



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 11:47 AM BST

PDB ID : 1TK8
Title : T7 DNA polymerase ternary complex with 8 oxo guanosine and dAMP at the elongation site
Authors : Briebe, L.G.; Eichman, B.F.; Kokoska, R.J.; Doublie, S.; Kunkel, T.A.; Ellenberger, T.
Deposited on : 2004-06-08
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

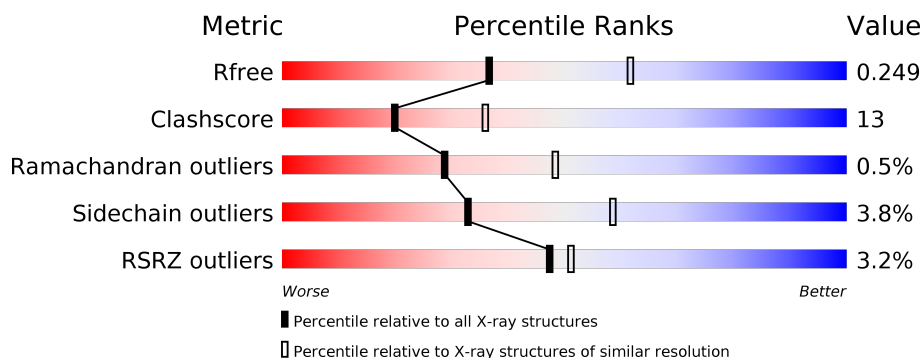
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	22	<div> <div>32%</div> <div> <div>9%</div> <div>59%</div> <div>9%</div> <div>23%</div> </div> </div>
2	T	26	<div> <div>27%</div> <div> <div>27%</div> <div>38%</div> <div>12%</div> <div>23%</div> </div> </div>
3	A	698	<div> <div>%</div> <div> <div>75%</div> <div>22%</div> <div>..</div> </div> </div>
4	B	108	<div> <div>3%</div> <div> <div>70%</div> <div>24%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7658 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(*CP*GP*AP*AP*AP*AP*CP*GP*AP*CP*GP*GP*CP*CP*AP*GP*TP*GP*CP*CP*AP*(2DA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	17	Total	C	N	O	P	0	0	0
			348	164	70	97	17			

- Molecule 2 is a DNA chain called 5'-D(*CP*CP*CP*AP*(8OG)P*TP*GP*GP*CP*AP*C P*TP*GP*GP*CP*CP*GP*TP*CP*GP*TP*TP*TP*TP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	20	Total	C	N	O	P	0	0	0
			410	194	73	123	20			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	692	Total	C	N	O	S	0	0	0
			5496	3498	952	1022	24			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	DELETION	UNP P00581
A	?	-	ARG	DELETION	UNP P00581
A	?	-	PHE	DELETION	UNP P00581
A	?	-	GLY	DELETION	UNP P00581
A	?	-	SER	DELETION	UNP P00581
A	?	-	HIS	DELETION	UNP P00581

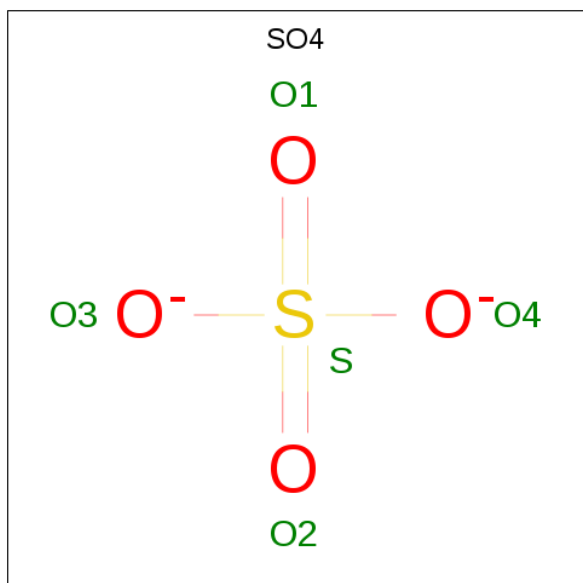
- Molecule 4 is a protein called Thioredoxin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	105	Total	C	N	O	S	0	0	0
			802	518	129	152	3			

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

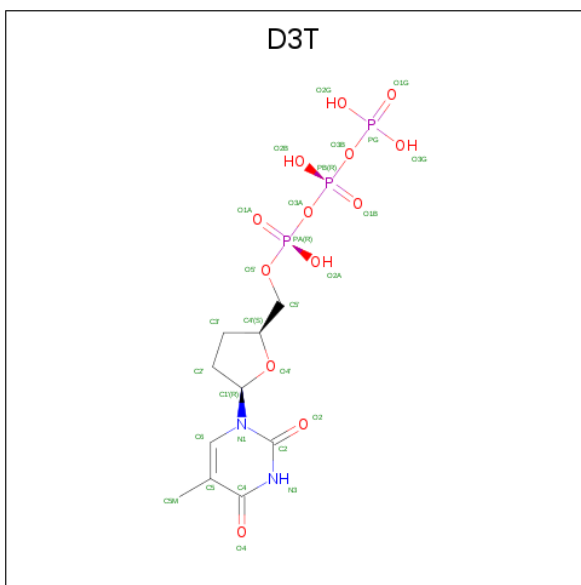
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Mg	0	0
			3	3		
5	T	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



