



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:15 PM UTC

PDB ID : 2FLL / pdb_00002fl
Title : Ternary complex of human DNA polymerase iota with DNA and dTTP
Authors : Nair, D.T.; Johnson, R.E.; Prakash, L.; Prakash, S.; Aggarwal, A.K.
Deposited on : 2006-01-06
Resolution : 2.60 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

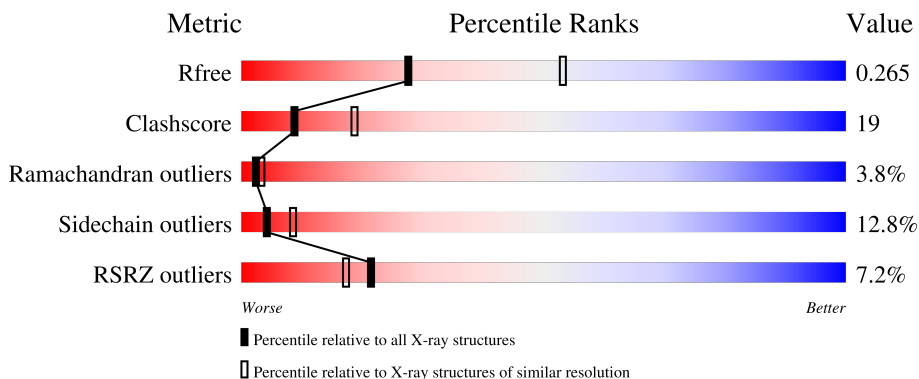
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	P	7	
2	T	11	
3	A	420	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3309 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 DNA chain called DNA primer strand.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	9	182	88	32	54	8	0	0	0

- Molecule 3 is a protein called DNA polymerase iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	373	2866	1802	502	541	21	0	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

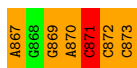
- Molecule 5 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).

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 primer strand

Chain P: 



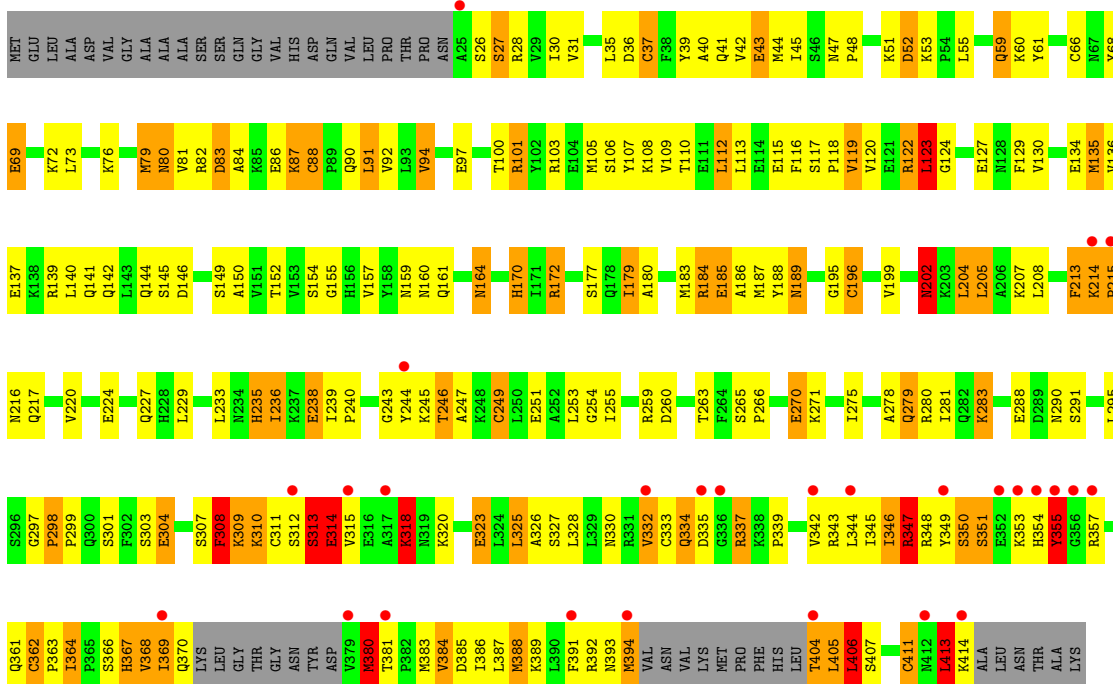
- Molecule 2: DNA template strand

Chain T: 



- Molecule 3: DNA polymerase iota

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.33Å 98.33Å 202.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.2 (50.00-2.60) 94.1 (50.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.29 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.223 , 0.277 (Not available) , 0.265	Depositor DCC
R_{free} test set	1450 reflections (7.83%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtrriage
Anisotropy	0.108	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3309	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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, 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	P	1.93	2/136 (1.5%)	2.51	9/208 (4.3%)
2	T	2.19	4/203 (2.0%)	2.34	16/312 (5.1%)
3	A	2.50	141/2904 (4.9%)	1.73	59/3922 (1.5%)
All	All	2.46	147/3243 (4.5%)	1.82	84/4442 (1.9%)

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	P	0	2
2	T	0	2
3	A	0	2
All	All	0	6

