



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 01:00 PM EDT

PDB ID : 1TK0
Title : T7 DNA polymerase ternary complex with 8 oxo guanosine and ddCTP at the insertion site
Authors : Brieba, L.G.; Eichman, B.F.; Kokoska, R.J.; Doublet, S.; Kunkel, T.A.; Ellenberger, T.
Deposited on : 2004-06-07
Resolution : 2.30 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

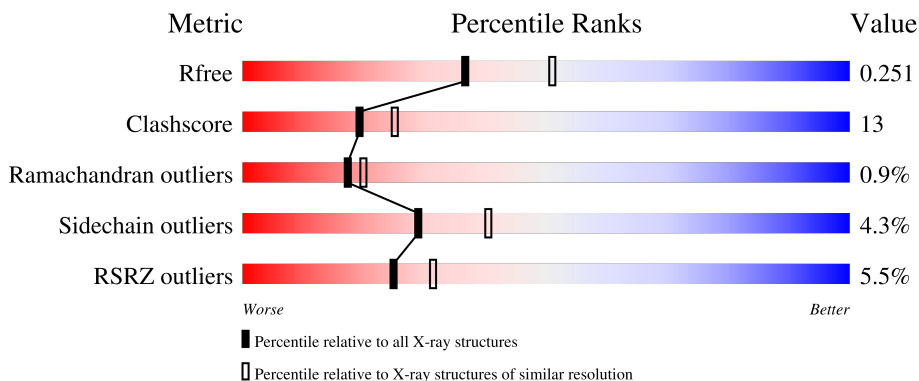
1 Overall quality at a glance

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 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	22	
2	T	26	
3	A	698	
4	B	108	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7428 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*A*CP*GP*GP*CP*CP*AP*GP*TP*GP*CP*CP*AP*(DDG))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	P	13	262	125	52	73	12	0	0	0

- Molecule 2 is a DNA chain called 5'-D(*CP*CP*CP*(8OG)P*CP*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
			Total	C	N	O	P			
2	T	16	319	149	57	97	16	0	0	0

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	686	5444	3468	939	1013	24	0	0	0

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
			Total	C	N	O	S			
4	B	105	802	518	129	152	3	0	0	0

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

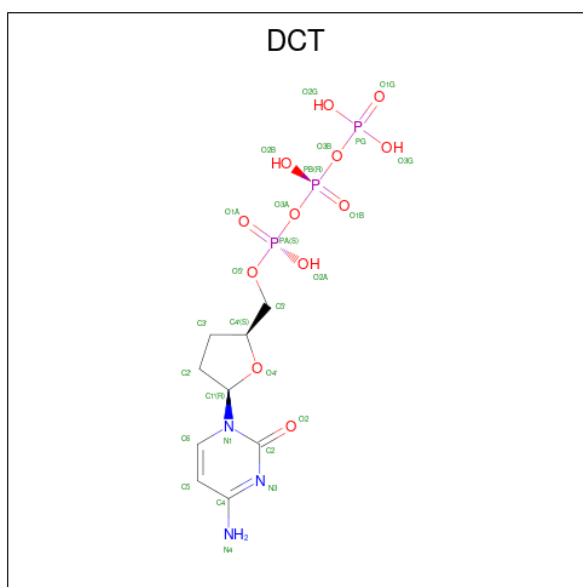
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Mg 3 3	0	0

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



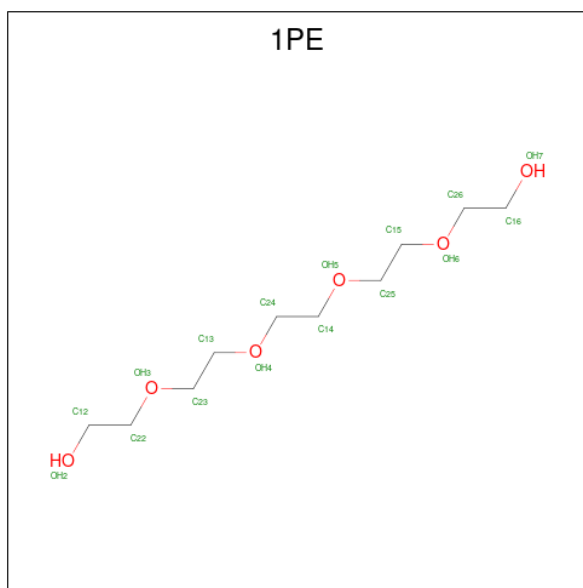
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0