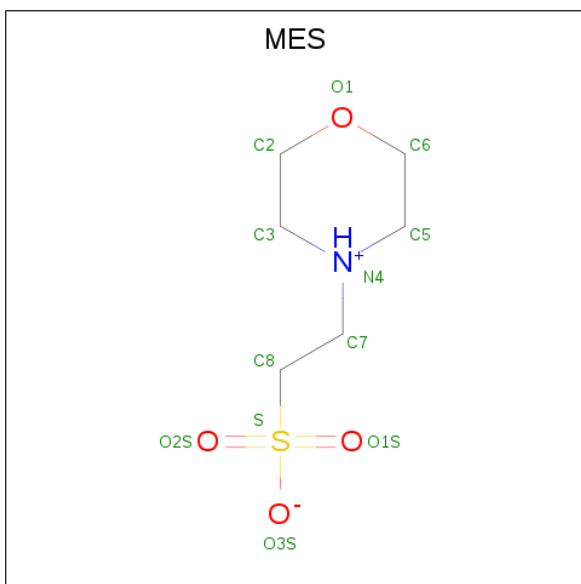
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2',3'-DIDEOXY-THYMIDINE-5'-TRIPHOSPHATE (three-letter code: D3T) (formula: C₁₀H₁₇N₂O₁₃P₃).



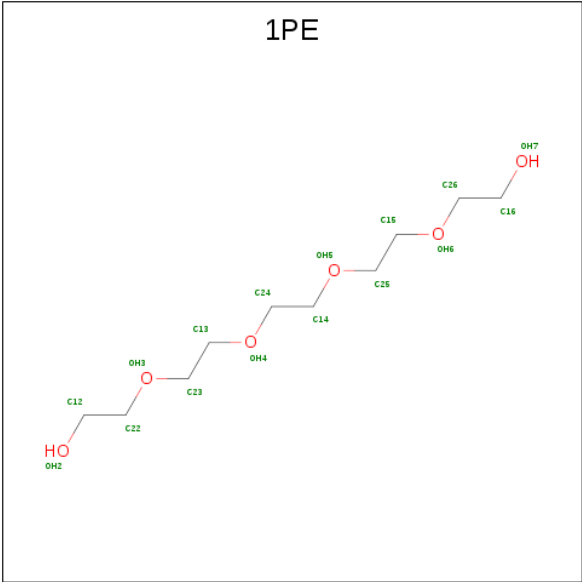
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			28	10	2	13	3		

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 9 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	C O	0	0
			16	10 6		

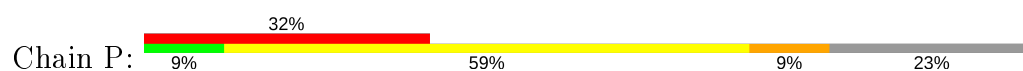
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	P	25	Total	O	0	0
			25	25		
10	T	41	Total	O	0	0
			41	41		
10	A	434	Total	O	0	0
			434	434		
10	B	32	Total	O	0	0
			32	32		

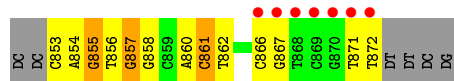
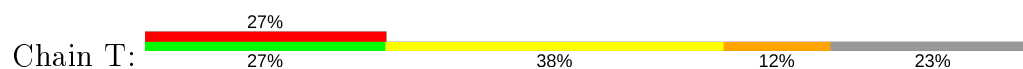
3 Residue-property plots

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.

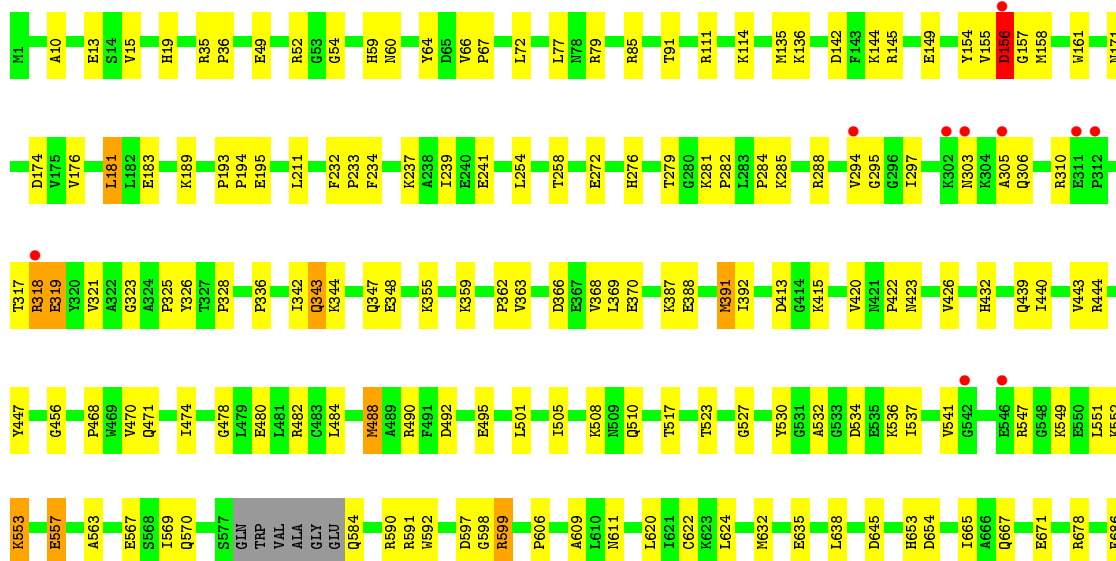
- Molecule 1: 5'-D(*CP*GP*AP*AP*AP*AP*CP*GP*AP*CP*GP*GP*CP*CP*AP*GP*TP*GP*CP*CP*AP*(2DA))-3'