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	214	LYS	CA-C	-15.31	1.33	1.52
3	A	44	MET	SD-CE	-13.23	1.46	1.79
3	A	186	ALA	CA-CB	-11.73	1.35	1.53
3	A	116	PHE	C-O	-11.19	1.11	1.24
3	A	185	GLU	CA-C	10.39	1.66	1.52
3	A	389	LYS	CA-CB	10.37	1.69	1.53
3	A	255	ILE	CA-CB	-10.01	1.42	1.53
3	A	27	SER	C-O	-9.74	1.11	1.23
3	A	310	LYS	CA-CB	9.71	1.69	1.53
3	A	109	VAL	CA-CB	-9.65	1.43	1.54
3	A	199	VAL	CA-CB	-9.51	1.42	1.54
3	A	394	MET	SD-CE	-9.34	1.56	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	405	LEU	CA-CB	-9.25	1.37	1.53
3	A	199	VAL	C-O	-9.18	1.14	1.24
3	A	298	PRO	C-O	-9.07	1.14	1.24
3	A	213	PHE	C-O	-8.93	1.13	1.24
3	A	263	THR	C-O	-8.90	1.12	1.24
2	T	843	DG	O4'-C1'	-8.83	1.24	1.41
3	A	82	ARG	CA-CB	8.80	1.67	1.53
3	A	216	ASN	N-CA	8.65	1.60	1.47
3	A	103	ARG	CZ-NH2	8.57	1.44	1.33
3	A	245	LYS	C-O	-8.48	1.14	1.24
3	A	184	ARG	CD-NE	-8.43	1.34	1.46
3	A	355	TYR	CA-C	8.20	1.63	1.52
3	A	45	ILE	CA-CB	8.17	1.65	1.54
3	A	347	ARG	CA-C	8.00	1.62	1.52
3	A	381	THR	CA-C	7.95	1.62	1.52
3	A	155	GLY	CA-C	7.91	1.61	1.52
3	A	220	VAL	C-O	7.87	1.32	1.24
3	A	355	TYR	CA-CB	7.86	1.66	1.53
3	A	40	ALA	CA-CB	-7.84	1.40	1.53
3	A	384	VAL	CA-CB	-7.81	1.46	1.54
3	A	260	ASP	C-O	-7.68	1.15	1.24
3	A	202	ASN	CA-CB	-7.55	1.40	1.53
3	A	309	LYS	CA-C	-7.38	1.43	1.52
3	A	42	VAL	C-O	-7.22	1.15	1.24
3	A	43	GLU	CA-C	-7.06	1.43	1.52
3	A	160	ASN	CA-C	7.05	1.64	1.52
3	A	239	ILE	C-O	-7.03	1.15	1.24
3	A	180	ALA	CA-C	-7.01	1.43	1.52
3	A	380	MET	CG-SD	7.00	1.98	1.80
3	A	123	LEU	N-CA	-6.98	1.38	1.46
3	A	136	VAL	CA-CB	-6.97	1.46	1.54
3	A	45	ILE	C-O	-6.93	1.15	1.24
3	A	80	ASN	C-O	-6.92	1.15	1.23
3	A	386	ILE	CA-CB	6.92	1.62	1.54
2	T	839	DT	O3'-P	6.91	1.71	1.61
3	A	411	CYS	CA-C	-6.86	1.43	1.53
3	A	215	PRO	N-CA	6.85	1.56	1.47
3	A	227	GLN	N-CA	6.65	1.54	1.46
3	A	144	GLN	CA-C	6.64	1.61	1.52
3	A	154	SER	N-CA	-6.64	1.38	1.46
3	A	281	ILE	C-O	-6.57	1.15	1.24
3	A	172	ARG	CD-NE	-6.56	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	179	ILE	CG1-CD1	-6.48	1.26	1.51
3	A	41	GLN	CA-C	-6.43	1.44	1.52
3	A	141	GLN	C-O	-6.43	1.16	1.24
3	A	189	ASN	CB-CG	6.42	1.68	1.52
3	A	117	SER	C-O	-6.38	1.16	1.24
3	A	179	ILE	CA-CB	-6.35	1.46	1.54
3	A	159	ASN	CA-C	-6.33	1.43	1.52
3	A	79	MET	SD-CE	6.33	1.95	1.79
3	A	135	MET	CA-C	6.32	1.60	1.52
3	A	135	MET	SD-CE	6.32	1.95	1.79
3	A	254	GLY	C-O	-6.31	1.15	1.24
1	P	872	DC	O4'-C1'	-6.30	1.29	1.41
3	A	243	GLY	N-CA	6.26	1.49	1.44
3	A	164	ASN	C-O	-6.26	1.16	1.24
3	A	129	PHE	CA-C	-6.19	1.45	1.52
3	A	183	MET	CA-C	6.18	1.60	1.52
3	A	346	ILE	CA-CB	6.17	1.63	1.55
3	A	122	ARG	CD-NE	-6.17	1.37	1.46
3	A	118	PRO	CA-CB	6.15	1.62	1.53
1	P	871	DC	O3'-P	6.13	1.70	1.61
3	A	30	ILE	CA-CB	-6.08	1.46	1.54
3	A	259	ARG	C-O	-6.08	1.16	1.24
3	A	313	SER	CA-C	6.06	1.60	1.52
3	A	297	GLY	N-CA	-6.03	1.36	1.44
3	A	271	LYS	CA-CB	6.00	1.61	1.53
3	A	278	ALA	CA-CB	6.00	1.62	1.53
3	A	150	ALA	CA-C	5.99	1.60	1.52
3	A	406	LEU	CA-C	5.99	1.59	1.52
3	A	140	LEU	C-O	-5.95	1.17	1.24
3	A	263	THR	CA-CB	5.88	1.64	1.53
3	A	187	MET	N-CA	-5.84	1.39	1.46
3	A	380	MET	SD-CE	5.80	1.94	1.79
3	A	105	MET	CG-SD	5.79	1.95	1.80
3	A	189	ASN	CG-OD1	5.79	1.34	1.23
3	A	323	GLU	N-CA	5.74	1.53	1.46
3	A	157	VAL	C-O	-5.74	1.18	1.24
3	A	120	VAL	CA-C	-5.69	1.46	1.52
3	A	351	SER	CA-C	5.69	1.60	1.52
3	A	202	ASN	CG-ND2	-5.66	1.21	1.33
2	T	844	DT	O3'-P	5.64	1.69	1.61
3	A	349	TYR	CA-CB	5.62	1.60	1.53
3	A	113	LEU	N-CA	5.62	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	28	ARG	N-CA	-5.61	1.38	1.45
3	A	188	TYR	CA-C	5.61	1.60	1.52
3	A	40	ALA	CA-C	5.59	1.60	1.52
3	A	177	SER	C-O	-5.58	1.17	1.24
3	A	216	ASN	C-O	-5.57	1.16	1.23
3	A	283	LYS	CE-NZ	5.55	1.66	1.49
3	A	290	ASN	CG-OD1	5.54	1.34	1.23
3	A	385	ASP	CA-C	5.51	1.60	1.52
3	A	134	GLU	CA-C	-5.48	1.45	1.52
3	A	233	LEU	C-O	5.42	1.30	1.23
3	A	30	ILE	C-O	5.42	1.29	1.24
3	A	44	MET	N-CA	5.39	1.53	1.46
3	A	139	ARG	CA-C	-5.35	1.45	1.52
3	A	244	TYR	N-CA	5.34	1.53	1.46
3	A	291	SER	CA-C	5.34	1.59	1.53
3	A	103	ARG	CA-CB	-5.33	1.44	1.53
3	A	196	CYS	C-O	5.31	1.30	1.23
3	A	39	TYR	CB-CG	5.31	1.63	1.51
3	A	172	ARG	CZ-NH2	5.30	1.40	1.33
3	A	115	GLU	C-O	-5.29	1.17	1.24
3	A	290	ASN	CB-CG	5.28	1.65	1.52
3	A	84	ALA	CA-CB	-5.26	1.44	1.53
3	A	380	MET	CA-C	-5.26	1.46	1.52
3	A	101	ARG	CD-NE	5.24	1.53	1.46
3	A	314	GLU	CA-CB	5.24	1.62	1.53
3	A	100	THR	N-CA	-5.23	1.40	1.46
3	A	59	GLN	C-O	-5.22	1.18	1.23
3	A	119	VAL	CA-C	-5.22	1.47	1.53
3	A	152	THR	CA-CB	5.22	1.62	1.53
3	A	122	ARG	CZ-NH1	-5.20	1.25	1.32
3	A	337	ARG	CA-CB	5.20	1.62	1.53
3	A	189	ASN	N-CA	-5.19	1.40	1.46
3	A	303	SER	CA-C	5.18	1.59	1.52
3	A	170	HIS	CA-C	-5.16	1.46	1.52
3	A	249	CYS	CA-C	-5.16	1.46	1.52
3	A	208	LEU	N-CA	-5.16	1.40	1.46
3	A	94	VAL	CA-C	-5.12	1.46	1.52
3	A	238	GLU	C-O	5.11	1.30	1.24
2	T	847	DT	O4'-C1'	-5.09	1.31	1.41
3	A	108	LYS	CE-NZ	5.07	1.64	1.49
3	A	110	THR	CA-C	5.07	1.59	1.52
3	A	80	ASN	N-CA	5.06	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	87	LYS	CA-C	-5.06	1.45	1.52
3	A	66	CYS	CA-CB	-5.05	1.45	1.53
3	A	183	MET	N-CA	-5.04	1.40	1.46
3	A	207	LYS	C-N	-5.03	1.27	1.33
3	A	86	GLU	CA-C	5.03	1.60	1.52
3	A	361	GLN	CA-C	5.03	1.60	1.53
3	A	184	ARG	CA-C	5.01	1.59	1.52
3	A	189	ASN	C-O	-5.00	1.18	1.24
3	A	280	ARG	CZ-NH2	5.00	1.40	1.33

