W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:37 AM GMT

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PDB ID	:	2DPJ
Title	:	structure of hPoli with DNA and dTTP
Authors	:	Nair, D.T.; Johnson, R.E.; Prakash, L.; Prakash, S.; Aggarwal, A.K.
Deposited on	:	2006-05-12
Resolution	:	2.30 Å(reported)

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 2.30 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.
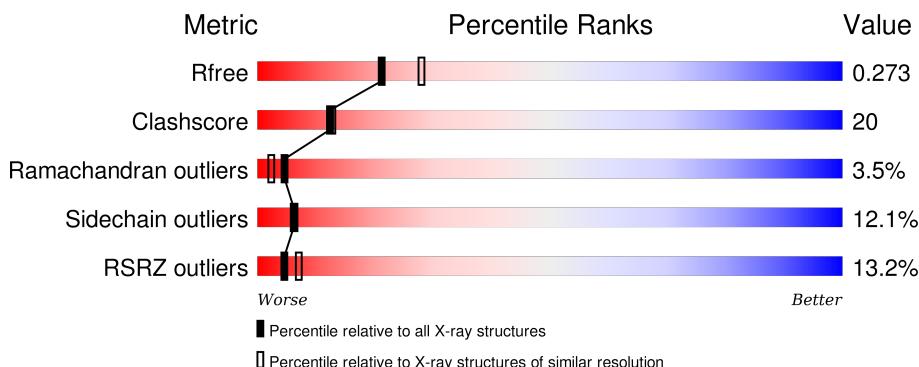
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	P	7	
2	T	9	
3	A	420	
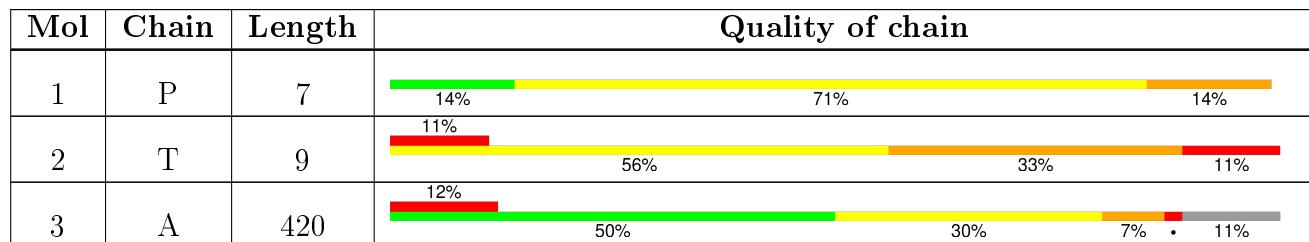
2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3357 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 5'-D(*AP*GP*GP*AP*CP*CP*(DOC))-3'.

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

- Molecule 2 is a DNA chain called 5'-D(*TP*(EDA)P*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
			184	90	32	54	8			

- Molecule 3 is a protein called DNA polymerase iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	373	Total	C	N	O	S	0	0	0
			2876	1809	504	542	21			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).
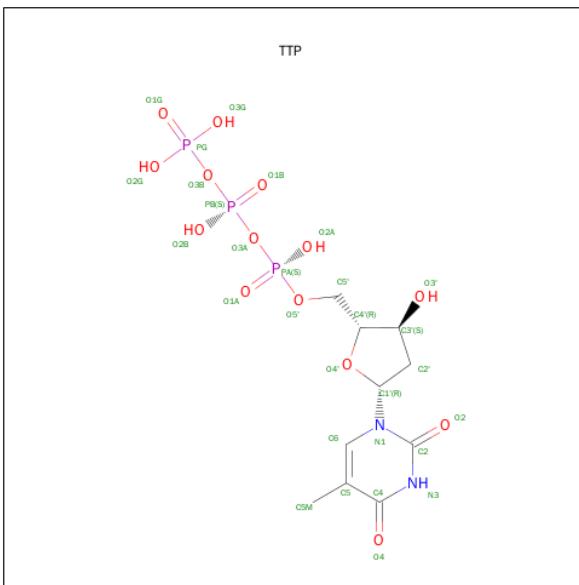
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	29	10	2	14	3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	3	Total 3	O 3	0	0
6	T	14	Total 14	O 14	0	0
6	A	110	Total 110	O 110	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 5'-D(*AP*GP*GP*AP*CP*CP*(DOC))-3'

Chain P:
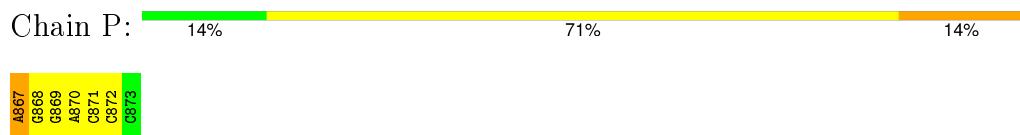
- Molecule 2: 5'-D(*TP*(EDA)P*GP*GP*GP*TP*CP*CP*T)-3'

Chain T:

