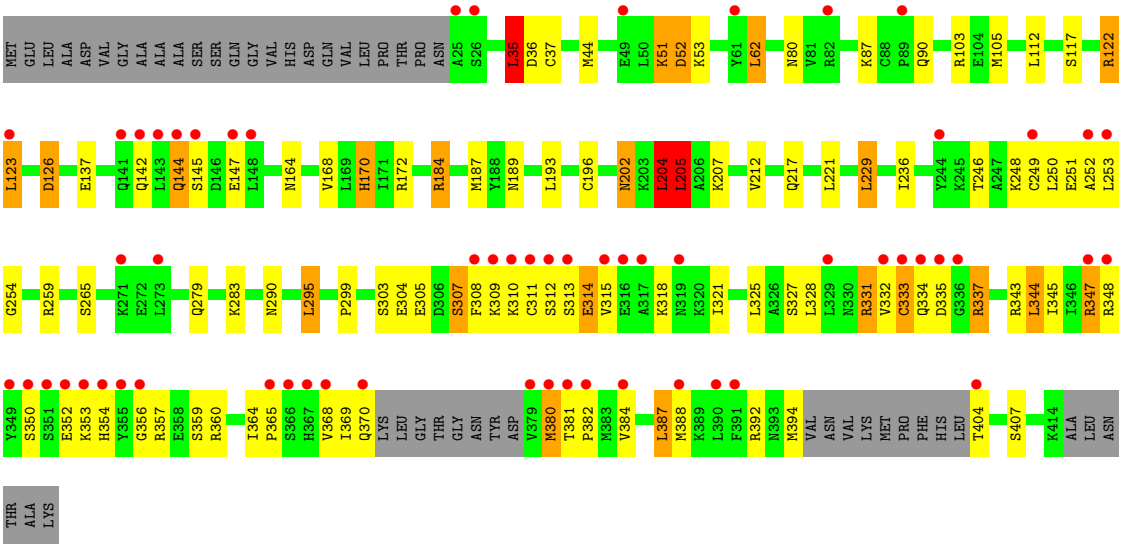
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	193	193	193	0	0
			Total	O		
6	P	7	7	7	0	0
			Total	O		
6	T	13	13	13	0	0

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.

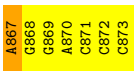
• Molecule 1: DNA polymerase iota

Chain A: 14% 63% 20% 5% • 11%



• Molecule 2: Primer DNA strand

Chain P: 86% 14%



• Molecule 3: Template DNA strand

Chain T: 36% 36% 27%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	98.11Å 98.11Å 202.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.61 – 2.10 36.61 – 2.02	Depositor EDS
% Data completeness (in resolution range)	97.1 (36.61-2.10) 96.5 (36.61-2.02)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.62 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, R_{free}	0.220 , 0.253 0.223 , 0.255	Depositor DCC
R_{free} test set	3086 reflections (8.07%)	wwPDB-VP
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3414	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TTP, DOC, MG, 3DR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.12	7/2914 (0.2%)	1.12	18/3934 (0.5%)
2	P	1.86	3/136 (2.2%)	2.83	16/208 (7.7%)
3	T	1.89	2/160 (1.2%)	2.79	16/245 (6.5%)
All	All	1.21	12/3210 (0.4%)	1.39	50/4387 (1.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	SER	CB-OG	6.87	1.51	1.42
2	P	867	DA	C2'-C1'	6.53	1.58	1.52
1	A	122	ARG	CD-NE	-6.50	1.35	1.46
1	A	249	CYS	CB-SG	6.18	1.92	1.82
1	A	207	LYS	CE-NZ	-6.10	1.33	1.49
3	T	842	DG	C3'-O3'	-5.90	1.36	1.44
1	A	122	ARG	CG-CD	5.36	1.65	1.51
1	A	212	VAL	CB-CG1	5.21	1.63	1.52
1	A	184	ARG	CD-NE	-5.11	1.37	1.46
3	T	844	DT	C3'-O3'	-5.08	1.37	1.44
2	P	867	DA	C5'-C4'	5.05	1.56	1.51
2	P	872	DC	C3'-O3'	-5.02	1.37	1.44