- Molecule 7 is 2',3'-DIDEOXYCYTIDINE 5'-TRIPHOSPHATE (three-letter code: DCT) (formula: C₉H₁₆N₃O₁₂P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
7	A	1	Total	C	N	O	P	0	0
			27	9	3	12	3		

- Molecule 8 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



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

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	P	18	Total	O	0	0
			18	18		
10	T	27	Total	O	0	0
			27	27		
10	A	461	Total	O	0	0
			461	461		
10	B	27	Total	O	0	0
			27	27		

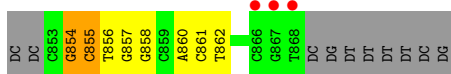
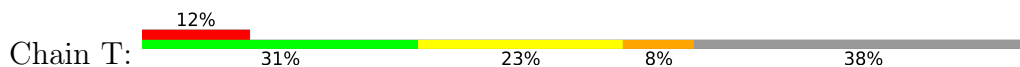
3 Residue-property plots i

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.

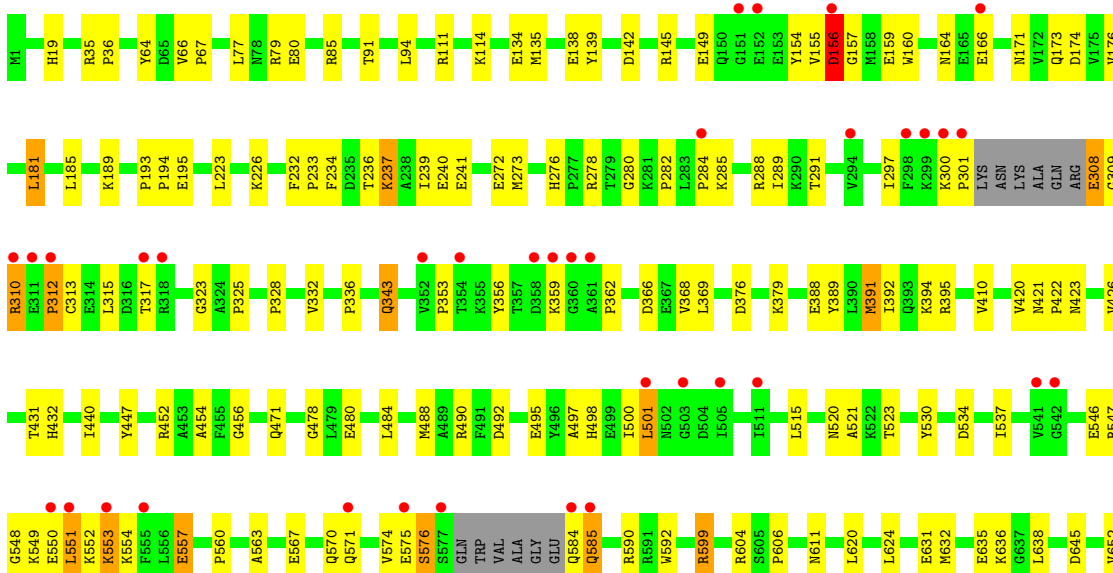
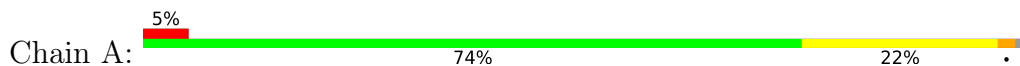
- Molecule 1: 5'-D(*CP*GP*AP*AP*AP*AP*CP*GP*A*CP*GP*GP*CP*CP*AP*GP*TP*GP*CP*CP*AP*(DDG))-3'