- Molecule 3: DNA polymerase iota

Chain A:
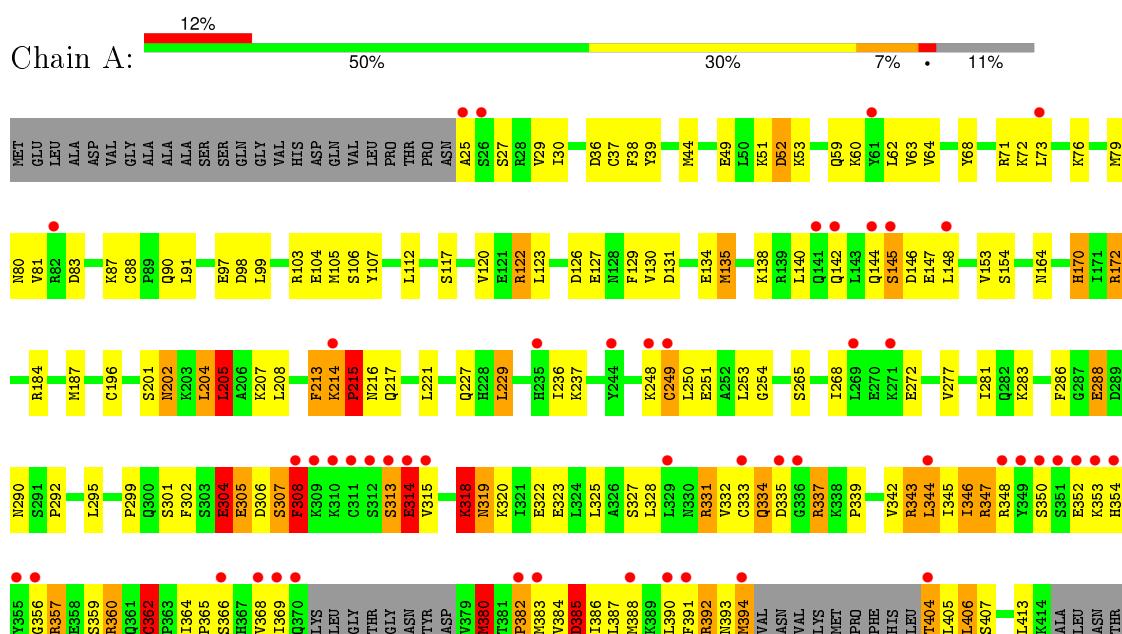
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	98.06Å 98.06Å 203.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.76 – 2.30 36.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.0 (36.76-2.30) 94.0 (36.64-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	8.14 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.238 , 0.277 0.232 , 0.273	Depositor DCC
R_{free} test set	2085 reflections (9.10%)	DCC
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 51.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Outliers	0 of 26427 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3357	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: DOC, MG, EDA, 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	P	2.98	11/136 (8.1%)	3.74	28/208 (13.5%)
2	T	3.66	32/178 (18.0%)	3.93	48/271 (17.7%)
3	A	1.75	44/2914 (1.5%)	1.34	27/3934 (0.7%)
All	All	1.97	87/3228 (2.7%)	1.79	103/4413 (2.3%)

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
2	T	0	1
3	A	0	3
All	All	0	4