- Molecule 2: 5'-D(*CP*CP*CP*AP*(8OG)P*TP*GP*GP*CP*AP*CP*TP*GP*GP*CP*CP*GP*TP*CP*GP*TP*TP*TP*TP*CP*G)-3'

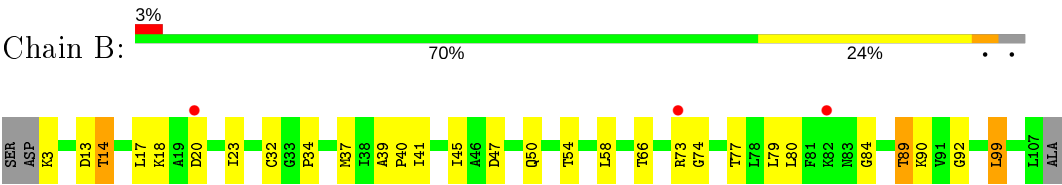


- Molecule 3: DNA polymerase





● Molecule 4: Thioredoxin 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.18Å 215.71Å 52.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.97 – 2.50 39.97 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.97-2.50) 96.5 (39.97-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.261 0.193 , 0.249	Depositor DCC
R_{free} test set	2514 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7658	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 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, D3T, 1PE, 8OG, 2DA, SO4, MES

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	0.44	0/368	0.79	0/565
2	T	0.46	0/431	0.85	0/659
3	A	0.33	0/5630	0.57	0/7618
4	B	0.31	0/817	0.58	0/1108
All	All	0.34	0/7246	0.61	0/9950