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	867	DA	O5'-C5'-C4'	13.57	131.16	110.80
2	T	847	DT	C4'-C3'-O3'	11.54	127.32	110.00
1	P	872	DC	C4'-C3'-O3'	11.05	126.58	110.00
1	P	871	DC	C4'-C3'-O3'	9.87	124.80	110.00
3	A	270	GLU	N-CA-C	-9.82	99.33	111.11
3	A	350	SER	N-CA-C	9.59	119.52	108.49
2	T	842	DG	C3'-C2'-C1'	9.09	115.23	101.60
3	A	407	SER	N-CA-C	8.93	122.09	108.52
2	T	842	DG	C4'-C3'-O3'	8.91	123.37	110.00
2	T	844	DT	C5'-C4'-C3'	-8.72	101.82	114.90
3	A	87	LYS	N-CA-C	-8.05	102.93	114.12
3	A	363	PRO	CA-C-N	7.76	127.88	122.60
3	A	363	PRO	C-N-CA	7.76	127.88	122.60
2	T	839	DT	P-O3'-C3'	7.67	131.71	120.20
3	A	271	LYS	N-CA-C	7.67	121.10	112.97
1	P	869	DG	P-O3'-C3'	-7.34	109.19	120.20
2	T	845	DC	C2'-C3'-O3'	7.33	122.50	111.50
3	A	406	LEU	N-CA-C	7.27	121.26	109.40
3	A	349	TYR	N-CA-C	7.24	120.07	108.41
3	A	394	MET	CB-CA-C	-7.04	96.73	110.10
3	A	389	LYS	N-CA-C	-6.89	103.84	111.36
3	A	279	GLN	N-CA-C	-6.83	104.42	112.89
3	A	215	PRO	CA-C-N	-6.55	113.15	123.24
3	A	215	PRO	C-N-CA	-6.55	113.15	123.24
3	A	47	ASN	CA-C-N	6.49	127.00	119.47
3	A	47	ASN	C-N-CA	6.49	127.00	119.47
3	A	309	LYS	CA-C-N	6.44	133.84	121.54
3	A	309	LYS	C-N-CA	6.44	133.84	121.54
3	A	88	CYS	CA-C-N	6.29	126.04	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	88	CYS	C-N-CA	6.29	126.04	119.05
3	A	388	MET	N-CA-C	6.26	118.19	111.36
2	T	839	DT	O5'-C5'-C4'	6.26	120.19	110.80
1	P	870	DA	C5'-C4'-O4'	-6.17	100.14	109.40
3	A	309	LYS	O-C-N	6.16	130.25	123.22
2	T	847	DT	C2'-C3'-O3'	6.14	120.71	111.50
1	P	867	DA	C1'-O4'-C4'	6.04	118.77	109.70
3	A	318	LYS	N-CA-C	-5.97	105.82	113.23
3	A	405	LEU	CA-C-N	5.95	131.87	122.94
3	A	405	LEU	C-N-CA	5.95	131.87	122.94
3	A	214	LYS	CA-C-O	-5.94	112.02	120.16
2	T	843	DG	C4'-C3'-C2'	-5.91	93.54	102.40
3	A	347	ARG	CB-CA-C	5.88	123.10	110.45
3	A	332	VAL	CB-CA-C	-5.88	103.47	112.05
3	A	380	MET	N-CA-C	-5.87	104.51	111.03
3	A	364	ILE	N-CA-C	5.86	112.90	107.56
3	A	215	PRO	N-CD-CG	-5.78	94.54	103.20
3	A	185	GLU	N-CA-C	-5.77	104.91	111.14
1	P	867	DA	O4'-C4'-C3'	-5.72	96.82	105.40
3	A	405	LEU	N-CA-C	5.68	122.89	110.80
2	T	843	DG	C4'-C3'-O3'	5.66	118.49	110.00
3	A	80	ASN	N-CA-CB	5.65	118.30	110.17
3	A	265	SER	N-CA-C	5.63	119.43	109.58
3	A	325	LEU	N-CA-C	5.63	117.28	111.03
3	A	79	MET	CA-C-O	-5.61	114.82	121.16
2	T	844	DT	C4-C5-C6	-5.61	110.79	119.20
3	A	124	GLY	N-CA-C	-5.59	102.16	112.62
3	A	411	CYS	O-C-N	5.58	130.14	122.72
2	T	840	DA	OP1-P-OP2	-5.55	103.35	120.00
3	A	312	SER	N-CA-C	5.53	118.38	107.98
3	A	61	TYR	N-CA-C	-5.52	104.97	112.26
3	A	320	LYS	N-CA-C	-5.49	105.29	111.28
3	A	381	THR	CB-CA-C	5.49	120.99	110.17
3	A	278	ALA	CA-C-N	-5.49	111.53	121.14
3	A	278	ALA	C-N-CA	-5.49	111.53	121.14
3	A	249	CYS	CB-CA-C	-5.35	101.75	110.85
3	A	312	SER	CA-C-O	-5.32	115.62	121.58
3	A	308	PHE	CA-C-N	-5.32	115.70	122.77
3	A	308	PHE	C-N-CA	-5.32	115.70	122.77
1	P	867	DA	P-O3'-C3'	5.24	128.06	120.20
2	T	845	DC	OP1-P-O3'	-5.20	92.39	108.00
1	P	867	DA	O4'-C1'-N9	5.20	116.20	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	839	DT	O3'-P-O5'	-5.19	96.21	104.00
3	A	215	PRO	O-C-N	-5.19	115.64	122.64
3	A	172	ARG	CG-CD-NE	-5.17	100.62	112.00
3	A	413	LEU	N-CA-C	5.15	118.10	110.48
3	A	79	MET	N-CA-CB	-5.14	102.63	110.85
3	A	179	ILE	CB-CA-C	-5.14	105.21	112.14
3	A	323	GLU	CB-CA-C	-5.12	103.08	110.96
2	T	842	DG	O3'-P-O5'	5.09	111.64	104.00
3	A	362	CYS	O-C-N	-5.09	117.87	121.84
2	T	839	DT	N1-C1'-C2'	-5.04	105.95	113.50
3	A	347	ARG	CA-CB-CG	5.03	124.16	114.10
3	A	304	GLU	N-CA-C	-5.02	101.74	109.52
3	A	72	LYS	N-CA-C	5.01	117.47	111.71