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

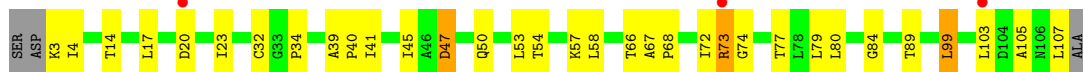


- Molecule 3: DNA polymerase





● 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	106.23Å 215.10Å 52.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.85 – 2.30 35.85 – 2.29	Depositor EDS
% Data completeness (in resolution range)	94.0 (35.85-2.30) 93.5 (35.85-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.29Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.263 0.203 , 0.251	Depositor DCC
R_{free} test set	2464 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtrriage
Anisotropy	0.509	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.1	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	0.94	EDS
Total number of atoms	7428	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: DCT, 1PE, MES, 8OG, SO4, DDG, MG

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	0.45	0/270	0.87	0/415
2	T	0.48	0/329	0.87	0/502
3	A	0.33	0/5577	0.58	0/7547
4	B	0.29	0/817	0.57	0/1108
All	All	0.34	0/6993	0.61	0/9572

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
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	820	DC	Sidechain
1	P	821	DA	Sidechain
2	T	855	DC	Sidechain
2	T	857	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	262	0	143	17	0
2	T	319	0	174	8	0
3	A	5444	0	5317	131	0
4	B	802	0	816	22	0
5	A	3	0	0	0	0
6	A	10	0	0	0	0
7	A	27	0	12	2	0
8	A	16	0	22	0	0
9	A	12	0	13	2	0
10	A	461	0	0	6	0
10	B	27	0	0	1	0
10	P	18	0	0	2	0
10	T	27	0	0	0	0
All	All	7428	0	6497	173	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 (173) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:816:DG:H2''	1:P:817:DT:H5'	1.38	1.01
1:P:812:DG:H2''	1:P:813:DC:H5'	1.38	1.00
3:A:111:ARG:HH21	3:A:114:LYS:HD2	1.32	0.94
1:P:812:DG:H2''	1:P:813:DC:C5'	1.98	0.93
3:A:297:ILE:HD12	3:A:297:ILE:H	1.34	0.91
3:A:570:GLN:HE22	3:A:606:PRO:HB3	1.38	0.88
1:P:815:DA:H2''	1:P:816:DG:H5'	1.54	0.88
3:A:164:ASN:OD1	3:A:166:GLU:HG2	1.79	0.83
1:P:816:DG:H2''	1:P:817:DT:C5'	2.08	0.82
3:A:35:ARG:HB3	3:A:36:PRO:HD2	1.62	0.80
1:P:815:DA:H2''	1:P:816:DG:C5'	2.11	0.80
3:A:301:PRO:HA	3:A:308:GLU:HG2	1.65	0.79
4:B:39:ALA:HB3	4:B:40:PRO:HD3	1.65	0.78