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	122	ARG	NE-CZ-NH2	-23.77	108.42	120.30
1	A	122	ARG	NE-CZ-NH1	16.84	128.72	120.30
2	P	870	DA	O4'-C1'-N9	14.77	118.34	108.00
1	A	184	ARG	NE-CZ-NH2	-11.57	114.52	120.30
3	T	843	DG	O5'-P-OP2	-11.01	95.79	105.70
3	T	842	DG	P-O5'-C5'	10.34	137.44	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	867	DA	O4'-C1'-N9	-9.86	101.10	108.00
3	T	841	DG	C5-C6-O6	-9.55	122.87	128.60
2	P	870	DA	O4'-C4'-C3'	8.77	111.26	106.00
2	P	869	DG	N1-C6-O6	-8.74	114.66	119.90
1	A	122	ARG	CD-NE-CZ	8.23	135.13	123.60
2	P	869	DG	O4'-C1'-N9	8.16	113.71	108.00
1	A	122	ARG	CG-CD-NE	-7.80	95.42	111.80
3	T	842	DG	O4'-C1'-N9	-7.70	102.61	108.00
2	P	870	DA	O5'-P-OP2	-7.47	98.98	105.70
3	T	841	DG	C5-C6-N1	7.17	115.09	111.50
2	P	868	DG	N3-C2-N2	-7.02	114.99	119.90
3	T	844	DT	C6-C5-C7	-6.91	118.76	122.90
3	T	847	DT	O4'-C1'-N1	-6.88	103.18	108.00
1	A	259	ARG	NE-CZ-NH1	6.85	123.73	120.30
3	T	844	DT	C4-C5-C7	6.85	123.11	119.00
3	T	846	DC	O4'-C1'-N1	-6.85	103.21	108.00
1	A	205	LEU	CB-CG-CD1	6.78	122.53	111.00
1	A	62	LEU	CA-CB-CG	6.64	130.58	115.30
1	A	184	ARG	NE-CZ-NH1	6.52	123.56	120.30
3	T	842	DG	O5'-P-OP2	-6.36	99.98	105.70
2	P	868	DG	N1-C2-N2	6.35	121.91	116.20
2	P	868	DG	O4'-C1'-N9	6.30	112.41	108.00
1	A	123	LEU	CB-CG-CD2	5.52	120.38	111.00
3	T	845	DC	P-O3'-C3'	5.44	126.23	119.70
1	A	204	LEU	CB-CG-CD2	5.44	120.25	111.00
2	P	868	DG	C5-C6-O6	-5.44	125.34	128.60
2	P	871	DC	OP1-P-OP2	-5.44	111.44	119.60
1	A	126	ASP	CB-CG-OD1	-5.38	113.45	118.30
1	A	295	LEU	CB-CG-CD2	5.38	120.14	111.00
1	A	331	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	103	ARG	NE-CZ-NH2	-5.28	117.66	120.30
3	T	842	DG	C5'-C4'-O4'	-5.28	99.28	109.30
1	A	347	ARG	NE-CZ-NH2	-5.25	117.67	120.30
3	T	846	DC	C6-N1-C2	5.24	122.40	120.30
2	P	870	DA	N1-C6-N6	-5.23	115.46	118.60
2	P	872	DC	O4'-C1'-N1	5.20	111.64	108.00
3	T	843	DG	P-O3'-C3'	5.20	125.94	119.70
2	P	869	DG	C5-C6-O6	5.17	131.70	128.60
1	A	35	LEU	CB-CG-CD1	5.16	119.78	111.00
1	A	348	ARG	NE-CZ-NH2	-5.15	117.72	120.30