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	213	PHE	Peptide
3	A	68	TYR	Sidechain
1	P	871	DC	Sidechain
1	P	872	DC	Sidechain
2	T	842	DG	Sidechain
2	T	843	DG	Sidechain

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	P	139	0	77	4	2
2	T	182	0	103	7	2
3	A	2866	0	2888	112	0
4	A	2	0	0	0	0
5	A	29	0	13	1	0
6	A	86	0	0	3	0
6	T	5	0	0	0	0
All	All	3309	0	3081	118	2

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 19.

All (118) 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)
3:A:391:PHE:O	3:A:394:MET:HB2	1.62	0.97
1:P:871:DC:OP1	3:A:246:THR:HG22	1.66	0.93
2:T:841:DG:H2''	2:T:842:DG:H5''	1.52	0.91
3:A:283:LYS:HE3	3:A:288:GLU:OE1	1.73	0.88
3:A:405:LEU:C	3:A:406:LEU:HD23	2.04	0.83
3:A:367:HIS:N	3:A:367:HIS:ND1	2.32	0.78
3:A:202:ASN:HD22	3:A:202:ASN:C	1.94	0.75
3:A:308:PHE:HB2	3:A:311:CYS:HB2	1.69	0.75
3:A:335:ASP:OD2	3:A:337:ARG:NH1	2.21	0.73
3:A:413:LEU:N	3:A:413:LEU:CD2	2.52	0.73
3:A:172:ARG:HD3	6:A:912:HOH:O	1.89	0.72
3:A:325:LEU:HD11	3:A:387:LEU:HD11	1.72	0.72
3:A:413:LEU:N	3:A:413:LEU:HD23	2.06	0.71
3:A:137:GLU:HG2	3:A:172:ARG:HH12	1.58	0.68
3:A:249:CYS:O	3:A:253:LEU:HD12	1.92	0.68
3:A:73:LEU:HD12	3:A:73:LEU:N	2.09	0.67
3:A:119:VAL:HB	6:A:1054:HOH:O	1.94	0.67
3:A:135:MET:HE2	3:A:179:ILE:HD12	1.77	0.66
3:A:406:LEU:HD23	3:A:406:LEU:N	2.11	0.66
3:A:283:LYS:CE	3:A:288:GLU:OE1	2.43	0.66
3:A:342:VAL:HG21	3:A:387:LEU:HD21	1.78	0.66
3:A:344:LEU:HD11	3:A:387:LEU:CD2	2.26	0.65
3:A:76:LYS:HB2	3:A:79:MET:HE3	1.80	0.63
3:A:325:LEU:HD23	3:A:380:MET:HE3	1.80	0.63
3:A:325:LEU:HD11	3:A:387:LEU:CD1	2.28	0.62
3:A:137:GLU:HG2	3:A:172:ARG:NH1	2.15	0.62
3:A:202:ASN:HD21	3:A:205:LEU:H	1.49	0.61
3:A:337:ARG:HG2	3:A:414:LYS:C	2.26	0.60
3:A:347:ARG:HD3	3:A:404:THR:HG23	1.83	0.60
3:A:88:CYS:SG	3:A:90:GLN:O	2.59	0.60
3:A:202:ASN:ND2	3:A:205:LEU:H	2.00	0.60
1:P:871:DC:OP1	3:A:246:THR:CG2	2.45	0.59
3:A:283:LYS:HE2	3:A:288:GLU:HB3	1.86	0.57
3:A:344:LEU:HD11	3:A:387:LEU:HD22	1.86	0.57
3:A:413:LEU:HD23	3:A:413:LEU:H	1.65	0.57
3:A:238:GLU:O	3:A:240:PRO:HD3	2.05	0.56
3:A:73:LEU:HD12	3:A:73:LEU:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:392:ARG:C	3:A:394:MET:H	2.15	0.55
3:A:346:ILE:HG12	3:A:394:MET:HE3	1.88	0.55
3:A:368:VAL:HG21	3:A:383:MET:CE	2.36	0.55
3:A:369:ILE:O	3:A:369:ILE:HG22	2.06	0.55
3:A:325:LEU:O	3:A:326:ALA:C	2.46	0.55
2:T:840:DA:OP1	3:A:309:LYS:HE3	2.08	0.53
2:T:841:DG:C2'	2:T:842:DG:H5''	2.32	0.53
3:A:347:ARG:HG2	3:A:404:THR:HG23	1.92	0.52
3:A:202:ASN:C	3:A:202:ASN:ND2	2.62	0.52
3:A:332:VAL:CG1	3:A:339:PRO:HD3	2.40	0.52
3:A:112:LEU:C	3:A:112:LEU:HD23	2.36	0.51
3:A:161:GLN:NE2	3:A:224:GLU:HB2	2.25	0.51
3:A:189:ASN:HB3	6:A:1028:HOH:O	2.11	0.51
1:P:873:DOC:H2'	5:A:875:TTP:HM52	1.92	0.50
3:A:137:GLU:CG	3:A:172:ARG:HH12	2.25	0.50
3:A:304:GLU:HG3	3:A:328:LEU:HG	1.94	0.49
3:A:51:LYS:C	3:A:53:LYS:H	2.20	0.49