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	313	SER	CB-OG	30.32	1.81	1.42
3	A	318	LYS	CE-NZ	14.28	1.84	1.49
2	T	843	DG	P-O5'	12.34	1.72	1.59
2	T	841	DG	P-O5'	11.60	1.71	1.59
1	P	869	DG	N7-C5	10.56	1.45	1.39
3	A	207	LYS	CE-NZ	-10.19	1.23	1.49
3	A	319	ASN	C-O	9.63	1.41	1.23
2	T	841	DG	C6-N1	9.10	1.46	1.39
2	T	843	DG	O4'-C1'	-8.96	1.31	1.42
1	P	868	DG	N7-C5	8.93	1.44	1.39
3	A	103	ARG	CZ-NH2	8.48	1.44	1.33
2	T	843	DG	C6-N1	8.42	1.45	1.39
2	T	844	DT	C3'-O3'	-8.29	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	122	ARG	CG-CD	8.15	1.72	1.51
3	A	104	GLU	CD-OE2	7.91	1.34	1.25
3	A	385	ASP	CG-OD1	7.74	1.43	1.25
2	T	839	DT	C1'-N1	7.67	1.59	1.49
1	P	872	DC	C3'-O3'	-7.41	1.34	1.44
3	A	134	GLU	CD-OE1	7.41	1.33	1.25
2	T	839	DT	C5'-C4'	7.24	1.59	1.51
1	P	871	DC	C2'-C1'	7.21	1.59	1.52
2	T	839	DT	N1-C6	7.20	1.43	1.38
2	T	845	DC	N1-C6	-7.19	1.32	1.37
3	A	68	TYR	CD2-CE2	-7.17	1.28	1.39
3	A	216	ASN	N-CA	7.04	1.60	1.46
2	T	847	DT	C1'-N1	6.96	1.58	1.49
2	T	839	DT	C5-C6	6.95	1.39	1.34
2	T	841	DG	C2-N3	6.93	1.38	1.32
3	A	214	LYS	CA-C	-6.82	1.35	1.52
1	P	872	DC	P-OP2	-6.74	1.37	1.49
3	A	25	ALA	CA-CB	6.67	1.66	1.52
2	T	844	DT	C2-O2	-6.59	1.17	1.22
3	A	64	VAL	CB-CG2	-6.58	1.39	1.52
2	T	839	DT	C5-C7	6.42	1.53	1.50
2	T	843	DG	C5'-C4'	-6.41	1.44	1.51
3	A	214	LYS	CE-NZ	-6.41	1.33	1.49
2	T	839	DT	C4'-O4'	6.36	1.51	1.45
2	T	844	DT	N1-C2	-6.23	1.33	1.38
3	A	249	CYS	CB-SG	6.17	1.92	1.82
3	A	122	ARG	CD-NE	-6.16	1.35	1.46
2	T	845	DC	C4'-C3'	6.14	1.59	1.53
3	A	29	VAL	CB-CG1	6.04	1.65	1.52
2	T	843	DG	P-OP2	-6.03	1.38	1.49
1	P	871	DC	O4'-C1'	-6.03	1.35	1.42
3	A	394	MET	CG-SD	6.00	1.96	1.81
3	A	382	PRO	N-CD	5.99	1.56	1.47
3	A	129	PHE	CG-CD1	5.95	1.47	1.38
2	T	841	DG	C5-C4	5.93	1.42	1.38
2	T	847	DT	C2'-C1'	5.93	1.58	1.52
2	T	843	DG	N1-C2	5.91	1.42	1.37
3	A	105	MET	CG-SD	5.86	1.96	1.81
3	A	201	SER	CB-OG	5.85	1.49	1.42
2	T	843	DG	O5'-C5'	-5.83	1.27	1.42
2	T	846	DC	C2-N3	5.82	1.40	1.35
2	T	844	DT	C5-C7	5.75	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	107	TYR	CD2-CE2	5.74	1.48	1.39
1	P	870	DA	C2'-C1'	5.71	1.58	1.52
3	A	127	GLU	CD-OE1	5.64	1.31	1.25
3	A	227	GLN	CG-CD	5.64	1.64	1.51
3	A	138	LYS	CD-CE	5.61	1.65	1.51
3	A	39	TYR	CE2-CZ	5.58	1.45	1.38
2	T	844	DT	C4'-O4'	5.53	1.50	1.45
3	A	385	ASP	C-O	5.50	1.33	1.23
3	A	301	SER	CB-OG	5.48	1.49	1.42
3	A	290	ASN	CB-CG	5.48	1.63	1.51
3	A	362	CYS	CB-SG	5.48	1.91	1.82
3	A	305	GLU	CD-OE1	-5.47	1.19	1.25
1	P	869	DG	O4'-C1'	5.46	1.48	1.42
3	A	64	VAL	CA-CB	5.43	1.66	1.54
2	T	844	DT	O3'-P	5.42	1.67	1.61
3	A	385	ASP	CB-CG	5.40	1.63	1.51
2	T	842	DG	C6-O6	-5.36	1.19	1.24
3	A	117	SER	CB-OG	5.34	1.49	1.42
3	A	213	PHE	CE2-CZ	5.31	1.47	1.37
1	P	872	DC	C4'-O4'	5.27	1.50	1.45
2	T	842	DG	N1-C2	-5.27	1.33	1.37
3	A	292	PRO	CG-CD	5.26	1.68	1.50
1	P	872	DC	P-O5'	5.21	1.65	1.59
1	P	870	DA	P-O5'	5.17	1.65	1.59
3	A	286	PHE	CG-CD1	5.15	1.46	1.38
3	A	38	PHE	CE2-CZ	5.12	1.47	1.37
2	T	845	DC	C2-O2	-5.10	1.19	1.24
3	A	134	GLU	CD-OE2	5.10	1.31	1.25
3	A	63	VAL	CB-CG1	-5.09	1.42	1.52
2	T	843	DG	C3'-C2'	-5.08	1.46	1.52
3	A	38	PHE	CB-CG	-5.04	1.42	1.51
3	A	288	GLU	CD-OE2	5.01	1.31	1.25