3	T	843	DG	C2'-C3'-O3'	-5.13	95.66	112.60
2	P	867	DA	N1-C6-N6	5.12	121.67	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	842	DG	C5-C6-N1	5.05	114.03	111.50
2	P	867	DA	O4'-C1'-C2'	-5.03	101.87	105.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2876	0	2899	80	0
2	P	139	0	79	0	1
3	T	155	0	88	3	1
4	A	29	0	13	0	0
5	A	2	0	0	0	0
6	A	193	0	0	6	0
6	P	7	0	0	0	0
6	T	13	0	0	0	0
All	All	3414	0	3079	81	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 (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASN:HB3	6:A:964:HOH:O	1.56	1.06
1:A:344:LEU:HD11	1:A:387:LEU:HD13	1.33	1.05
1:A:347:ARG:HD2	1:A:404:THR:HG23	1.44	0.98
1:A:347:ARG:HD2	1:A:404:THR:CG2	1.98	0.93
1:A:331:ARG:HD2	6:A:1004:HOH:O	1.70	0.93
1:A:164:ASN:H	1:A:170:HIS:HD2	1.18	0.91
1:A:335:ASP:OD2	1:A:337:ARG:HD3	1.78	0.84
1:A:44:MET:HE3	1:A:51:LYS:HA	1.61	0.81
1:A:308:PHE:CD1	1:A:311:CYS:HB2	2.16	0.80
1:A:144:GLN:HG3	1:A:147:GLU:HG2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LYS:HE3	3:T:840:3DR:OP2	1.87	0.73
1:A:236:ILE:HD12	1:A:250:LEU:HD13	1.71	0.73
1:A:144:GLN:HG3	1:A:147:GLU:CG	2.21	0.71
1:A:164:ASN:H	1:A:170:HIS:CD2	2.06	0.71
1:A:365:PRO:HD2	1:A:368:VAL:HG21	1.73	0.70
1:A:44:MET:CE	1:A:51:LYS:HA	2.23	0.68
1:A:307:SER:HB2	3:T:841:DG:OP2	1.95	0.66
1:A:318:LYS:HB2	1:A:388:MET:SD	2.36	0.66
1:A:344:LEU:HD11	1:A:387:LEU:CD1	2.19	0.63
1:A:308:PHE:HD1	1:A:311:CYS:HB2	1.64	0.63
1:A:308:PHE:O	1:A:404:THR:HA	2.00	0.60
1:A:380:MET:HE2	1:A:384:VAL:HG23	1.83	0.60
1:A:137:GLU:HG3	6:A:1108:HOH:O	2.00	0.60
1:A:308:PHE:HE1	1:A:312:SER:CB	2.15	0.59
1:A:112:LEU:C	1:A:112:LEU:HD23	2.23	0.59
1:A:308:PHE:CE1	1:A:312:SER:HB2	2.38	0.58
1:A:347:ARG:HH11	1:A:404:THR:HG23	1.69	0.58
1:A:308:PHE:HE1	1:A:312:SER:HB2	1.67	0.58
1:A:202:ASN:ND2	1:A:205:LEU:H	2.01	0.57
1:A:365:PRO:HD2	1:A:368:VAL:CG2	2.34	0.56
1:A:335:ASP:CG	1:A:337:ARG:HD3	2.26	0.55
1:A:304:GLU:HG3	1:A:328:LEU:HG	1.89	0.55
1:A:304:GLU:O	1:A:407:SER:HB2	2.07	0.54
1:A:202:ASN:HD22	1:A:202:ASN:C	2.12	0.53
1:A:364:ILE:HG23	1:A:368:VAL:HG23	1.91	0.52