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	1
2	T	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	821	DA	Sidechain
2	T	857	DG	Sidechain
2	T	861	DC	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	348	0	189	23	0
2	T	410	0	226	16	0
3	A	5496	0	5373	123	0
4	B	802	0	816	23	0
5	A	3	0	0	0	0
5	T	1	0	0	0	0
6	A	10	0	0	0	0
7	A	28	0	13	2	0
8	A	12	0	13	1	0
9	A	16	0	22	2	0
10	A	434	0	0	8	0
10	B	32	0	0	2	0
10	P	25	0	0	0	0
10	T	41	0	0	1	0
All	All	7658	0	6652	174	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (174) 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)
2:T:856:DT:H2"	2:T:857:DG:H5"	1.28	1.09
1:P:816:DG:H2"	1:P:817:DT:H5'	1.38	1.05
3:A:189:LYS:HG2	3:A:194:PRO:HG3	1.36	1.01
3:A:111:ARG:HH21	3:A:114:LYS:HD2	1.29	0.97
1:P:812:DG:H2"	1:P:813:DC:H5'	1.47	0.96
1:P:815:DA:H2"	1:P:816:DG:H5'	1.53	0.89
1:P:815:DA:H2"	1:P:816:DG:C5'	2.09	0.82
3:A:328:PRO:HB3	4:B:73:ARG:HH12	1.44	0.82
3:A:343:GLN:HG3	3:A:362:PRO:HG3	1.63	0.79
3:A:570:GLN:HE22	3:A:606:PRO:HB3	1.49	0.77
3:A:344:LYS:O	3:A:348:GLU:HG3	1.86	0.75
2:T:856:DT:C2'	2:T:857:DG:H5"	2.15	0.74
1:P:820:DC:H2"	1:P:821:DA:H5'	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:35:ARG:HB3	3:A:36:PRO:HD2	1.70	0.73
4:B:39:ALA:HB3	4:B:40:PRO:HD3	1.71	0.71
1:P:816:DG:H2''	1:P:817:DT:C5'	2.18	0.69
3:A:484:LEU:O	3:A:488:MET:HG2	1.92	0.69
2:T:860:DA:H2''	2:T:861:DC:H5'	1.74	0.69
4:B:45:ILE:HG13	4:B:99:LEU:HD13	1.74	0.69
3:A:599:ARG:HD3	3:A:620:LEU:HD11	1.75	0.69
2:T:854:DA:H2'	2:T:855:8OG:C2	2.22	0.69
3:A:279:THR:HG22	3:A:281:LYS:H	1.58	0.68
3:A:547:ARG:CZ	3:A:551:LEU:HD11	2.24	0.67
3:A:570:GLN:NE2	3:A:606:PRO:HB3	2.10	0.67
3:A:13:GLU:CD	3:A:13:GLU:H	1.97	0.66
1:P:806:DA:H2''	1:P:807:DC:H5'	1.76	0.66
1:P:817:DT:H2''	1:P:818:DG:H5'	1.78	0.65
2:T:856:DT:H2''	2:T:857:DG:C5'	2.16	0.65
3:A:111:ARG:NH2	3:A:114:LYS:HD2	2.07	0.64
3:A:343:GLN:HG3	3:A:362:PRO:CG	2.26	0.64
2:T:853:DC:H5''	2:T:854:DA:OP2	1.98	0.64
3:A:276:HIS:HD2	3:A:279:THR:H	1.45	0.63
3:A:66:VAL:HB	3:A:67:PRO:HD3	1.81	0.63
3:A:135:MET:HG3	3:A:174:ASP:OD1	2.01	0.61
3:A:318:ARG:O	3:A:319:GLU:HB2	1.99	0.61
3:A:237:LYS:O	3:A:241:GLU:HG3	2.00	0.60
1:P:817:DT:OP1	3:A:359:LYS:HB3	2.01	0.60
3:A:328:PRO:HB3	4:B:73:ARG:NH1	2.15	0.60
3:A:64:TYR:O	3:A:67:PRO:HD2	2.02	0.60
3:A:305:ALA:HB1	3:A:310:ARG:CB	2.32	0.59
3:A:638:LEU:N	3:A:638:LEU:HD22	2.17	0.59
3:A:79:ARG:HD3	10:A:1556:HOH:O	2.03	0.59
1:P:812:DG:H2''	1:P:813:DC:C5'	2.27	0.58
3:A:553:LYS:O	3:A:557:GLU:HB2	2.03	0.58
2:T:866:DC:H2''	2:T:867:DG:C8	2.39	0.58
3:A:91:THR:HB	3:A:181:LEU:HD13	1.85	0.57
3:A:584:GLN:NE2	10:A:1538:HOH:O	2.36	0.57
3:A:534:ASP:CG	3:A:549:LYS:HG2	2.25	0.57
3:A:391:MET:HE2	3:A:392:ILE:HD13	1.86	0.56
3:A:321:VAL:HG23	4:B:90:LYS:HD2	1.86	0.56
3:A:480:GLU:CD	7:A:823:D3T:H2'2	2.26	0.56
3:A:370:GLU:OE1	3:A:387:LYS:HE3	2.06	0.55
1:P:817:DT:H2''	1:P:818:DG:C5'	2.36	0.55
3:A:645:ASP:HB3	3:A:665:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:815:DA:H2''	1:P:816:DG:H5''	1.89	0.54
3:A:597:ASP:OD1	3:A:599:ARG:HD2	2.08	0.54
4:B:73:ARG:O	4:B:73:ARG:HD2	2.09	0.53
2:T:858:DG:H4'	3:A:432:HIS:O	2.08	0.53
3:A:15:VAL:HG22	3:A:72:LEU:HD21	1.89	0.52
3:A:368:VAL:HG23	3:A:369:LEU:N	2.24	0.52
3:A:279:THR:HG22	3:A:281:LYS:N	2.24	0.52
3:A:413:ASP:O	3:A:415:LYS:HD2	2.10	0.52
3:A:233:PRO:HB2	3:A:456:GLY:O	2.09	0.52
3:A:553:LYS:NZ	3:A:553:LYS:HB2	2.24	0.51
3:A:323:GLY:O	3:A:325:PRO:HD3	2.11	0.51
3:A:284:PRO:HA	3:A:288:ARG:HH21	1.76	0.51
1:P:822:2DA:H5''	10:A:1008:HOH:O	2.11	0.51
1:P:816:DG:C2'	1:P:817:DT:H5'	2.27	0.51
3:A:632:MET:HA	3:A:635:GLU:HG2	1.92	0.50
3:A:19:HIS:O	3:A:36:PRO:HD3	2.12	0.50
3:A:294:VAL:HG12	3:A:295:GLY:N	2.27	0.50
3:A:318:ARG:O	3:A:319:GLU:CB	2.58	0.50
3:A:490:ARG:HG3	10:A:1238:HOH:O	2.12	0.50
1:P:820:DC:H2''	1:P:821:DA:C5'	2.41	0.50
3:A:285:LYS:HE2	3:A:285:LYS:HA	1.94	0.49
3:A:234:PHE:CZ	3:A:239:ILE:HG13	2.47	0.49
3:A:284:PRO:HA	3:A:288:ARG:NH2	2.27	0.49
3:A:368:VAL:CG2	3:A:369:LEU:N	2.76	0.48
3:A:678:ARG:NH1	3:A:691:ASP:OD1	2.45	0.48
2:T:854:DA:O5'	3:A:532:ALA:HA	2.14	0.48