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	870	DA	O4'-C1'-N9	15.09	118.57	108.00
2	T	843	DG	O4'-C1'-C2'	-14.57	94.24	105.90
1	P	870	DA	O4'-C4'-C3'	14.44	114.66	106.00
2	T	843	DG	C4'-C3'-C2'	-13.25	91.17	103.10
1	P	867	DA	O4'-C4'-C3'	-11.95	98.83	106.00
1	P	867	DA	O5'-C5'-C4'	11.81	140.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	847	DT	C2-N3-C4	-11.73	120.16	127.20
1	P	869	DG	O4'-C1'-N9	11.73	116.21	108.00
1	P	870	DA	O5'-P-OP2	-11.56	95.29	105.70
2	T	842	DG	O4'-C1'-N9	-11.46	99.98	108.00
1	P	872	DC	O4'-C4'-C3'	10.51	112.31	106.00
3	A	122	ARG	NE-CZ-NH2	-10.45	115.08	120.30
2	T	842	DG	O4'-C1'-C2'	-10.08	97.84	105.90
1	P	870	DA	N1-C2-N3	9.90	134.25	129.30
1	P	871	DC	O4'-C4'-C3'	9.42	111.65	106.00
2	T	843	DG	O4'-C4'-C3'	9.42	111.65	106.00
2	T	846	DC	O4'-C1'-N1	-9.37	101.44	108.00
2	T	839	DT	O4'-C4'-C3'	-9.05	100.57	106.00
3	A	103	ARG	NE-CZ-NH2	-9.04	115.78	120.30
2	T	846	DC	O4'-C4'-C3'	-8.71	100.77	106.00
2	T	846	DC	C5-C6-N1	8.66	125.33	121.00
2	T	843	DG	N9-C4-C5	8.50	108.80	105.40
1	P	871	DC	OP1-P-OP2	-8.49	106.87	119.60
3	A	215	PRO	N-CD-CG	-8.49	90.47	103.20
3	A	73	LEU	CB-CG-CD1	8.41	125.29	111.00
2	T	843	DG	O4'-C1'-N9	-8.14	102.30	108.00
2	T	844	DT	C4-C5-C7	8.11	123.87	119.00
2	T	847	DT	N1-C2-N3	8.09	119.45	114.60
3	A	71	ARG	NE-CZ-NH1	7.88	124.24	120.30
2	T	839	DT	O4'-C1'-N1	7.73	113.41	108.00
2	T	844	DT	N1-C2-N3	7.72	119.23	114.60
2	T	844	DT	C6-N1-C2	-7.70	117.45	121.30
1	P	867	DA	C1'-O4'-C4'	7.63	117.73	110.10
2	T	839	DT	C5'-C4'-O4'	7.59	123.72	109.30
3	A	71	ARG	NE-CZ-NH2	-7.57	116.52	120.30
3	A	343	ARG	NE-CZ-NH2	-7.53	116.54	120.30
3	A	385	ASP	CB-CG-OD1	7.50	125.05	118.30
2	T	843	DG	N9-C1'-C2'	-7.41	98.52	112.60
2	T	846	DC	C6-N1-C2	-7.25	117.40	120.30
3	A	122	ARG	CG-CD-NE	-7.23	96.61	111.80
1	P	872	DC	O4'-C1'-N1	-7.21	102.95	108.00
2	T	843	DG	C4-C5-N7	-7.21	107.92	110.80
1	P	869	DG	P-O3'-C3'	-7.15	111.12	119.70
2	T	847	DT	C4-C5-C7	7.09	123.25	119.00
2	T	846	DC	C4'-C3'-C2'	6.86	109.28	103.10
3	A	172	ARG	NE-CZ-NH2	-6.86	116.87	120.30
2	T	841	DG	C5-C6-O6	-6.83	124.50	128.60
3	A	83	ASP	CB-CG-OD2	6.82	124.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	843	DG	C6-N1-C2	-6.75	121.05	125.10
3	A	52	ASP	CB-CG-OD2	6.74	124.37	118.30
2	T	847	DT	C6-C5-C7	-6.72	118.87	122.90
2	T	842	DG	C4'-C3'-O3'	6.62	126.25	109.70
2	T	847	DT	N3-C4-C5	6.60	119.16	115.20
2	T	843	DG	C8-N9-C4	-6.59	103.76	106.40
3	A	205	LEU	CB-CG-CD1	6.57	122.16	111.00
3	A	331	ARG	NE-CZ-NH1	6.53	123.56	120.30
3	A	103	ARG	NH1-CZ-NH2	6.51	126.56	119.40
2	T	843	DG	C3'-C2'-C1'	6.51	110.31	102.50
2	T	844	DT	C5'-C4'-C3'	-6.41	102.56	114.10
1	P	872	DC	C5-C6-N1	-6.36	117.82	121.00
2	T	842	DG	C3'-C2'-C1'	6.28	110.04	102.50
2	T	843	DG	C2-N3-C4	6.26	115.03	111.90
2	T	839	DT	C6-N1-C2	-6.24	118.18	121.30
1	P	870	DA	C6-N1-C2	-6.16	114.91	118.60
3	A	343	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	P	870	DA	O4'-C1'-C2'	6.12	110.79	105.90
2	T	844	DT	C6-C5-C7	-6.09	119.25	122.90
1	P	868	DG	O4'-C1'-N9	6.08	112.26	108.00
2	T	847	DT	O4'-C1'-N1	-6.04	103.77	108.00
2	T	841	DG	C5-C6-N1	6.03	114.52	111.50
3	A	215	PRO	O-C-N	-6.00	113.10	122.70
1	P	872	DC	C3'-C2'-C1'	5.97	109.67	102.50
3	A	357	ARG	NE-CZ-NH1	5.95	123.28	120.30
2	T	843	DG	C8-N9-C1'	5.92	134.69	127.00
2	T	847	DT	O5'-P-OP2	5.85	117.72	110.70
2	T	841	DG	C6-N1-C2	-5.84	121.59	125.10
1	P	872	DC	C4'-C3'-O3'	5.82	124.24	109.70
2	T	843	DG	C4-N9-C1'	-5.78	118.98	126.50
1	P	871	DC	C2-N3-C4	-5.73	117.03	119.90
3	A	302	PHE	N-CA-C	-5.71	95.58	111.00
3	A	135	MET	CG-SD-CE	-5.67	91.13	100.20
2	T	847	DT	C5-C4-O4	-5.62	120.97	124.90
1	P	871	DC	C1'-O4'-C4'	-5.57	104.53	110.10
2	T	842	DG	C1'-O4'-C4'	5.53	115.62	110.10
1	P	870	DA	C2-N3-C4	-5.50	107.85	110.60
3	A	304	GLU	OE1-CD-OE2	5.49	129.89	123.30
3	A	308	PHE	N-CA-C	-5.45	96.29	111.00
2	T	847	DT	N1-C2-O2	-5.45	118.74	123.10
1	P	870	DA	OP2-P-O3'	5.40	117.08	105.20
1	P	867	DA	O4'-C1'-N9	5.39	111.77	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	103	ARG	NE-CZ-NH1	-5.33	117.64	120.30
3	A	319	ASN	CA-C-N	-5.28	105.59	117.20
1	P	868	DG	C8-N9-C4	5.20	108.48	106.40
3	A	306	ASP	CB-CG-OD1	5.13	122.92	118.30
1	P	867	DA	C6-N1-C2	-5.08	115.55	118.60
1	P	868	DG	N7-C8-N9	-5.07	110.57	113.10
3	A	214	LYS	N-CA-CB	5.05	119.69	110.60
2	T	847	DT	O4'-C4'-C3'	5.03	109.02	106.00
1	P	871	DC	C5-C4-N4	-5.03	116.68	120.20
2	T	845	DC	N3-C4-C5	-5.03	119.89	121.90
2	T	839	DT	O5'-C5'-C4'	5.02	123.54	111.00
3	A	98	ASP	CB-CG-OD2	5.01	122.81	118.30
2	T	845	DC	C4-C5-C6	5.01	119.90	117.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	213	PHE	Peptide
3	A	346	ILE	Peptide
3	A	380	MET	Peptide
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	79	0	1
2	T	184	0	104	10	1
3	A	2876	0	2899	121	0
4	A	2	0	0	0	0
5	A	29	0	13	0	0
6	A	110	0	0	4	0
6	P	3	0	0	0	0
6	T	14	0	0	1	0
All	All	3357	0	3095	124	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 20.

