



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:11 PM UTC

PDB ID : 3G6Y / pdb_00003g6y
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 ⓘ 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

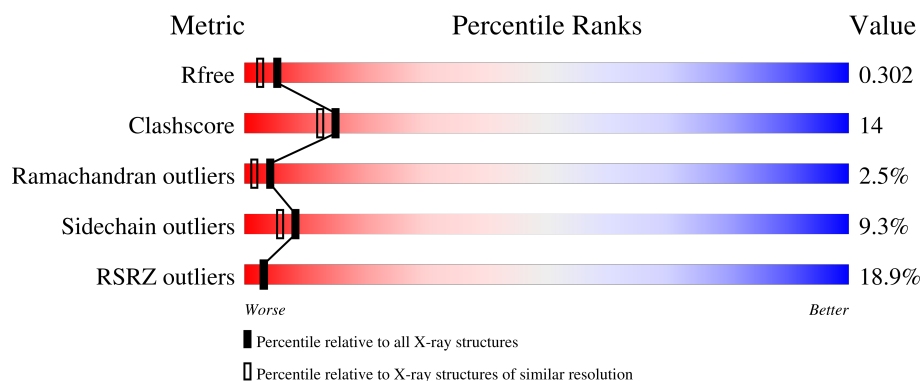
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. 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	A	420	17% 62% 21% 5% 11%
2	P	7	14% 57% 29% 14%
3	T	11	18% 36% 18% 27%

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
1	A	373	Total	C	N	O	S	0	0	0
			2876	1809	504	542	21			

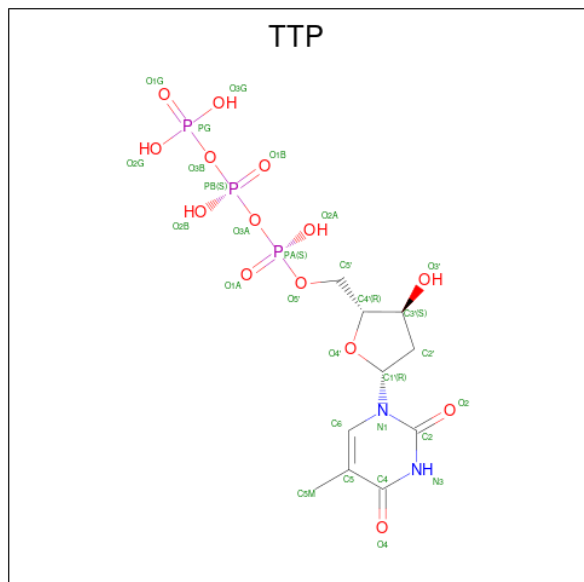
- Molecule 2 is a DNA chain called Primer DNA strand.

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

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

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

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



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

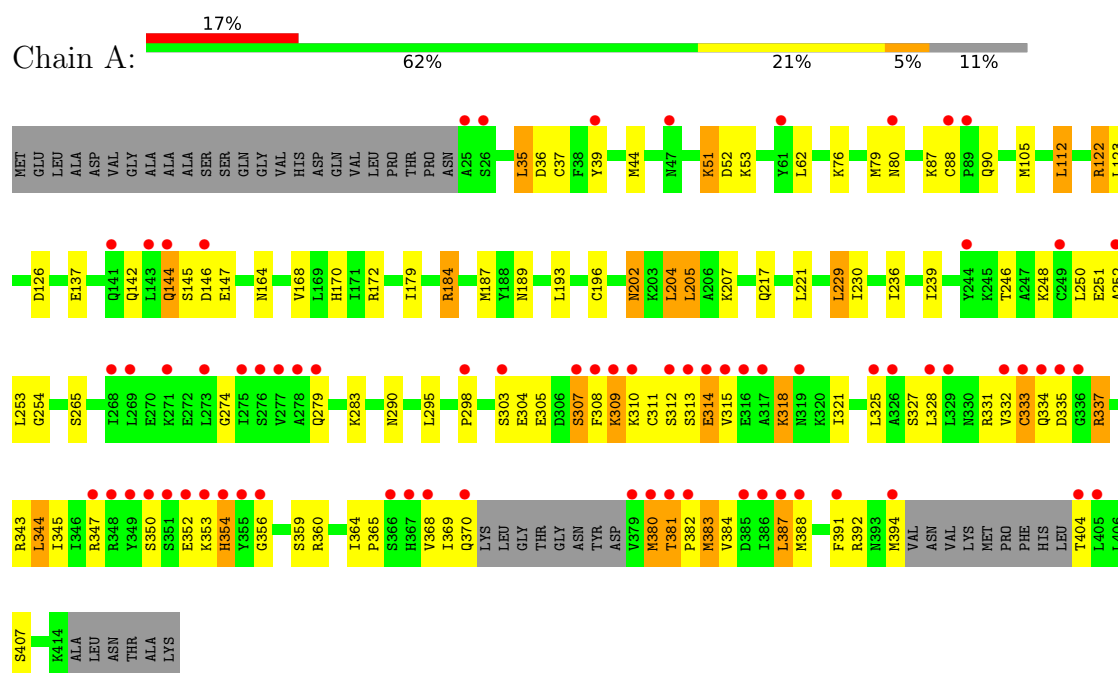
- Molecule 6 is water.