2:T:861:DC:H2'	2:T:862:DT:H71	1.94	0.48
2:T:854:DA:C4	3:A:527:GLY:HA2	2.47	0.48
3:A:563:ALA:O	3:A:567:GLU:HG3	2.14	0.48
2:T:856:DT:H2'	10:T:1086:HOH:O	2.12	0.48
4:B:77:THR:HG22	4:B:79:LEU:HD13	1.96	0.48
4:B:13:ASP:HB3	10:B:1368:HOH:O	2.13	0.47
3:A:211:LEU:HD21	3:A:598:GLY:C	2.35	0.47
3:A:136:LYS:HD2	9:A:992:1PE:H122	1.96	0.47
3:A:391:MET:HE2	3:A:392:ILE:HA	1.96	0.47
4:B:17:LEU:HA	4:B:84:GLY:HA2	1.97	0.47
3:A:317:THR:O	3:A:318:ARG:C	2.52	0.47
3:A:505:ILE:HD12	3:A:508:LYS:NZ	2.30	0.47
3:A:77:LEU:O	8:A:991:MES:H31	2.15	0.46
3:A:537:ILE:O	3:A:541:VAL:HG22	2.15	0.46
1:P:817:DT:H1'	1:P:818:DG:H5''	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:49:GLU:OE1	3:A:52:ARG:NH1	2.48	0.46
4:B:58:LEU:HD21	4:B:66:THR:HB	1.97	0.46
3:A:183:GLU:HG2	10:A:1365:HOH:O	2.16	0.46
3:A:233:PRO:HA	3:A:415:LYS:HG3	1.96	0.46
4:B:37:MET:O	4:B:40:PRO:HD2	2.16	0.46
2:T:853:DC:H42	3:A:584:GLN:HE22	1.64	0.46
3:A:478:GLY:HA2	7:A:823:D3T:O1B	2.16	0.46
1:P:816:DG:H1'	1:P:817:DT:H5'	1.97	0.46
3:A:590:ARG:HD2	3:A:592:TRP:O	2.16	0.46
4:B:79:LEU:HD12	4:B:89:THR:HB	1.97	0.46
3:A:272:GLU:O	3:A:288:ARG:HD3	2.15	0.45
3:A:195:GLU:H	3:A:195:GLU:CD	2.20	0.45
3:A:569:ILE:HG21	3:A:609:ALA:HB1	1.99	0.45
3:A:303:ASN:HB2	3:A:306:GLN:CB	2.47	0.45
3:A:326:TYR:HB3	4:B:92:GLY:HA2	1.99	0.45
3:A:456:GLY:HA2	3:A:471:GLN:OE1	2.15	0.45
3:A:49:GLU:OE2	3:A:54:GLY:HA3	2.16	0.45
3:A:591:ARG:O	3:A:591:ARG:HG2	2.16	0.45
3:A:632:MET:O	3:A:635:GLU:HG2	2.17	0.45
3:A:276:HIS:CD2	3:A:279:THR:H	2.31	0.45
4:B:41:ILE:O	4:B:45:ILE:HG12	2.17	0.45
3:A:155:VAL:O	3:A:156:ASP:C	2.55	0.45
3:A:570:GLN:HG2	10:A:1080:HOH:O	2.16	0.45
4:B:32:CYS:SG	4:B:34:PRO:HD2	2.57	0.45
3:A:638:LEU:H	3:A:638:LEU:HD22	1.82	0.44
3:A:667:GLN:O	3:A:671:GLU:HG3	2.17	0.44
1:P:816:DG:C2'	1:P:817:DT:C5'	2.91	0.44
3:A:590:ARG:HD3	3:A:592:TRP:CE2	2.52	0.44
3:A:423:ASN:OD1	3:A:599:ARG:NH2	2.50	0.44
4:B:23:ILE:HD13	4:B:54:THR:HB	2.00	0.44
3:A:678:ARG:HD3	3:A:690:LEU:O	2.18	0.44
3:A:388:GLU:O	3:A:392:ILE:HG12	2.18	0.43
3:A:282:PRO:C	3:A:284:PRO:HD3	2.38	0.43
4:B:3:LYS:HD3	4:B:50:GLN:NE2	2.32	0.43
4:B:23:ILE:CD1	4:B:54:THR:HB	2.49	0.43
3:A:297:ILE:HD12	3:A:297:ILE:N	2.34	0.43
1:P:821:DA:O4'	3:A:439:GLN:HA	2.17	0.43
3:A:336:PRO:O	3:A:342:ILE:HD11	2.19	0.43
2:T:871:DT:C2'	2:T:872:DT:H71	2.49	0.43
3:A:10:ALA:C	9:A:992:1PE:H231	2.40	0.43
3:A:158:MET:HA	3:A:161:TRP:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:145:ARG:O	3:A:149:GLU:HG3	2.19	0.42
1:P:810:DC:H2''	1:P:811:DG:C8	2.54	0.42
3:A:174:ASP:HB3	10:A:1251:HOH:O	2.19	0.42
3:A:355:LYS:HE2	3:A:363:VAL:HG21	2.01	0.42
3:A:443:VAL:HG23	3:A:444:ARG:HG3	2.00	0.42
4:B:14:THR:HG23	10:B:1368:HOH:O	2.19	0.42
3:A:391:MET:HE2	3:A:392:ILE:N	2.34	0.42
3:A:478:GLY:O	3:A:482:ARG:HG3	2.20	0.42
2:T:854:DA:H2'	2:T:855:8OG:N3	2.34	0.42
3:A:420:VAL:O	3:A:422:PRO:HD3	2.20	0.42
3:A:391:MET:HE1	3:A:447:TYR:CD2	2.55	0.42
3:A:474:ILE:HD12	3:A:474:ILE:N	2.35	0.42
3:A:59:HIS:O	3:A:60:ASN:HB3	2.19	0.42
3:A:144:LYS:HG2	3:A:154:TYR:CD1	2.55	0.42
3:A:158:MET:HA	3:A:161:TRP:CE2	2.55	0.42
3:A:468:PRO:HG2	10:A:1299:HOH:O	2.18	0.42
4:B:13:ASP:OD1	4:B:18:LYS:HE3	2.19	0.42
1:P:807:DC:H2''	1:P:808:DG:C8	2.54	0.42
3:A:470:VAL:HG12	3:A:471:GLN:N	2.34	0.41
3:A:534:ASP:OD1	3:A:549:LYS:HG2	2.20	0.41
4:B:74:GLY:O	4:B:77:THR:OG1	2.34	0.41
1:P:821:DA:H5''	3:A:440:ILE:O	2.20	0.41
4:B:80:LEU:C	4:B:80:LEU:HD23	2.40	0.41
3:A:638:LEU:N	3:A:638:LEU:CD2	2.83	0.41
3:A:189:LYS:HE2	3:A:194:PRO:CG	2.51	0.41
2:T:854:DA:H2'	2:T:855:8OG:N2	2.35	0.41
3:A:622:CYS:SG	3:A:654:ASP:HA	2.61	0.40
3:A:343:GLN:HG2	3:A:347:GLN:HE21	1.87	0.40
3:A:193:PRO:HA	3:A:194:PRO:HD3	1.80	0.40
3:A:279:THR:CG2	3:A:281:LYS:HB3	2.51	0.40
3:A:510:GLN:NE2	3:A:517:THR:C	2.75	0.40
3:A:530:TYR:CE1	3:A:611:ASN:HA	2.57	0.40
4:B:77:THR:CG2	4:B:79:LEU:HD13	2.51	0.40
3:A:155:VAL:O	3:A:157:GLY:N	2.54	0.40
3:A:254:LEU:O	3:A:258:THR:HG23	2.21	0.40
3:A:492:ASP:OD2	3:A:495:GLU:HB3	2.22	0.40
3:A:552:LYS:HB3	3:A:552:LYS:HE2	1.96	0.40
1:P:813:DC:H2''	1:P:814:DC:O5'	2.22	0.40