All (124) 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:318:LYS:CE	3:A:318:LYS:NZ	1.84	1.38
3:A:313:SER:OG	3:A:313:SER:CB	1.81	1.27
3:A:344:LEU:HD11	3:A:387:LEU:HD22	1.21	1.08
2:T:842:DG:H2"	2:T:843:DG:H5'	1.44	0.97
3:A:249:CYS:O	3:A:253:LEU:HD12	1.69	0.93
3:A:308:PHE:O	3:A:308:PHE:HD1	1.49	0.92
3:A:308:PHE:CD1	3:A:308:PHE:O	2.22	0.91
3:A:344:LEU:CD1	3:A:387:LEU:HD22	2.02	0.88
3:A:392:ARG:C	3:A:394:MET:H	1.83	0.80
3:A:365:PRO:O	3:A:368:VAL:HG22	1.85	0.77
3:A:331:ARG:HD2	6:A:1014:HOH:O	1.87	0.73
3:A:347:ARG:NH1	3:A:404:THR:OG1	2.21	0.73
3:A:319:ASN:O	3:A:322:GLU:N	2.22	0.72
3:A:391:PHE:O	3:A:394:MET:HB2	1.88	0.72
2:T:841:DG:OP2	3:A:307:SER:HB2	1.89	0.72
3:A:392:ARG:C	3:A:394:MET:N	2.40	0.71
3:A:343:ARG:HD2	3:A:345:ILE:HD11	1.72	0.71
3:A:335:ASP:OD2	3:A:337:ARG:HD3	1.91	0.70
2:T:841:DG:H2"	2:T:842:DG:H5"	1.72	0.69
3:A:318:LYS:HB2	3:A:388:MET:CE	2.24	0.67
3:A:392:ARG:O	3:A:394:MET:N	2.28	0.67
3:A:405:LEU:C	3:A:406:LEU:HD23	2.15	0.67
3:A:283:LYS:HE3	3:A:288:GLU:OE1	1.96	0.66
3:A:386:ILE:O	3:A:390:LEU:HD12	1.96	0.65
3:A:164:ASN:H	3:A:170:HIS:HD2	1.42	0.65
3:A:344:LEU:HD11	3:A:387:LEU:CD2	2.12	0.65
3:A:332:VAL:CG1	3:A:339:PRO:HD3	2.26	0.65
3:A:382:PRO:O	3:A:383:MET:C	2.35	0.64
3:A:304:GLU:HG3	3:A:328:LEU:HG	1.79	0.64
3:A:236:ILE:HD12	3:A:250:LEU:HD13	1.82	0.62
3:A:346:ILE:HG22	3:A:406:LEU:HD22	1.81	0.62
3:A:318:LYS:HB2	3:A:388:MET:HE1	1.81	0.61
3:A:305:GLU:HG3	3:A:407:SER:HB3	1.81	0.61
3:A:380:MET:HE2	3:A:384:VAL:HG22	1.82	0.61
2:T:840:EDA:H5"	3:A:60:LYS:HB2	1.82	0.60
3:A:347:ARG:HD3	3:A:404:THR:OG1	2.01	0.60
3:A:335:ASP:OD2	3:A:337:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:196:CYS:SG	3:A:214:LYS:O	2.59	0.60
3:A:304:GLU:O	3:A:407:SER:HB2	2.00	0.60
3:A:388:MET:HE3	3:A:388:MET:HA	1.84	0.59
3:A:394:MET:C	6:A:989:HOH:O	2.41	0.59
3:A:365:PRO:HB2	3:A:368:VAL:HG13	1.85	0.58
3:A:359:SER:O	3:A:360:ARG:HD3	2.05	0.57
3:A:237:LYS:HD3	3:A:237:LYS:O	2.04	0.57
3:A:404:THR:HA	6:A:994:HOH:O	2.05	0.56
3:A:352:GLU:O	3:A:354:HIS:N	2.38	0.56
3:A:335:ASP:CG	3:A:337:ARG:HH11	2.08	0.56
3:A:251:GLU:C	3:A:253:LEU:N	2.57	0.55
3:A:347:ARG:NH1	3:A:404:THR:HG1	2.04	0.55
3:A:388:MET:O	3:A:391:PHE:HB3	2.08	0.54
3:A:380:MET:O	3:A:384:VAL:HG23	2.06	0.54
3:A:308:PHE:HZ	3:A:406:LEU:HG	1.72	0.54
3:A:332:VAL:HG13	3:A:339:PRO:HD3	1.89	0.53
3:A:313:SER:O	3:A:314:GLU:OE2	2.26	0.53
3:A:347:ARG:HD3	3:A:404:THR:HG23	1.91	0.52
3:A:36:ASP:OD1	3:A:215:PRO:O	2.28	0.52
3:A:76:LYS:HB2	3:A:79:MET:CE	2.39	0.52
2:T:842:DG:H2"	2:T:843:DG:C5'	2.29	0.52
3:A:406:LEU:N	3:A:406:LEU:HD23	2.24	0.52
2:T:840:EDA:H8	3:A:59:GLN:OE1	2.10	0.52
3:A:51:LYS:C	3:A:53:LYS:H	2.12	0.52
2:T:841:DG:OP1	3:A:97:GLU:HG2	2.09	0.51
3:A:202:ASN:ND2	3:A:205:LEU:H	2.08	0.51