3:A:300:LYS:HG3	3:A:301:PRO:HD2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:817:DT:H2''	1:P:818:DG:H5'	1.66	0.76
3:A:570:GLN:NE2	3:A:606:PRO:HB3	2.04	0.72
3:A:328:PRO:HB3	4:B:73:ARG:HH12	1.56	0.70
3:A:480:GLU:CD	7:A:823:DCT:H2''	2.12	0.70
3:A:79:ARG:HD3	10:A:1108:HOH:O	1.92	0.69
2:T:860:DA:H2''	2:T:861:DC:H5'	1.74	0.68
3:A:343:GLN:HG3	3:A:362:PRO:HG3	1.77	0.67
3:A:546:GLU:H	3:A:546:GLU:CD	1.99	0.66
3:A:284:PRO:HA	3:A:288:ARG:NH2	2.10	0.66
3:A:563:ALA:O	3:A:567:GLU:HG3	1.96	0.65
4:B:45:ILE:HG13	4:B:99:LEU:HD13	1.77	0.65
3:A:391:MET:HE2	3:A:392:ILE:HA	1.78	0.65
3:A:678:ARG:NH1	3:A:691:ASP:OD1	2.23	0.65
4:B:3:LYS:HE3	4:B:50:GLN:CD	2.18	0.64
3:A:276:HIS:CD2	3:A:278:ARG:HB3	2.32	0.63
3:A:484:LEU:O	3:A:488:MET:HG2	1.99	0.63
4:B:23:ILE:HD13	4:B:54:THR:HB	1.78	0.63
3:A:91:THR:HB	3:A:181:LEU:HD13	1.80	0.62
3:A:94:LEU:HB3	3:A:185:LEU:HD13	1.80	0.62
3:A:285:LYS:HA	3:A:285:LYS:HE2	1.81	0.62
3:A:276:HIS:O	3:A:280:GLY:HA2	2.00	0.62
1:P:817:DT:H2''	1:P:818:DG:C5'	2.30	0.62
3:A:631:GLU:O	3:A:635:GLU:HG2	1.99	0.61
3:A:139:TYR:HE1	3:A:166:GLU:HG3	1.65	0.61
3:A:154:TYR:OH	3:A:157:GLY:HA2	2.00	0.61
3:A:276:HIS:HD2	3:A:278:ARG:H	1.47	0.61
3:A:145:ARG:O	3:A:149:GLU:HB2	2.02	0.60
3:A:85:ARG:HD3	10:A:1180:HOH:O	2.01	0.60
1:P:820:DC:H2''	1:P:821:DA:H5'	1.83	0.59
2:T:858:DG:H4'	3:A:432:HIS:O	2.03	0.59
3:A:64:TYR:O	3:A:67:PRO:HD2	2.03	0.58
3:A:584:GLN:O	3:A:585:GLN:O	2.21	0.58
3:A:237:LYS:O	3:A:241:GLU:HG3	2.04	0.58
3:A:135:MET:HG3	3:A:174:ASP:OD1	2.04	0.57
1:P:812:DG:H2''	1:P:813:DC:H5''	1.86	0.57
3:A:297:ILE:HD12	3:A:297:ILE:N	2.14	0.57
3:A:667:GLN:O	3:A:671:GLU:HG3	2.05	0.57
10:P:1650:HOH:O	3:A:394:LYS:HE2	2.07	0.55
3:A:19:HIS:O	3:A:36:PRO:HD3	2.06	0.55
4:B:14:THR:HG21	10:B:1190:HOH:O	2.07	0.54
3:A:599:ARG:HD3	3:A:620:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:23:ILE:CD1	4:B:54:THR:HB	2.37	0.54
3:A:391:MET:O	3:A:391:MET:HE3	2.08	0.54
3:A:575:GLU:O	3:A:576:SER:HB3	2.08	0.54
4:B:77:THR:HG22	4:B:79:LEU:HD13	1.90	0.53
3:A:343:GLN:HG3	3:A:362:PRO:CG	2.38	0.53
3:A:282:PRO:O	3:A:284:PRO:HD3	2.08	0.53
3:A:515:LEU:HD12	3:A:521:ALA:HA	1.90	0.52
3:A:421:ASN:HB3	3:A:431:THR:OG1	2.10	0.52
4:B:32:CYS:SG	4:B:34:PRO:HD2	2.50	0.52
3:A:134:GLU:O	3:A:138:GLU:HB2	2.10	0.51
3:A:557:GLU:O	3:A:560:PRO:HD3	2.10	0.51