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

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.

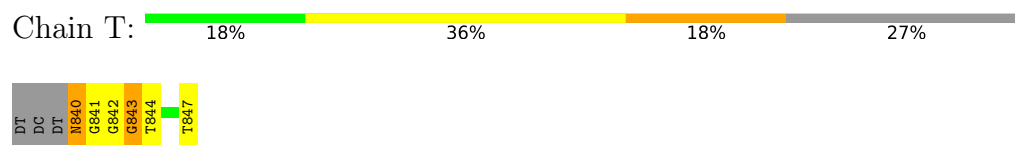
- Molecule 1: DNA polymerase iota



- Molecule 2: Primer DNA strand



- Molecule 3: Template DNA strand



4 Data and refinement statistics

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 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.1 (36.61-2.10) 97.1 (36.61-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.62 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, R_{free}	0.220 , 0.253 (Not available) , 0.302	Depositor DCC
R_{free} test set	3086 reflections (7.98%)	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 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.36	9/2914 (0.3%)	1.27	15/3934 (0.4%)
2	P	0.87	0/136	1.82	2/208 (1.0%)
3	T	1.00	0/160	2.09	7/245 (2.9%)
All	All	1.33	9/3210 (0.3%)	1.36	24/4387 (0.5%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	ARG	CD-NE	-7.75	1.35	1.46
1	A	179	ILE	CG1-CD1	-7.02	1.24	1.51
1	A	383	MET	C-O	-6.36	1.16	1.24
1	A	230	ILE	CA-CB	6.33	1.62	1.54
1	A	184	ARG	CD-NE	-6.06	1.37	1.46
1	A	39	TYR	N-CA	5.57	1.53	1.46
1	A	239	ILE	CA-C	5.45	1.58	1.52
1	A	207	LYS	CE-NZ	-5.18	1.33	1.49
1	A	391	PHE	C-O	5.13	1.29	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ARG	NE-CZ-NH2	-11.98	108.42	119.20
3	T	842	DG	P-O5'-C5'	11.63	137.44	120.00
3	T	843	DG	C2'-C3'-O3'	-10.56	95.66	111.50
2	P	867	DA	O5'-C5'-C4'	8.42	123.43	110.80
1	A	318	LYS	N-CA-C	-8.12	104.52	114.75
1	A	122	ARG	CD-NE-CZ	7.66	135.13	124.40
1	A	122	ARG	CG-CD-NE	-7.54	95.42	112.00
1	A	122	ARG	NE-CZ-NH1	7.22	128.72	121.50
3	T	842	DG	C5'-C4'-O4'	-6.75	99.28	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	870	DA	O4'-C1'-N9	6.63	118.34	108.40
1	A	274	GLY	N-CA-C	-6.39	104.74	112.48
3	T	842	DG	C2'-C3'-O3'	-6.39	101.91	111.50
3	T	843	DG	N9-C1'-C2'	-6.17	104.24	113.50
3	T	842	DG	O3'-P-O5'	5.82	112.72	104.00
1	A	88	CYS	CA-C-N	5.79	125.65	119.28
1	A	88	CYS	C-N-CA	5.79	125.65	119.28
3	T	844	DT	N1-C1'-C2'	-5.78	104.84	113.50
1	A	126	ASP	N-CA-C	5.73	120.09	112.30
1	A	179	ILE	CB-CA-C	-5.68	104.70	111.97
1	A	381	THR	CA-C-N	-5.62	113.23	119.19
1	A	381	THR	C-N-CA	-5.62	113.23	119.19
1	A	298	PRO	O-C-N	5.38	123.68	121.15
1	A	184	ARG	NE-CZ-NH2	-5.20	114.52	119.20
1	A	354	HIS	N-CA-C	5.06	121.58	110.80