1:A:308:PHE:HB2	1:A:311:CYS:SG	2.50	0.52
1:A:344:LEU:CD1	1:A:387:LEU:HD22	2.40	0.51
1:A:365:PRO:O	1:A:368:VAL:HG22	2.10	0.51
1:A:344:LEU:HD11	1:A:387:LEU:HD22	1.93	0.50
1:A:352:GLU:O	1:A:354:HIS:N	2.44	0.50
1:A:51:LYS:C	1:A:53:LYS:H	2.15	0.50
1:A:343:ARG:HD2	1:A:345:ILE:HD11	1.93	0.50
1:A:168:VAL:HG22	1:A:172:ARG:HD2	1.94	0.49
1:A:321:ILE:HG23	1:A:387:LEU:HD12	1.94	0.49
1:A:290:ASN:ND2	6:A:1130:HOH:O	2.41	0.49
1:A:360:ARG:HG2	1:A:394:MET:HG3	1.94	0.49
1:A:251:GLU:O	1:A:252:ALA:C	2.50	0.48
1:A:313:SER:O	1:A:314:GLU:HB2	2.13	0.48
1:A:380:MET:HE2	1:A:384:VAL:CG2	2.43	0.48
1:A:105:MET:CG	1:A:193:LEU:HD11	2.44	0.48
1:A:122:ARG:HD3	6:A:1043:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ARG:HH11	1:A:404:THR:CG2	2.27	0.48
1:A:184:ARG:HA	1:A:187:MET:HE2	1.95	0.47
1:A:381:THR:N	1:A:382:PRO:HD2	2.29	0.47
1:A:44:MET:HE2	1:A:51:LYS:HG2	1.98	0.46
1:A:309:LYS:O	1:A:310:LYS:HB2	2.16	0.46
1:A:318:LYS:HD2	1:A:388:MET:SD	2.55	0.46
1:A:364:ILE:HG23	1:A:368:VAL:CG2	2.45	0.45
1:A:333:CYS:O	1:A:335:ASP:N	2.50	0.45
1:A:347:ARG:HD2	1:A:404:THR:HG21	1.93	0.44
1:A:305:GLU:HA	1:A:407:SER:HB3	2.00	0.44
1:A:36:ASP:O	1:A:37:CYS:C	2.56	0.44
1:A:308:PHE:HB2	1:A:311:CYS:HB2	1.99	0.43
1:A:344:LEU:O	1:A:359:SER:HA	2.18	0.43
1:A:251:GLU:O	1:A:254:GLY:N	2.44	0.43
1:A:380:MET:O	1:A:384:VAL:HG23	2.18	0.43
1:A:196:CYS:HA	1:A:217:GLN:O	2.19	0.43
1:A:221:LEU:HD22	1:A:229:LEU:HD12	2.00	0.43
1:A:303:SER:O	1:A:331:ARG:NH2	2.52	0.42
6:A:937:HOH:O	3:T:843:DG:H5”	2.19	0.42
1:A:360:ARG:HG2	1:A:394:MET:CG	2.49	0.42
1:A:251:GLU:O	1:A:253:LEU:N	2.52	0.42
1:A:364:ILE:HG22	1:A:369:ILE:HG13	2.02	0.41
1:A:248:LYS:HD3	1:A:248:LYS:HA	1.72	0.41
1:A:144:GLN:HG3	1:A:147:GLU:CD	2.40	0.41
1:A:304:GLU:HG2	1:A:331:ARG:HH21	1.85	0.41
1:A:381:THR:N	1:A:382:PRO:CD	2.84	0.40
1:A:305:GLU:HG2	1:A:407:SER:HB3	2.03	0.40
1:A:35:LEU:HD12	1:A:35:LEU:HA	1.93	0.40
1:A:202:ASN:HD21	1:A:204:LEU:HB3	1.86	0.40
1:A:51:LYS:O	1:A:53:LYS:N	2.52	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:P:867:DA:O5’	3:T:847:DT:O3’[10_665]	1.77	0.43