There are no symmetry-related clashes.

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	688/698 (99%)	667 (97%)	17 (2%)	4 (1%)	25	43
4	B	103/108 (95%)	100 (97%)	3 (3%)	0	100	100
All	All	791/806 (98%)	767 (97%)	20 (2%)	4 (0%)	29	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	156	ASP
3	A	318	ARG
3	A	319	GLU
3	A	653	HIS

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	
3	A	569/579 (98%)	549 (96%)	20 (4%)	36	62
4	B	85/87 (98%)	80 (94%)	5 (6%)	19	37
All	All	654/666 (98%)	629 (96%)	25 (4%)	33	58

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	85	ARG
3	A	142	ASP

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Mol	Chain	Res	Type
3	A	156	ASP
3	A	171	ASN
3	A	176	VAL
3	A	181	LEU
3	A	232	PHE
3	A	343	GLN
3	A	366	ASP
3	A	391	MET
3	A	426	VAL
3	A	488	MET
3	A	501	LEU
3	A	523	THR
3	A	536	LYS
3	A	553	LYS
3	A	557	GLU
3	A	599	ARG
3	A	624	LEU
3	A	686	PHE
4	B	14	THR
4	B	20	ASP
4	B	47	ASP
4	B	89	THR
4	B	99	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	276	HIS
3	A	343	GLN
3	A	347	GLN
3	A	510	GLN
3	A	570	GLN
3	A	584	GLN
3	A	607	HIS
4	B	50	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	8OG	T	855	1,2	18,25,26	1.20	2 (11%)	21,37,40	2.52	5 (23%)
1	2DA	P	822	1,2	17,22,23	0.72	1 (5%)	13,31,34	0.87	1 (7%)

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	8OG	T	855	1,2	-	2/3/21/22	0/3/3/3
1	2DA	P	822	1,2	-	0/3/18/19	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	855	8OG	C6-N1	3.48	1.39	1.33
2	T	855	8OG	C8-N7	-3.09	1.30	1.34
1	P	822	2DA	C8-N7	-2.01	1.31	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	855	8OG	C5-C6-N1	-8.61	111.65	123.43
2	T	855	8OG	C6-N1-C2	5.81	125.16	115.93
2	T	855	8OG	C2-N3-C4	-3.01	111.92	115.36
2	T	855	8OG	N3-C2-N1	-2.47	123.93	127.22
2	T	855	8OG	C6-C5-C4	-2.07	118.82	120.80
1	P	822	2DA	C5-C6-N6	2.06	123.48	120.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	855	8OG	O4'-C4'-C5'-O5'
2	T	855	8OG	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	855	8OG	3	0
1	P	822	2DA	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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
8	MES	A	991	-	12,12,12	0.51	0	14,16,16	0.89	0
6	SO4	A	905	-	4,4,4	0.29	0	6,6,6	0.08	0
9	1PE	A	992	-	15,15,15	0.86	0	14,14,14	0.89	0
7	D3T	A	823	5	22,29,29	1.07	1 (4%)	25,45,45	3.20	4 (16%)
6	SO4	A	906	-	4,4,4	0.25	0	6,6,6	0.07	0