3:A:391:MET:HE2	3:A:392:ILE:HD13	1.92	0.51
2:T:855:DC:C6	2:T:856:DT:H72	2.46	0.51
3:A:315:LEU:HD21	4:B:105:ALA:HB1	1.91	0.51
1:P:816:DG:C2'	1:P:817:DT:C5'	2.86	0.51
3:A:173:GLN:O	3:A:176:VAL:HG22	2.11	0.51
3:A:195:GLU:H	3:A:195:GLU:CD	2.13	0.51
4:B:73:ARG:HD2	4:B:73:ARG:O	2.11	0.51
3:A:189:LYS:HD2	3:A:194:PRO:HG2	1.93	0.50
4:B:74:GLY:O	4:B:77:THR:OG1	2.29	0.50
3:A:234:PHE:CZ	3:A:239:ILE:HG13	2.46	0.50
1:P:815:DA:H2''	1:P:816:DG:H5''	1.92	0.50
4:B:41:ILE:O	4:B:45:ILE:HG12	2.11	0.50
3:A:368:VAL:HG23	3:A:369:LEU:N	2.26	0.49
4:B:17:LEU:HA	4:B:84:GLY:HA2	1.94	0.49
3:A:478:GLY:HA2	7:A:823:DCT:O1B	2.12	0.49
2:T:855:DC:H2'	2:T:856:DT:H72	1.94	0.49
3:A:698:PRO:HD2	3:A:702:ILE:HD12	1.94	0.49
3:A:328:PRO:HB3	4:B:73:ARG:NH1	2.24	0.49
3:A:645:ASP:HB3	3:A:665:ILE:HD13	1.95	0.49
3:A:552:LYS:HE3	10:A:1412:HOH:O	2.12	0.48
3:A:549:LYS:O	3:A:553:LYS:HG2	2.12	0.48
3:A:550:GLU:O	3:A:554:LYS:HB2	2.13	0.48
3:A:391:MET:HE1	3:A:447:TYR:CD2	2.48	0.48
3:A:456:GLY:HA2	3:A:471:GLN:OE1	2.14	0.48
4:B:3:LYS:CD	4:B:47:ASP:HA	2.44	0.48
3:A:66:VAL:HB	3:A:67:PRO:HD3	1.96	0.47
3:A:272:GLU:CD	3:A:291:THR:H	2.17	0.47
3:A:282:PRO:C	3:A:284:PRO:HD3	2.35	0.47
3:A:530:TYR:CE1	3:A:611:ASN:HA	2.50	0.47
1:P:820:DC:H2''	1:P:821:DA:C5'	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:811:DG:H2''	1:P:812:DG:C8	2.50	0.47
3:A:77:LEU:HD13	9:A:902:MES:O2S	2.15	0.47
3:A:111:ARG:HH21	3:A:114:LYS:CD	2.14	0.47
4:B:103:LEU:O	4:B:107:LEU:HD13	2.14	0.47
4:B:3:LYS:HE3	4:B:50:GLN:NE2	2.29	0.46
3:A:77:LEU:O	9:A:902:MES:H31	2.14	0.46
3:A:189:LYS:HD2	3:A:194:PRO:CG	2.46	0.46
3:A:284:PRO:HA	3:A:288:ARG:HH21	1.81	0.46
3:A:420:VAL:O	3:A:422:PRO:HD3	2.16	0.46
3:A:548:GLY:O	3:A:552:LYS:HG2	2.15	0.46
3:A:111:ARG:NH2	3:A:114:LYS:HD2	2.14	0.46
3:A:297:ILE:H	3:A:297:ILE:CD1	2.12	0.46
3:A:368:VAL:CG2	3:A:369:LEU:N	2.78	0.46
1:P:816:DG:H1'	1:P:817:DT:H5''	1.97	0.46
3:A:35:ARG:HH11	3:A:35:ARG:HG3	1.80	0.46
3:A:79:ARG:HG2	3:A:80:GLU:N	2.31	0.46
3:A:574:VAL:HG12	3:A:576:SER:H	1.80	0.46
3:A:388:GLU:O	3:A:392:ILE:HG12	2.16	0.45
3:A:239:ILE:HD11	3:A:454:ALA:CB	2.46	0.45
2:T:854:8OG:H2''	2:T:855:DC:C6	2.51	0.45
3:A:223:LEU:O	3:A:226:LYS:HB3	2.16	0.45
3:A:376:ASP:OD2	3:A:379:LYS:HG3	2.16	0.45
3:A:35:ARG:HB3	3:A:36:PRO:CD	2.41	0.45