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	A	367/420 (87%)	339 (92%)	19 (5%)	9 (2%)	5 2

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	314	GLU
1	A	315	VAL
1	A	334	GLN
1	A	350	SER
1	A	353	LYS
1	A	52	ASP
1	A	333	CYS
1	A	145	SER
1	A	356	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	321/376 (85%)	288 (90%)	33 (10%)	7 4

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	51	LYS

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Mol	Chain	Res	Type
1	A	52	ASP
1	A	62	LEU
1	A	80	ASN
1	A	87	LYS
1	A	90	GLN
1	A	123	LEU
1	A	126	ASP
1	A	142	GLN
1	A	144	GLN
1	A	170	HIS
1	A	202	ASN
1	A	204	LEU
1	A	205	LEU
1	A	229	LEU
1	A	246	THR
1	A	265	SER
1	A	279	GLN
1	A	283	LYS
1	A	295	LEU
1	A	299	PRO
1	A	307	SER
1	A	325	LEU
1	A	327	SER
1	A	332	VAL
1	A	337	ARG
1	A	344	LEU
1	A	357	ARG
1	A	370	GLN
1	A	380	MET
1	A	387	LEU
1	A	392	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	80	ASN
1	A	90	GLN
1	A	170	HIS
1	A	202	ASN
1	A	262	GLN
1	A	300	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
3	3DR	T	840	3	8,11,12	1.55	2 (25%)	9,14,17	1.82	3 (33%)
2	DOC	P	873	3,2	16,19,20	1.12	1 (6%)	20,26,29	1.64	4 (20%)

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
3	3DR	T	840	3	-	2/3/15/16	0/1/1/1
2	DOC	P	873	3,2	-	0/7/18/19	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	840	3DR	O4'-C4'	-2.98	1.39	1.44
2	P	873	DOC	C6-C5	2.55	1.41	1.35
3	T	840	3DR	O5'-C5'	-2.53	1.38	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	873	DOC	C3'-C2'-C1'	4.52	108.01	102.78
3	T	840	3DR	O4'-C1'-C2'	-3.22	99.87	106.37
2	P	873	DOC	O4'-C1'-N1	3.12	113.43	107.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	873	DOC	O4'-C4'-C3'	3.01	109.80	104.80
3	T	840	3DR	O3'-C3'-C2'	-2.67	105.17	111.54
2	P	873	DOC	C2'-C1'-N1	-2.61	107.45	112.40
3	T	840	3DR	C1'-C2'-C3'	-2.50	100.39	103.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	T	840	3DR	C3'-C4'-C5'-O5'
3	T	840	3DR	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	840	3DR	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	TTP	A	875	5	26,30,30	1.71	5 (19%)	39,47,47	2.24	13 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TTP	A	875	5	-	4/22/34/34	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	875	TTP	C6-C5	5.22	1.43	1.34
4	A	875	TTP	C4-N3	-3.32	1.32	1.38
4	A	875	TTP	O2-C2	2.32	1.27	1.23
4	A	875	TTP	C2-N1	2.28	1.42	1.38
4	A	875	TTP	C4-C5	2.14	1.48	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	875	TTP	N3-C2-N1	6.14	123.03	114.89
4	A	875	TTP	C5-C4-N3	5.64	120.12	115.31
4	A	875	TTP	C4-N3-C2	-5.03	120.85	127.35
4	A	875	TTP	O2-C2-N1	-4.14	117.29	122.79
4	A	875	TTP	C5-C6-N1	-3.55	119.69	123.34
4	A	875	TTP	O4-C4-C5	-3.06	121.36	124.90
4	A	875	TTP	C6-N1-C2	-2.77	118.49	121.30
4	A	875	TTP	PB-O3B-PG	-2.42	124.50	132.83
4	A	875	TTP	PB-O3A-PA	-2.33	124.83	132.83
4	A	875	TTP	C5M-C5-C6	2.30	125.92	122.85
4	A	875	TTP	O2A-PA-O5'	2.17	117.82	107.75
4	A	875	TTP	C5M-C5-C4	-2.14	116.42	118.77
4	A	875	TTP	O3G-PG-O2G	2.09	115.62	107.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