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
8	MES	A	991	-	-	3/6/14/14	0/1/1/1
9	1PE	A	992	-	-	3/13/13/13	-
7	D3T	A	823	5	-	3/19/31/31	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	823	D3T	C4-N3	3.04	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	823	D3T	C4-N3-C2	14.66	127.52	115.14
7	A	823	D3T	PB-O3B-PG	-2.98	122.61	132.83
7	A	823	D3T	O2G-PG-O1G	2.24	119.44	110.68
7	A	823	D3T	C5M-C5-C6	2.04	122.98	118.68

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	991	MES	C7-C8-S-O1S
8	A	991	MES	C7-C8-S-O3S
9	A	992	1PE	OH2-C12-C22-OH3
9	A	992	1PE	OH7-C16-C26-OH6
7	A	823	D3T	PG-O3B-PB-O2B
8	A	991	MES	C7-C8-S-O2S
7	A	823	D3T	PB-O3A-PA-O2A
9	A	992	1PE	C25-C15-OH6-C26
7	A	823	D3T	PG-O3B-PB-O1B

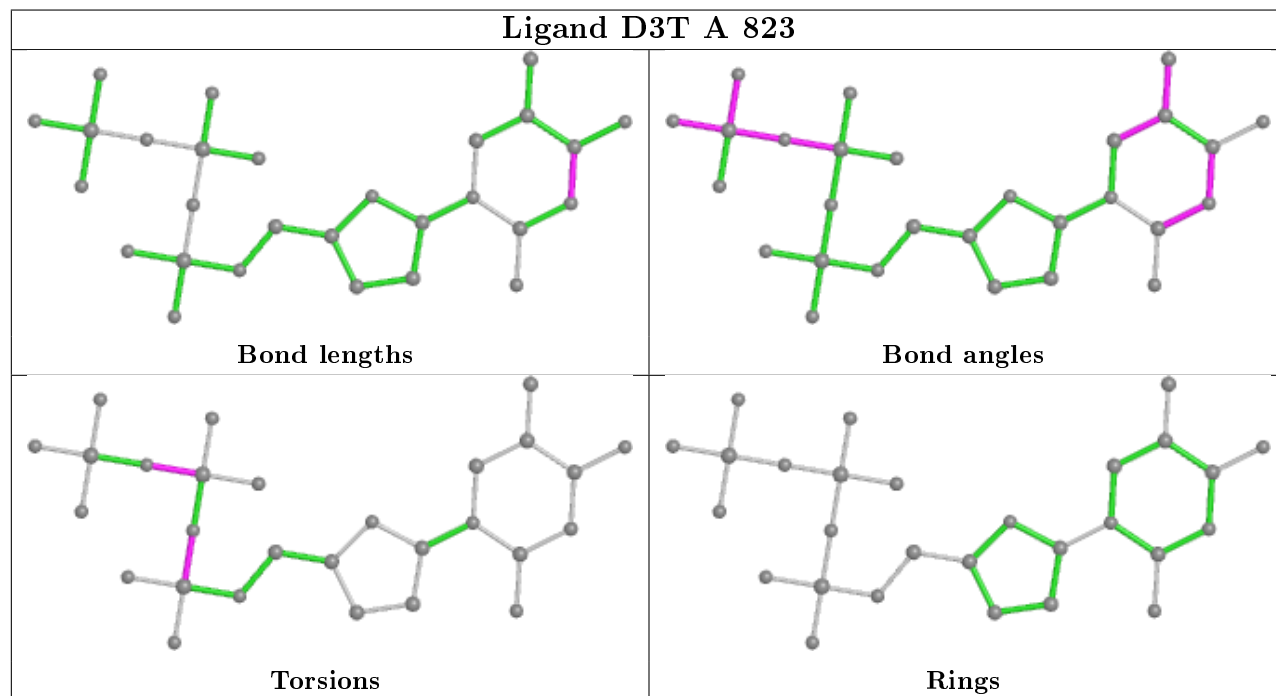
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	991	MES	1	0
9	A	992	1PE	2	0
7	A	823	D3T	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	P	16/22 (72%)	1.43	7 (43%) 0 0	14, 52, 100, 100	0
2	T	19/26 (73%)	1.31	7 (36%) 0 0	13, 30, 100, 100	0
3	A	692/698 (99%)	-0.24	10 (1%) 75 77	7, 20, 52, 77	0
4	B	105/108 (97%)	-0.16	3 (2%) 51 55	16, 30, 50, 55	0
All	All	832/854 (97%)	-0.16	27 (3%) 47 51	7, 22, 57, 100	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	808	DG	5.3
1	P	806	DA	4.9
2	T	871	DT	4.6
2	T	872	DT	4.4
2	T	869	DC	4.2
2	T	870	DG	4.1
1	P	807	DC	4.0
3	A	294	VAL	3.5
3	A	305	ALA	3.2
1	P	810	DC	3.0
4	B	20	ASP	3.0
1	P	809	DA	2.9
2	T	867	DG	2.7
3	A	311	GLU	2.7
3	A	303	ASN	2.5
3	A	542	GLY	2.5
1	P	811	DG	2.5
2	T	868	DT	2.3
3	A	318	ARG	2.3
2	T	866	DC	2.3
3	A	156	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	812	DG	2.2
3	A	312	PRO	2.2
3	A	546	GLU	2.1
4	B	73	ARG	2.1
3	A	302	LYS	2.1
4	B	82	LYS	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	8OG	T	855	23/24	0.95	0.14	11,19,26,28	0
1	2DA	P	822	20/21	0.97	0.15	10,11,15,17	0