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	85	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	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 14.

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: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: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
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:380:MET:HE2	1:A:384:VAL:HG23	1.76	0.67
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:44:MET:HE2	1:A:51:LYS:HG2	1.78	0.66
1:A:112:LEU:C	1:A:112:LEU:HD23	2.23	0.64
1:A:44:MET:HE2	1:A:51:LYS:HA	1.80	0.63
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:380:MET:HE2	1:A:384:VAL:CG2	2.30	0.61
1:A:308:PHE:O	1:A:404:THR:HA	2.00	0.60
1:A:335:ASP:CG	1:A:337:ARG:HD3	2.26	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: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:HD22	1:A:202:ASN:C	2.12	0.57
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:184:ARG:HA	1:A:187:MET:HE3	1.89	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:51:LYS:C	1:A:53:LYS:H	2.15	0.54
1:A:251:GLU:O	1:A:252:ALA:C	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:44:MET:HE3	1:A:51:LYS:HA	1.93	0.49
1:A:36:ASP:O	1:A:37:CYS:C	2.56	0.48
1:A:76:LYS:HB2	1:A:79:MET:HE3	1.95	0.48
1:A:105:MET:CG	1:A:193:LEU:HD11	2.44	0.48
1:A:313:SER:O	1:A:314:GLU:HB2	2.13	0.48
1:A:122:ARG:HD3	6:A:1043:HOH:O	2.12	0.48
1:A:347:ARG:HH11	1:A:404:THR:CG2	2.27	0.48
1:A:381:THR:N	1:A:382:PRO:HD2	2.29	0.47
1:A:144:GLN:HG3	1:A:147:GLU:CD	2.40	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: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:144:GLN:C	1:A:146:ASP:H	2.27	0.43
1:A:303:SER:O	1:A:331:ARG:NH2	2.52	0.42
1:A:251:GLU:C	1:A:253:LEU:N	2.74	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:304:GLU:HG2	1:A:331:ARG:HH21	1.85	0.41
1:A:364:ILE:HG12	1:A:383:MET:HE1	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	4 1