3:A:196:CYS:SG	3:A:214:LYS:O	2.71	0.49
3:A:380:MET:HE2	3:A:384:VAL:HG22	1.95	0.49
3:A:266:PRO:O	3:A:270:GLU:HB2	2.13	0.49
2:T:840:DA:H1'	3:A:59:GLN:OE1	2.13	0.48
3:A:83:ASP:O	3:A:87:LYS:HB2	2.14	0.48
3:A:275:ILE:HG12	3:A:279:GLN:NE2	2.27	0.48
3:A:299:PRO:O	3:A:337:ARG:NH2	2.47	0.48
3:A:380:MET:CE	3:A:384:VAL:HG22	2.43	0.48
3:A:170:HIS:HE1	3:A:224:GLU:OE2	1.97	0.47
3:A:369:ILE:C	3:A:370:GLN:CG	2.86	0.47
3:A:164:ASN:H	3:A:170:HIS:HD2	1.61	0.47
3:A:308:PHE:HB2	3:A:311:CYS:CB	2.42	0.47
3:A:73:LEU:N	3:A:73:LEU:CD1	2.77	0.47
3:A:69:GLU:O	3:A:73:LEU:CD1	2.62	0.47
3:A:344:LEU:HD11	3:A:387:LEU:HD23	1.97	0.47
3:A:350:SER:OG	3:A:351:SER:N	2.47	0.46
2:T:844:DT:OP2	3:A:301:SER:OG	2.33	0.46
3:A:106:SER:OG	3:A:122:ARG:NH2	2.48	0.46
3:A:392:ARG:C	3:A:394:MET:N	2.73	0.46
3:A:404:THR:O	3:A:405:LEU:CB	2.60	0.46
3:A:36:ASP:O	3:A:37:CYS:C	2.60	0.45
3:A:235:HIS:HD2	3:A:238:GLU:OE2	1.99	0.45
3:A:184:ARG:HD2	3:A:195:GLY:O	2.17	0.45
3:A:308:PHE:CZ	3:A:405:LEU:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:43:GLU:OE1	3:A:101:ARG:NH2	2.51	0.44
3:A:51:LYS:O	3:A:52:ASP:CG	2.60	0.44
3:A:55:LEU:HD12	3:A:92:VAL:O	2.17	0.44
3:A:170:HIS:CE1	3:A:224:GLU:OE2	2.71	0.44
3:A:308:PHE:CD1	3:A:308:PHE:O	2.69	0.44
3:A:73:LEU:H	3:A:73:LEU:CD1	2.31	0.44
3:A:330:ASN:O	3:A:333:CYS:HB3	2.18	0.44
3:A:318:LYS:HD2	3:A:388:MET:HE2	2.00	0.44
3:A:388:MET:O	3:A:391:PHE:HB3	2.18	0.44
3:A:88:CYS:O	3:A:91:LEU:HB2	2.17	0.43
3:A:204:LEU:HD13	3:A:205:LEU:HD13	2.00	0.43
3:A:353:LYS:O	3:A:355:TYR:N	2.52	0.43
3:A:196:CYS:HA	3:A:217:GLN:O	2.18	0.43
3:A:283:LYS:HE2	3:A:288:GLU:CB	2.47	0.43
2:T:844:DT:O5'	2:T:844:DT:H2'	2.18	0.43
3:A:31:VAL:HG12	3:A:130:VAL:HB	1.99	0.43
3:A:275:ILE:HG12	3:A:279:GLN:HE21	1.83	0.43
3:A:327:SER:O	3:A:328:LEU:C	2.57	0.43
3:A:368:VAL:C	3:A:370:GLN:H	2.27	0.43
3:A:384:VAL:O	3:A:388:MET:HG2	2.19	0.43
3:A:364:ILE:O	3:A:364:ILE:HG22	2.18	0.42
3:A:380:MET:HE2	3:A:384:VAL:CG2	2.49	0.42
3:A:298:PRO:HA	3:A:299:PRO:HD3	1.84	0.42
2:T:840:DA:N3	2:T:840:DA:H2'	2.35	0.42
3:A:369:ILE:C	3:A:370:GLN:HG3	2.43	0.42
3:A:405:LEU:O	3:A:406:LEU:HD23	2.19	0.42
3:A:247:ALA:O	3:A:251:GLU:HG3	2.20	0.42
3:A:308:PHE:CE1	3:A:405:LEU:HA	2.55	0.42
3:A:60:LYS:NZ	3:A:97:GLU:CD	2.78	0.41
3:A:123:LEU:O	3:A:127:GLU:HB2	2.20	0.41
3:A:369:ILE:O	3:A:369:ILE:CG2	2.67	0.41
3:A:236:ILE:H	3:A:236:ILE:HG12	1.60	0.41
3:A:334:GLN:HE21	3:A:334:GLN:HB3	1.51	0.41
3:A:342:VAL:CG2	3:A:387:LEU:HD21	2.49	0.41
3:A:343:ARG:HD2	3:A:345:ILE:HD11	2.02	0.41
3:A:270:GLU:HG2	3:A:275:ILE:HG13	2.03	0.41
3:A:283:LYS:HD2	3:A:283:LYS:HA	1.88	0.40
1:P:869:DG:H2''	1:P:870:DA:H5'	2.03	0.40
3:A:318:LYS:HB2	3:A:388:MET:CE	2.51	0.40
3:A:107:TYR:OH	3:A:299:PRO:HG3	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:867:DA:O5'	2:T:847:DT:O3'[10_665]	1.65	0.55
1:P:867:DA:C5'	2:T:847:DT:O3'[10_665]	2.02	0.18