6.3 Carbohydrates [i](#)

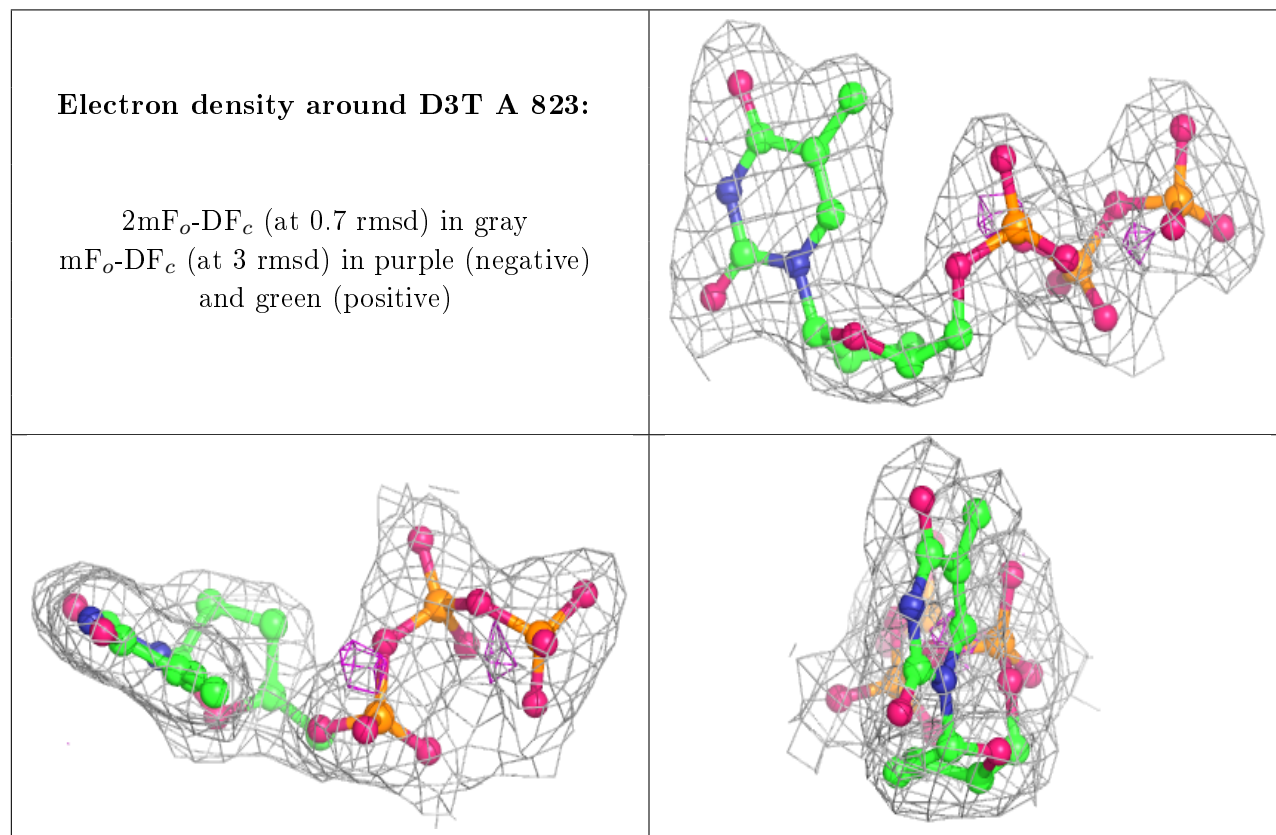
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	1PE	A	992	16/16	0.80	0.24	39,45,52,52	0
5	MG	T	904	1/1	0.85	0.09	34,34,34,34	0
6	SO4	A	905	5/5	0.92	0.19	58,59,60,60	0
5	MG	A	901	1/1	0.93	0.12	24,24,24,24	0
5	MG	A	902	1/1	0.95	0.10	24,24,24,24	0
8	MES	A	991	12/12	0.95	0.17	37,38,41,43	0
6	SO4	A	906	5/5	0.97	0.14	64,65,65,65	0
7	D3T	A	823	28/28	0.97	0.12	15,19,22,24	0
5	MG	A	903	1/1	0.98	0.06	16,16,16,16	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.