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 ⓘ

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%)	291 (91%)	30 (9%)	8 6

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	51	LYS
1	A	62	LEU
1	A	80	ASN
1	A	87	LYS
1	A	90	GLN
1	A	112	LEU
1	A	123	LEU
1	A	142	GLN
1	A	144	GLN
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	307	SER
1	A	309	LYS
1	A	325	LEU
1	A	327	SER
1	A	332	VAL
1	A	337	ARG
1	A	344	LEU
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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	90	GLN
1	A	170	HIS
1	A	202	ASN
1	A	216	ASN
1	A	256	ASN
1	A	262	GLN
1	A	300	GLN
1	A	330	ASN
1	A	334	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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$
2	DOC	P	873	2,3	16,19,20	1.13	2 (12%)	20,26,29	1.64	4 (20%)
3	3DR	T	840	3	8,11,12	1.42	1 (12%)	7,14,17	1.97	3 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DOC	P	873	2,3	-	0/7/18/19	0/2/2/2
3	3DR	T	840	3	-	2/3/15/16	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	840	3DR	O4'-C4'	-2.92	1.39	1.44
2	P	873	DOC	C6-C5	2.53	1.41	1.35
2	P	873	DOC	C6-N1	-2.00	1.33	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	873	DOC	C3'-C2'-C1'	4.46	108.01	102.87
3	T	840	3DR	O4'-C1'-C2'	-3.29	99.87	106.34
2	P	873	DOC	O4'-C1'-N1	3.14	113.43	107.86
2	P	873	DOC	O4'-C4'-C3'	3.04	109.80	104.81
3	T	840	3DR	C1'-C2'-C3'	-2.68	100.39	103.26
3	T	840	3DR	O3'-C3'-C2'	-2.67	105.17	111.43
2	P	873	DOC	C2'-C1'-N1	-2.61	107.45	112.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	T	840	3DR	O4'-C4'-C5'-O5'
3	T	840	3DR	C3'-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 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
4	TTP	A	875	5	29,30,30	2.07	7 (24%)	43,47,47	2.38	16 (37%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	875	TTP	C6-C5	5.26	1.43	1.34
4	A	875	TTP	PA-O3A	4.89	1.64	1.59
4	A	875	TTP	PB-O3B	4.54	1.64	1.59
4	A	875	TTP	C4-N3	-3.30	1.32	1.38
4	A	875	TTP	O2-C2	2.39	1.27	1.23
4	A	875	TTP	C2-N1	2.33	1.42	1.38
4	A	875	TTP	C4-C5	2.16	1.48	1.44

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	875	TTP	N3-C2-N1	6.26	123.03	114.89
4	A	875	TTP	C5-C4-N3	5.52	120.12	115.32
4	A	875	TTP	C4-N3-C2	-4.95	120.85	127.34
4	A	875	TTP	O2B-PB-O3A	4.49	119.42	107.27
4	A	875	TTP	O2-C2-N1	-4.23	117.29	122.80
4	A	875	TTP	O2A-PA-O3A	-3.99	96.48	107.27
4	A	875	TTP	O2B-PB-O3B	3.79	117.51	107.27
4	A	875	TTP	C5-C6-N1	-3.34	119.69	123.31
4	A	875	TTP	O4-C4-C5	-3.11	121.36	124.92
4	A	875	TTP	C6-N1-C2	-2.82	118.49	121.30
4	A	875	TTP	C5M-C5-C6	2.26	125.92	122.85
4	A	875	TTP	O2A-PA-O5'	2.26	117.82	107.57
4	A	875	TTP	O3B-PB-O1B	-2.23	104.01	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	875	TTP	C5M-C5-C4	-2.22	116.42	118.78
4	A	875	TTP	O2B-PB-O1B	-2.16	102.39	112.44
4	A	875	TTP	O3G-PG-O2G	2.08	115.62	107.80

There are no chirality outliers.

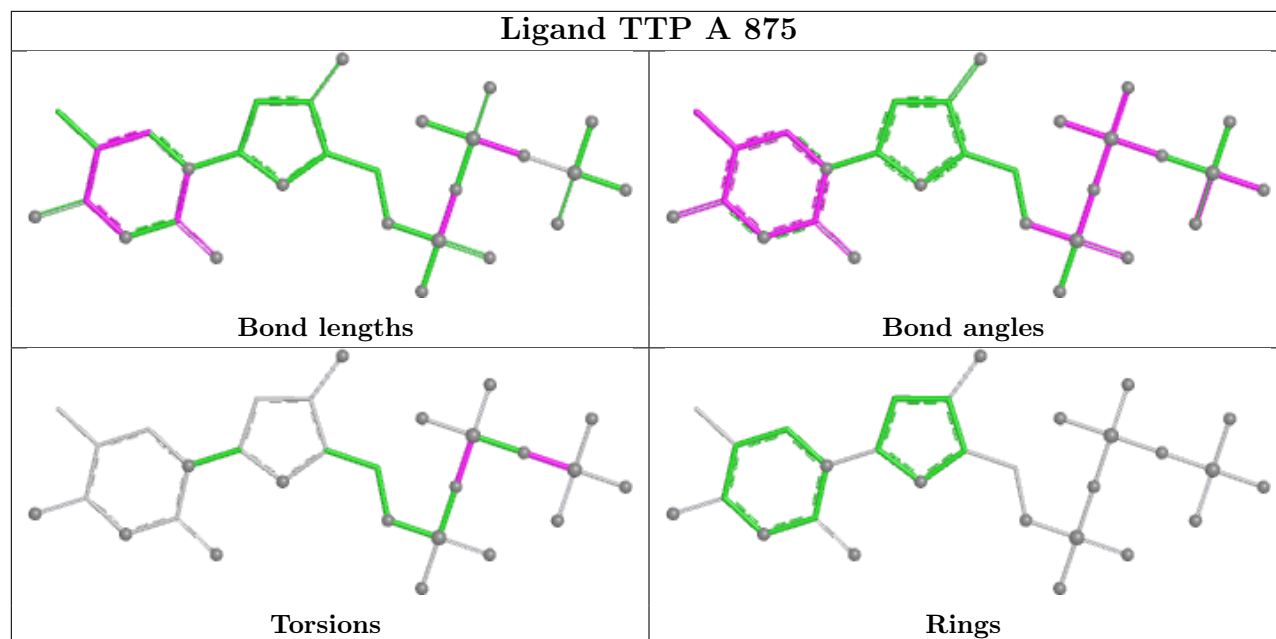
All (4) torsion outliers are listed below:

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 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	A	373/420 (88%)	0.98	72 (19%) 3 3	11, 27, 51, 65	0
2	P	6/7 (85%)	1.29	1 (16%) 4 4	21, 32, 36, 36	0
3	T	7/11 (63%)	0.32	0 100 100	15, 20, 22, 26	0
All	All	386/438 (88%)	0.97	73 (18%) 3 3	11, 27, 50, 65	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	25	ALA	7.2
1	A	354	HIS	7.1
1	A	379	VAL	6.2
1	A	349	TYR	6.1
1	A	367	HIS	5.4
1	A	351	SER	5.4
1	A	146	ASP	5.3
1	A	355	TYR	5.3
1	A	317	ALA	5.1
1	A	249	CYS	5.0
1	A	252	ALA	4.8
1	A	404	THR	4.8
1	A	350	SER	4.4
1	A	89	PRO	4.4
1	A	315	VAL	4.4
1	A	386	ILE	3.8
1	A	276	SER	3.8
1	A	88	CYS	3.7
1	A	244	TYR	3.7
1	A	316	GLU	3.6
1	A	144	GLN	3.6
1	A	366	SER	3.5
1	A	405	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	26	SER	3.4
1	A	353	LYS	3.4
1	A	314	GLU	3.3
1	A	334	GLN	3.3
1	A	381	THR	3.3
1	A	312	SER	3.2
1	A	80	ASN	3.2
1	A	370	GLN	3.2
1	A	391	PHE	3.2
1	A	336	GLY	3.2
1	A	326	ALA	3.1
1	A	313	SER	3.0
1	A	298	PRO	3.0
1	A	333	CYS	3.0
1	A	356	GLY	3.0
1	A	388	MET	3.0
1	A	309	LYS	2.9
1	A	310	LYS	2.8
1	A	61	TYR	2.8
1	A	273	LEU	2.8
1	A	278	ALA	2.8
1	A	348	ARG	2.7
1	A	385	ASP	2.7
1	A	308	PHE	2.7
1	A	279	GLN	2.7
1	A	368	VAL	2.7
1	A	268	ILE	2.7
2	P	867	DA	2.6
1	A	335	ASP	2.6
1	A	382	PRO	2.6
1	A	141	GLN	2.5
1	A	325	LEU	2.5
1	A	271	LYS	2.5
1	A	387	LEU	2.4
1	A	319	ASN	2.4
1	A	277	VAL	2.4
1	A	347	ARG	2.4
1	A	275	ILE	2.3
1	A	380	MET	2.3
1	A	394	MET	2.3
1	A	328	LEU	2.2
1	A	352	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	47	ASN	2.2
1	A	332	VAL	2.2
1	A	329	LEU	2.2
1	A	307	SER	2.2
1	A	143	LEU	2.1
1	A	39	TYR	2.1
1	A	269	LEU	2.0
1	A	303	SER	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	0.92	0.14	14,18,22,22	0
3	3DR	T	840	11/12	0.94	0.10	18,30,45,46	0