3:A:380:MET:HE2	3:A:384:VAL:CG2	2.40	0.51
3:A:221:LEU:HD22	3:A:229:LEU:HD12	1.92	0.51
3:A:76:LYS:HB2	3:A:79:MET:HE3	1.93	0.51
3:A:184:ARG:HA	3:A:187:MET:HE2	1.92	0.50
3:A:343:ARG:HG2	3:A:344:LEU:N	2.26	0.50
3:A:214:LYS:HB2	3:A:215:PRO:HD3	1.93	0.50
3:A:318:LYS:O	3:A:319:ASN:C	2.50	0.50
3:A:304:GLU:HG2	3:A:328:LEU:HD21	1.94	0.50
3:A:202:ASN:C	3:A:202:ASN:HD22	2.15	0.50
3:A:332:VAL:HG11	3:A:339:PRO:HD3	1.94	0.50
3:A:388:MET:CE	3:A:388:MET:HA	2.41	0.49
2:T:842:DG:H4'	3:A:99:LEU:HD12	1.94	0.49
3:A:362:CYS:SG	3:A:390:LEU:HD11	2.53	0.48
3:A:325:LEU:HD23	3:A:380:MET:CE	2.43	0.48
3:A:59:GLN:O	3:A:60:LYS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:325:LEU:HD23	3:A:380:MET:HE3	1.94	0.48
2:T:840:EDA:C5'	3:A:60:LYS:HB2	2.44	0.48
3:A:88:CYS:SG	3:A:91:LEU:HB2	2.53	0.48
3:A:36:ASP:O	3:A:37:CYS:C	2.53	0.47
3:A:51:LYS:O	3:A:53:LYS:N	2.47	0.47
3:A:299:PRO:O	3:A:337:ARG:NH2	2.44	0.47
3:A:44:MET:HE2	3:A:51:LYS:HA	1.96	0.47
3:A:265:SER:OG	3:A:268:ILE:HG13	2.15	0.47
3:A:72:LYS:NZ	6:A:949:HOH:O	2.42	0.47
3:A:319:ASN:O	3:A:322:GLU:CB	2.63	0.47
2:T:840:EDA:H5"	3:A:60:LYS:CB	2.44	0.47
3:A:388:MET:HE1	3:A:391:PHE:CD1	2.51	0.46
3:A:313:SER:OG	3:A:314:GLU:N	2.37	0.46
3:A:153:VAL:HG22	3:A:154:SER:N	2.31	0.46
3:A:347:ARG:O	3:A:404:THR:N	2.49	0.46
3:A:106:SER:OG	3:A:122:ARG:NH2	2.44	0.46
3:A:320:LYS:O	3:A:323:GLU:HB2	2.17	0.45
3:A:346:ILE:HA	3:A:405:LEU:O	2.17	0.45
3:A:196:CYS:HA	3:A:217:GLN:O	2.17	0.45
3:A:364:ILE:HG22	3:A:369:ILE:HG13	1.99	0.44
3:A:204:LEU:HD13	3:A:205:LEU:HD13	2.00	0.44
3:A:164:ASN:H	3:A:170:HIS:CD2	2.28	0.44
3:A:204:LEU:HD22	3:A:208:LEU:CD1	2.47	0.44
3:A:388:MET:CE	3:A:391:PHE:CD1	3.01	0.44
3:A:345:ILE:HG12	3:A:359:SER:HB3	2.00	0.43
3:A:120:VAL:HG22	3:A:130:VAL:HG22	2.00	0.43
3:A:272:GLU:HG3	3:A:272:GLU:O	2.18	0.43
3:A:112:LEU:HD23	3:A:112:LEU:C	2.39	0.43
3:A:325:LEU:HD11	3:A:387:LEU:HD11	1.99	0.43
3:A:251:GLU:O	3:A:254:GLY:N	2.42	0.43
3:A:30:ILE:HD13	3:A:131:ASP:HA	2.00	0.43
3:A:49:GLU:O	3:A:53:LYS:HD2	2.19	0.42
3:A:382:PRO:O	3:A:385:ASP:N	2.53	0.42
3:A:327:SER:O	3:A:328:LEU:C	2.57	0.42
3:A:364:ILE:HG23	3:A:368:VAL:CG2	2.50	0.42
3:A:236:ILE:HD13	3:A:236:ILE:HG21	1.65	0.42
3:A:140:LEU:HD23	3:A:140:LEU:HA	1.73	0.42
3:A:335:ASP:CG	3:A:337:ARG:NH1	2.73	0.41
3:A:268:ILE:O	3:A:272:GLU:HB2	2.20	0.41
3:A:44:MET:CE	3:A:51:LYS:HA	2.50	0.41
3:A:144:GLN:O	3:A:146:ASP:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:144:GLN:HG3	3:A:147:GLU:HG2	2.01	0.41
3:A:318:LYS:HG2	3:A:319:ASN:N	2.36	0.40
6:T:957:HOH:O	3:A:122:ARG:HD3	2.21	0.40
3:A:277:VAL:O	3:A:281:ILE:HG12	2.21	0.40
3:A:248:LYS:HD3	3:A:248:LYS:HA	1.90	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)
1:P:867:DA:O5'	2:T:847:DT:O3'[10_665]	1.91	0.29