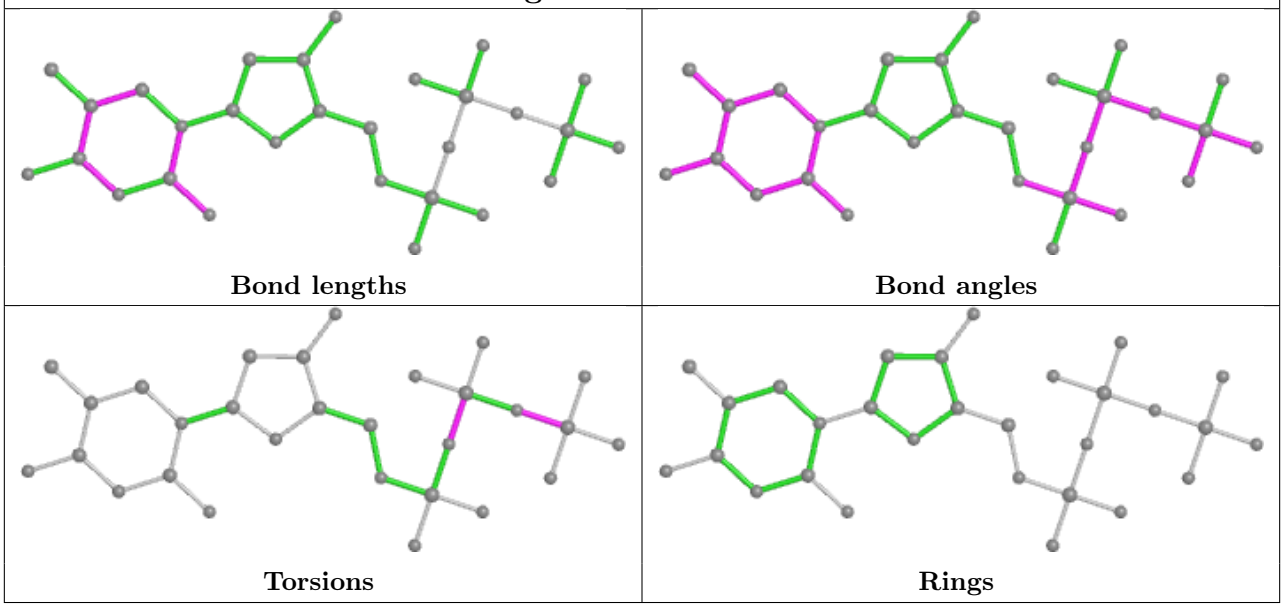
Mol	Chain	Res	Type	Atoms
4	A	875	TTP	PA-O3A-PB-O2B
4	A	875	TTP	PB-O3B-PG-O2G
4	A	875	TTP	PA-O3A-PB-O1B
4	A	875	TTP	PB-O3B-PG-O1G

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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.