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
3	A	367/420 (87%)	322 (88%)	31 (8%)	14 (4%)	2 3

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	310	LYS
3	A	313	SER
3	A	314	GLU
3	A	315	VAL
3	A	354	HIS
3	A	355	TYR
3	A	37	CYS
3	A	52	ASP
3	A	215	PRO
3	A	146	ASP
3	A	308	PHE
3	A	393	ASN
3	A	334	GLN
3	A	369	ILE

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
3	A	321/376 (85%)	280 (87%)	41 (13%)	4 8

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	26	SER
3	A	27	SER
3	A	35	LEU
3	A	48	PRO
3	A	69	GLU
3	A	80	ASN
3	A	81	VAL
3	A	83	ASP
3	A	91	LEU
3	A	94	VAL
3	A	112	LEU
3	A	123	LEU
3	A	142	GLN
3	A	145	SER
3	A	149	SER
3	A	185	GLU
3	A	202	ASN
3	A	204	LEU
3	A	205	LEU
3	A	229	LEU
3	A	235	HIS
3	A	236	ILE
3	A	246	THR
3	A	295	LEU
3	A	307	SER
3	A	313	SER
3	A	314	GLU
3	A	318	LYS
3	A	323	GLU
3	A	347	ARG
3	A	348	ARG
3	A	357	ARG
3	A	362	CYS
3	A	366	SER
3	A	367	HIS

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Mol	Chain	Res	Type
3	A	368	VAL
3	A	380	MET
3	A	404	THR
3	A	406	LEU
3	A	411	CYS
3	A	413	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	47	ASN
3	A	58	GLN
3	A	80	ASN
3	A	128	ASN
3	A	144	GLN
3	A	170	HIS
3	A	189	ASN
3	A	202	ASN
3	A	216	ASN
3	A	235	HIS
3	A	256	ASN
3	A	262	GLN
3	A	279	GLN
3	A	334	GLN
3	A	412	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](#)