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	
3	A	367/420 (87%)	329 (90%)	25 (7%)	13 (4%)	4	2

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	308	PHE
3	A	314	GLU
3	A	315	VAL
3	A	333	CYS
3	A	353	LYS
3	A	52	ASP
3	A	215	PRO
3	A	334	GLN
3	A	337	ARG
3	A	350	SER
3	A	393	ASN

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Mol	Chain	Res	Type
3	A	145	SER
3	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	
3	A	321/376 (85%)	282 (88%)	39 (12%)	6	6

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	27	SER
3	A	62	LEU
3	A	80	ASN
3	A	81	VAL
3	A	87	LYS
3	A	90	GLN
3	A	123	LEU
3	A	126	ASP
3	A	135	MET
3	A	142	GLN
3	A	145	SER
3	A	148	LEU
3	A	170	HIS
3	A	172	ARG
3	A	202	ASN
3	A	204	LEU
3	A	205	LEU
3	A	229	LEU
3	A	295	LEU
3	A	304	GLU
3	A	307	SER
3	A	308	PHE
3	A	314	GLU
3	A	318	LYS

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Mol	Chain	Res	Type
3	A	334	GLN
3	A	342	VAL
3	A	344	LEU
3	A	347	ARG
3	A	348	ARG
3	A	357	ARG
3	A	360	ARG
3	A	362	CYS
3	A	366	SER
3	A	380	MET
3	A	385	ASP
3	A	392	ARG
3	A	404	THR
3	A	406	LEU
3	A	413	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	80	ASN
3	A	170	HIS
3	A	202	ASN
3	A	262	GLN
3	A	279	GLN
3	A	334	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
1	DOC	P	873	1,2	11,19,20	2.31	5 (45%)	14,26,29	2.18	6 (42%)
2	EDA	T	840	2	15,26,27	1.37	2 (13%)	18,38,41	2.07	5 (27%)