6.3 Carbohydrates [i](#)

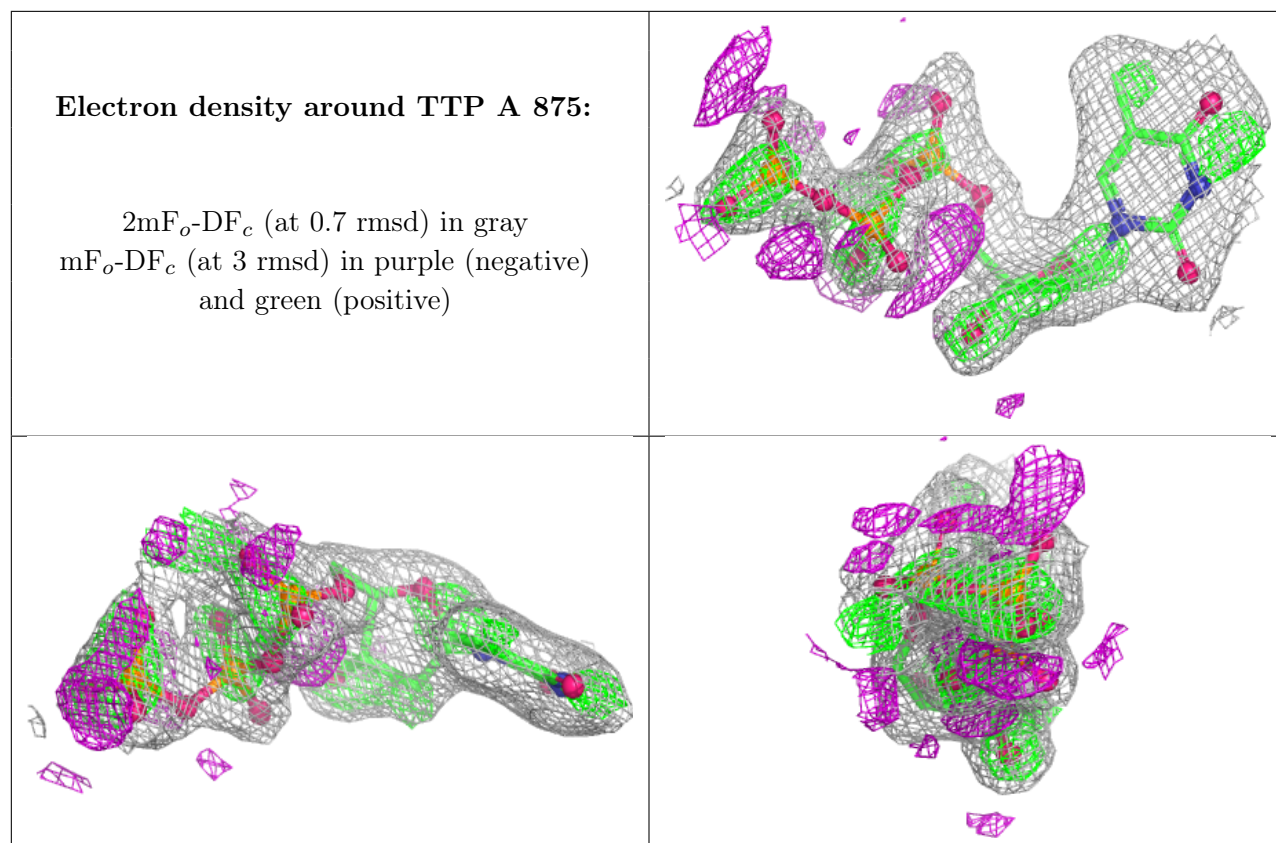
There are no oligosaccharides in this entry.

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
5	MG	A	871	1/1	0.52	0.23	12,12,12,12	0
5	MG	A	872	1/1	0.80	0.28	74,74,74,74	0
4	TTP	A	875	29/29	0.84	0.19	19,28,31,35	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.