1 non-standard protein/DNA/RNA residue is 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
1	DOC	P	873	1,2	16,19,20	2.61	6 (37%)	20,26,29	2.09	8 (40%)

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
1	DOC	P	873	1,2	-	1/7/18/19	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	873	DOC	O4'-C1'	-5.55	1.30	1.42
1	P	873	DOC	C1'-N1	5.18	1.61	1.48
1	P	873	DOC	C6-C5	-3.76	1.26	1.35
1	P	873	DOC	C2-N1	-3.27	1.33	1.40
1	P	873	DOC	O5'-C5'	-2.93	1.35	1.44
1	P	873	DOC	C3'-C2'	-2.63	1.46	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	873	DOC	C2'-C1'-N1	-4.43	104.00	112.40
1	P	873	DOC	O4'-C1'-C2'	-3.22	102.60	106.41
1	P	873	DOC	C4'-O4'-C1'	2.97	112.61	109.81
1	P	873	DOC	C5-C6-N1	2.84	126.45	121.84
1	P	873	DOC	C4-N3-C2	2.54	124.26	120.26
1	P	873	DOC	O4'-C4'-C5'	2.27	113.43	109.34
1	P	873	DOC	N1-C2-N3	-2.26	114.88	118.80
1	P	873	DOC	O2-C2-N3	2.00	125.49	122.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	P	873	DOC	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	873	DOC	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$
5	TTP	A	875	4	29,30,30	2.14	9 (31%)	43,47,47	2.34	13 (30%)

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	A	875	4	-	4/22/34/34	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	875	TTP	C5M-C5	-6.51	1.34	1.50
5	A	875	TTP	C4-N3	-4.46	1.30	1.38
5	A	875	TTP	C6-C5	3.05	1.39	1.34
5	A	875	TTP	C5'-C4'	-3.05	1.42	1.51
5	A	875	TTP	O4-C4	2.96	1.29	1.23
5	A	875	TTP	PA-O1A	-2.59	1.41	1.50
5	A	875	TTP	PB-O3A	2.45	1.62	1.59
5	A	875	TTP	C3'-C4'	-2.26	1.47	1.53
5	A	875	TTP	O5'-C5'	2.25	1.53	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	875	TTP	C6-N1-C2	-7.55	113.79	121.30
5	A	875	TTP	N3-C2-N1	6.14	122.89	114.89
5	A	875	TTP	C1'-N1-C6	5.91	130.67	120.74
5	A	875	TTP	O5'-C5'-C4'	3.61	121.29	108.99
5	A	875	TTP	C4-N3-C2	-3.45	122.82	127.34
5	A	875	TTP	C5-C4-N3	3.42	118.29	115.32
5	A	875	TTP	O2-C2-N3	-3.25	115.50	121.49
5	A	875	TTP	O3A-PB-O1B	-3.08	101.44	110.70
5	A	875	TTP	C5M-C5-C4	2.30	121.24	118.78
5	A	875	TTP	O2B-PB-O3A	2.17	113.15	107.27
5	A	875	TTP	O4'-C4'-C5'	2.12	116.13	109.33
5	A	875	TTP	C2'-C1'-N1	-2.03	108.75	113.81
5	A	875	TTP	C3'-C2'-C1'	2.02	107.53	102.60

There are no chirality outliers.

All (4) torsion outliers are listed below:

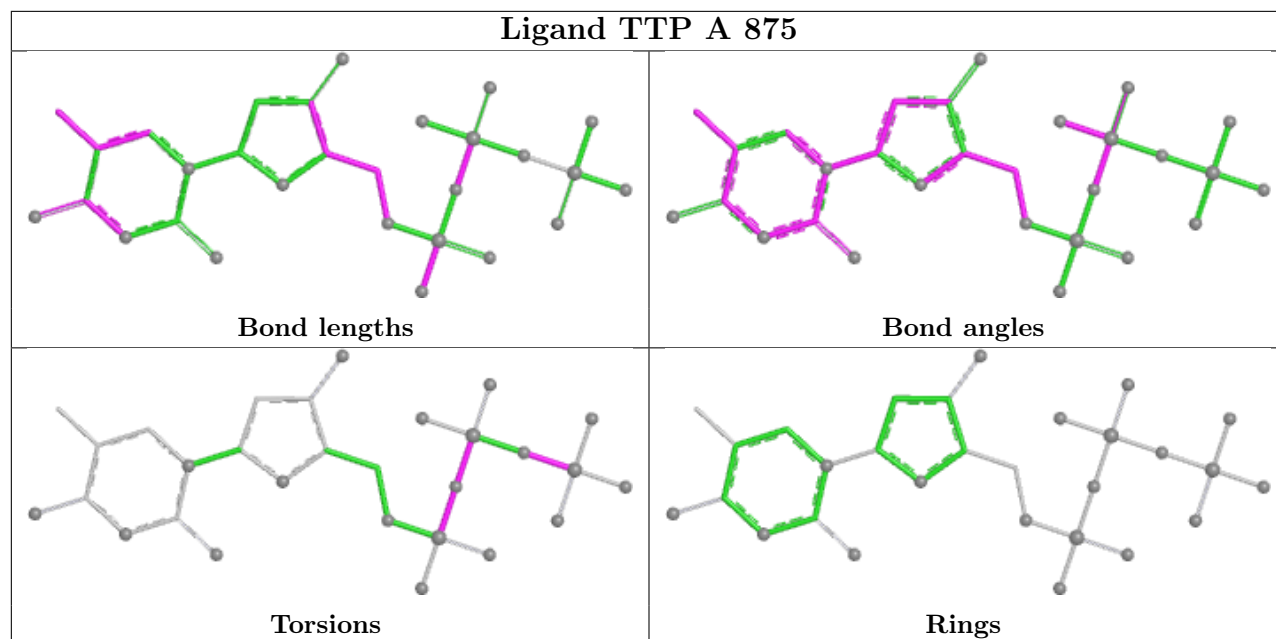
Mol	Chain	Res	Type	Atoms
5	A	875	TTP	PB-O3B-PG-O2G
5	A	875	TTP	PA-O3A-PB-O1B
5	A	875	TTP	PB-O3A-PA-O2A
5	A	875	TTP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	875	TTP	1	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	P	6/7 (85%)	-0.46	0 100 100	24, 38, 44, 44	0
2	T	9/11 (81%)	0.60	1 (11%) 10 8	29, 33, 51, 90	0
3	A	373/420 (88%)	0.23	27 (7%) 21 17	15, 43, 84, 102	0
All	All	388/438 (88%)	0.23	28 (7%) 21 17	15, 42, 84, 102	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	355	TYR	8.8
3	A	25	ALA	6.8
2	T	839	DT	6.2
3	A	354	HIS	5.9
3	A	349	TYR	4.9
3	A	332	VAL	4.1
3	A	353	LYS	4.0
3	A	356	GLY	3.6
3	A	394	MET	3.0
3	A	352	GLU	2.9
3	A	317	ALA	2.7
3	A	414	LYS	2.7
3	A	344	LEU	2.6
3	A	214	LYS	2.5
3	A	336	GLY	2.4
3	A	357	ARG	2.4
3	A	412	ASN	2.3
3	A	335	ASP	2.3
3	A	404	THR	2.2
3	A	315	VAL	2.2
3	A	381	THR	2.1
3	A	342	VAL	2.1
3	A	379	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	A	391	PHE	2.1
3	A	244	TYR	2.1
3	A	312	SER	2.0
3	A	215	PRO	2.0
3	A	369	ILE	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
1	DOC	P	873	18/19	0.96	0.08	11,25,41,43	0