Ligand TTP A 875



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, 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	A	373/420 (88%)	0.96	60 (16%)	1	2	11, 27, 51, 65	0
2	P	6/7 (85%)	0.54	0	100	100	21, 32, 36, 36	0
3	T	7/11 (63%)	0.17	0	100	100	15, 20, 22, 26	0
All	All	386/438 (88%)	0.94	60 (15%)	2	2	11, 27, 50, 65	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	354	HIS	16.7
1	A	355	TYR	15.6
1	A	25	ALA	11.0
1	A	350	SER	9.1
1	A	351	SER	8.2
1	A	312	SER	5.9
1	A	353	LYS	5.5
1	A	310	LYS	5.5
1	A	333	CYS	5.4
1	A	349	TYR	5.4
1	A	252	ALA	5.2
1	A	352	GLU	5.1
1	A	336	GLY	5.1
1	A	144	GLN	4.9
1	A	244	TYR	4.7
1	A	368	VAL	4.6
1	A	404	THR	4.5
1	A	249	CYS	4.2
1	A	388	MET	4.2
1	A	367	HIS	4.1
1	A	391	PHE	4.0
1	A	273	LEU	4.0
1	A	309	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	145	SER	3.9
1	A	315	VAL	3.7
1	A	348	ARG	3.7
1	A	334	GLN	3.6
1	A	82	ARG	3.6
1	A	370	GLN	3.5
1	A	61	TYR	3.5
1	A	366	SER	3.4
1	A	26	SER	3.3
1	A	356	GLY	3.2
1	A	89	PRO	3.2
1	A	143	LEU	3.1
1	A	390	LEU	3.1
1	A	317	ALA	3.0
1	A	311	CYS	3.0
1	A	335	ASP	3.0
1	A	148	LEU	2.9
1	A	308	PHE	2.9
1	A	319	ASN	2.9
1	A	142	GLN	2.9
1	A	141	GLN	2.7
1	A	380	MET	2.6
1	A	332	VAL	2.5
1	A	313	SER	2.5
1	A	381	THR	2.5
1	A	271	LYS	2.5
1	A	147	GLU	2.4
1	A	49	GLU	2.3
1	A	384	VAL	2.3
1	A	253	LEU	2.2
1	A	379	VAL	2.2
1	A	365	PRO	2.2
1	A	347	ARG	2.1
1	A	382	PRO	2.0
1	A	316	GLU	2.0
1	A	329	LEU	2.0
1	A	123	LEU	2.0

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. 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
2	DOC	P	873	18/19	0.97	0.19	14,18,22,22	0
3	3DR	T	840	11/12	0.97	0.14	18,30,45,46	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

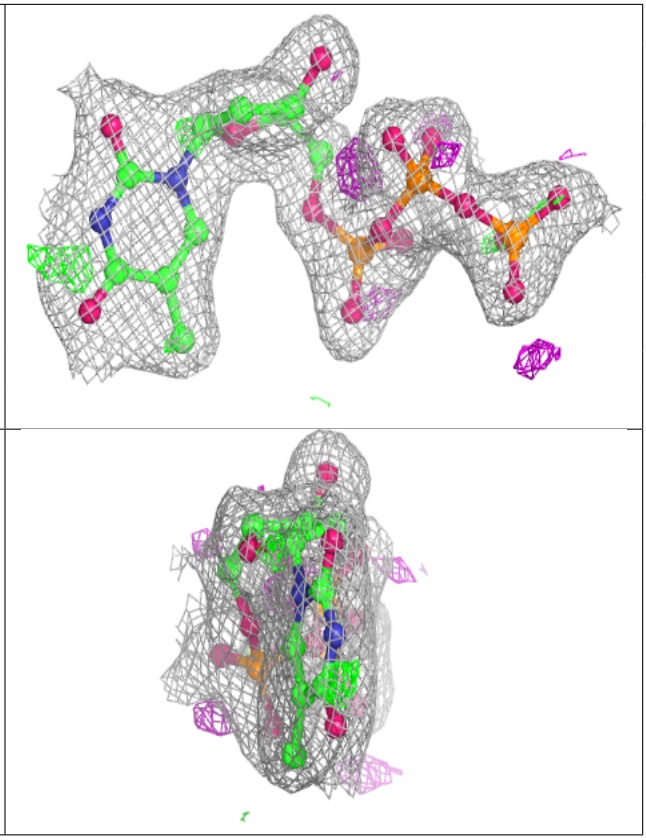
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	872	1/1	0.79	0.43	74,74,74,74	0
4	TTP	A	875	29/29	0.94	0.16	19,28,31,35	0
5	MG	A	871	1/1	0.95	0.11	12,12,12,12	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.

Electron density around TTP A 875:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.