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	-	0/3/18/19	0/2/2/2
2	EDA	T	840	2	-	0/3/21/22	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	873	DOC	C3'-C2'	-3.76	1.43	1.54
2	T	840	EDA	C5-C6	-2.97	1.35	1.41
1	P	873	DOC	O4'-C1'	-2.54	1.36	1.42
1	P	873	DOC	C6-C5	-2.11	1.33	1.38
2	T	840	EDA	C2'-C1'	2.50	1.59	1.52
1	P	873	DOC	C2'-C1'	3.55	1.60	1.51
1	P	873	DOC	O4'-C4'	3.77	1.52	1.44

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	840	EDA	O4'-C1'-N9	-5.71	97.83	107.72
1	P	873	DOC	C3'-C4'-C5'	-3.02	103.76	116.05
2	T	840	EDA	C4'-O4'-C1'	-2.94	102.02	109.47
1	P	873	DOC	O4'-C1'-N1	-2.22	103.87	107.72
1	P	873	DOC	C2'-C1'-N1	-2.02	108.39	112.49
2	T	840	EDA	C2-N3-C4	2.37	120.07	116.40
2	T	840	EDA	O4'-C4'-C3'	2.64	112.32	105.67
2	T	840	EDA	C2'-C1'-N9	3.08	121.66	114.16
1	P	873	DOC	O4'-C4'-C5'	3.11	114.14	109.54
1	P	873	DOC	O4'-C4'-C3'	3.74	110.96	104.69
1	P	873	DOC	C2-N3-C4	4.20	121.53	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	840	EDA	4	0

5.5 Carbohydrates (i)

There are no carbohydrates 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	21,30,30	1.53	6 (28%)	31,47,47	2.06	6 (19%)

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	-	0/18/34/34	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	875	TTP	PA-O1A	-2.66	1.41	1.51
5	A	875	TTP	C2'-C3'	-2.37	1.46	1.52
5	A	875	TTP	C5'-C4'	-2.01	1.45	1.51
5	A	875	TTP	C6-N1	2.07	1.38	1.35
5	A	875	TTP	C4-N3	2.69	1.38	1.33
5	A	875	TTP	O4'-C1'	3.50	1.50	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	875	TTP	C5-C4-N3	-6.01	118.45	125.14
5	A	875	TTP	PB-O3B-PG	-2.50	124.28	132.67
5	A	875	TTP	O3G-PG-O2G	2.45	116.71	107.38
5	A	875	TTP	C2'-C3'-C4'	2.59	108.15	102.77
5	A	875	TTP	O2B-PB-O3A	2.87	118.12	105.09
5	A	875	TTP	C4-N3-C2	6.15	120.56	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å²)	Q<0.9
1	P	6/7 (85%)	0.34	0	100	100	26, 31, 37, 39	0
2	T	8/9 (88%)	0.60	1 (12%)	5	8	20, 22, 25, 88	0
3	A	373/420 (88%)	0.68	50 (13%)	4	7	8, 37, 79, 97	0
All	All	387/436 (88%)	0.67	51 (13%)	4	7	8, 36, 79, 97	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	354	HIS	14.4
3	A	355	TYR	13.8
3	A	25	ALA	12.2
3	A	353	LYS	7.0
3	A	350	SER	6.3
3	A	352	GLU	5.5
3	A	244	TYR	5.2
3	A	144	GLN	4.9
3	A	333	CYS	4.8
3	A	368	VAL	4.7
3	A	336	GLY	4.7
3	A	370	GLN	4.7
3	A	310	LYS	4.4
3	A	249	CYS	4.3
3	A	73	LEU	4.3
3	A	309	LYS	4.2
3	A	349	TYR	4.2
3	A	26	SER	4.1
3	A	312	SER	4.1
2	T	839	DT	4.1
3	A	351	SER	4.1
3	A	311	CYS	3.8
3	A	142	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
3	A	61	TYR	3.6
3	A	214	LYS	3.6
3	A	382	PRO	3.6
3	A	235	HIS	3.4
3	A	145	SER	3.3
3	A	82	ARG	3.1
3	A	141	GLN	3.1
3	A	315	VAL	3.0
3	A	388	MET	3.0
3	A	335	ASP	3.0
3	A	148	LEU	3.0
3	A	314	GLU	2.9
3	A	308	PHE	2.7
3	A	329	LEU	2.7
3	A	313	SER	2.7
3	A	344	LEU	2.7
3	A	383	MET	2.7
3	A	348	ARG	2.3
3	A	248	LYS	2.3
3	A	390	LEU	2.3
3	A	356	GLY	2.2
3	A	404	THR	2.2
3	A	269	LEU	2.2
3	A	271	LYS	2.2
3	A	366	SER	2.2
3	A	391	PHE	2.1
3	A	394	MET	2.1
3	A	369	ILE	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
1	DOC	P	873	18/19	0.97	0.19	-	15,18,27,29	0
2	EDA	T	840	23/24	0.91	0.15	-	24,38,61,65	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors($Å^2$)	Q<0.9
5	TTP	A	875	29/29	0.97	0.14	-0.02	13,18,22,24	0
4	MG	A	871	1/1	0.98	0.10	-0.93	18,18,18,18	0
4	MG	A	872	1/1	0.93	0.24	-	78,78,78,78	0

6.5 Other polymers (i)

There are no such residues in this entry.