6.3 Carbohydrates [i](#)

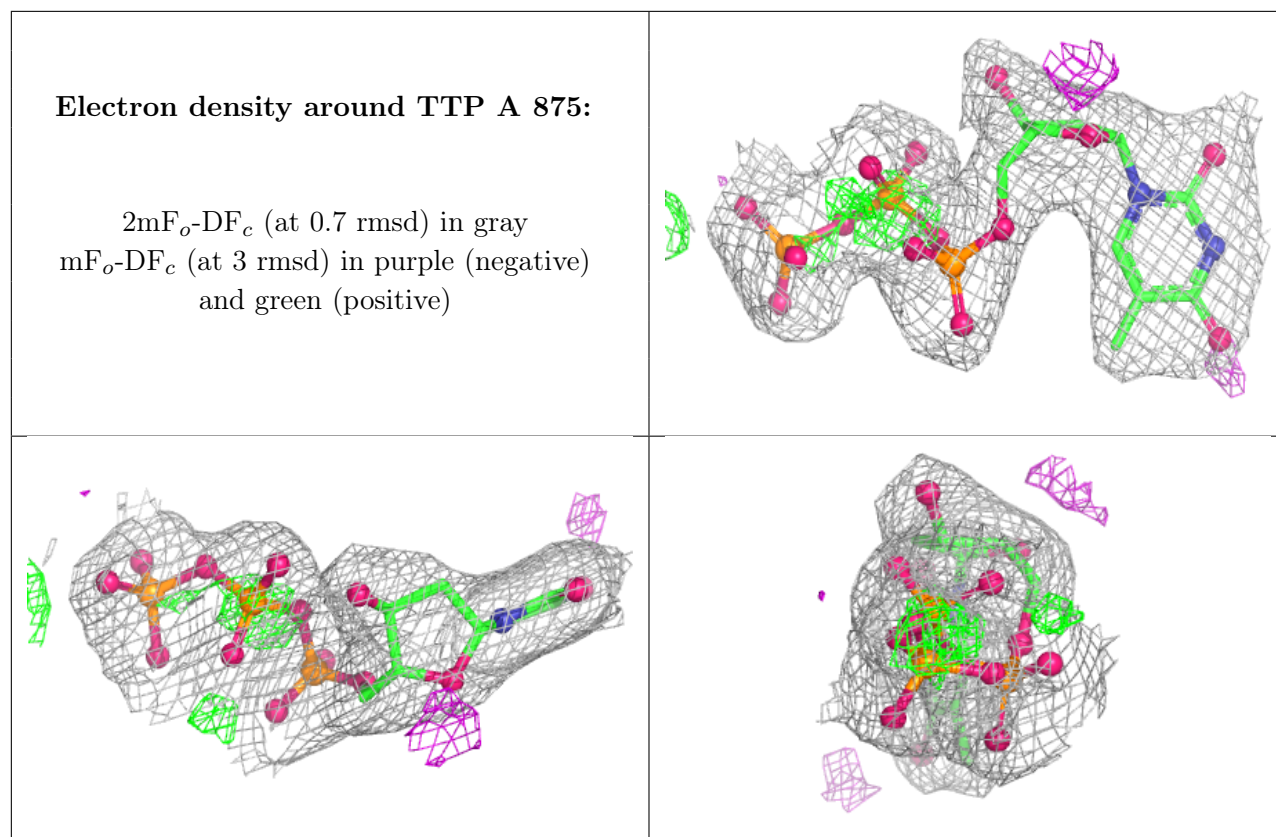
There are no oligosaccharides in this entry.

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
4	MG	A	872	1/1	0.91	0.20	102,102,102,102	0
5	TTP	A	875	29/29	0.97	0.08	17,21,24,27	0
4	MG	A	871	1/1	0.99	0.09	3,3,3,3	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.