3:A:410:VAL:HG23	3:A:410:VAL:O	2.16	0.45
3:A:155:VAL:O	3:A:157:GLY:N	2.50	0.45
3:A:276:HIS:CD2	3:A:278:ARG:H	2.32	0.45
3:A:423:ASN:OD1	3:A:599:ARG:NH2	2.50	0.44
3:A:273:MET:CE	3:A:284:PRO:HG3	2.47	0.44
3:A:537:ILE:HG13	3:A:552:LYS:HD3	2.00	0.44
3:A:574:VAL:HG12	3:A:575:GLU:N	2.32	0.44
3:A:233:PRO:HB2	3:A:456:GLY:O	2.17	0.44
3:A:236:THR:O	3:A:240:GLU:HG3	2.17	0.44
3:A:534:ASP:CG	3:A:549:LYS:HG2	2.38	0.44
3:A:497:ALA:O	3:A:500:ILE:HG22	2.18	0.44
3:A:276:HIS:HD2	3:A:278:ARG:N	2.15	0.44
3:A:336:PRO:HB2	3:A:389:TYR:CD1	2.53	0.44
3:A:520:ASN:HA	3:A:523:THR:HG22	1.99	0.44
3:A:391:MET:HE3	3:A:395:ARG:HG2	2.00	0.44
2:T:861:DC:H2'	2:T:862:DT:H71	1.99	0.43
3:A:490:ARG:HD3	10:A:1146:HOH:O	2.17	0.43
3:A:193:PRO:HA	3:A:194:PRO:HD3	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:58:LEU:HD21	4:B:66:THR:HB	2.00	0.43
3:A:155:VAL:CG1	3:A:156:ASP:N	2.81	0.43
2:T:854:8OG:H5''	2:T:854:8OG:O8	2.19	0.43
3:A:574:VAL:HG12	3:A:576:SER:N	2.34	0.43
3:A:155:VAL:O	3:A:156:ASP:C	2.57	0.43
3:A:145:ARG:HH11	3:A:145:ARG:HB2	1.83	0.43
3:A:632:MET:O	3:A:636:LYS:HG3	2.19	0.43
3:A:590:ARG:HD2	3:A:592:TRP:O	2.19	0.43
3:A:391:MET:HE2	3:A:392:ILE:CA	2.46	0.42
3:A:547:ARG:O	3:A:551:LEU:HD22	2.19	0.42
2:T:855:DC:H2'	2:T:856:DT:C7	2.49	0.42
3:A:492:ASP:OD2	3:A:495:GLU:HB3	2.19	0.42
3:A:554:LYS:O	3:A:554:LYS:HD3	2.19	0.42
3:A:155:VAL:HG12	3:A:156:ASP:N	2.33	0.42
3:A:276:HIS:O	3:A:280:GLY:CA	2.66	0.42
3:A:323:GLY:O	3:A:325:PRO:HD3	2.20	0.42
3:A:343:GLN:CG	3:A:362:PRO:HG3	2.46	0.42
3:A:570:GLN:HG2	10:A:1272:HOH:O	2.19	0.42
3:A:426:VAL:CG1	3:A:604:ARG:NH2	2.83	0.42
3:A:652:VAL:HB	3:A:655:GLU:HG2	2.02	0.42
4:B:67:ALA:HB3	4:B:68:PRO:HD3	2.01	0.42
1:P:821:DA:H5''	3:A:440:ILE:O	2.20	0.42
4:B:4:ILE:HG21	4:B:57:LYS:HG3	2.01	0.41
3:A:353:PRO:HB2	3:A:356:TYR:OH	2.20	0.41
3:A:309:GLY:O	3:A:310:ARG:CB	2.68	0.41
3:A:317:THR:HG22	3:A:317:THR:O	2.20	0.41
3:A:159:GLU:HG2	3:A:160:TRP:CD1	2.56	0.41
3:A:308:GLU:HG3	3:A:313:CYS:SG	2.61	0.41
3:A:410:VAL:HG22	10:A:1178:HOH:O	2.21	0.41
3:A:135:MET:CE	3:A:135:MET:HA	2.51	0.41
3:A:452:ARG:HG3	3:A:700:TRP:HB3	2.01	0.41
3:A:391:MET:HE1	3:A:447:TYR:HD2	1.84	0.41
3:A:498:HIS:O	3:A:501:LEU:HD12	2.21	0.41
1:P:815:DA:H5'	10:P:1478:HOH:O	2.20	0.41
4:B:72:ILE:CD1	4:B:77:THR:HG21	2.51	0.40
3:A:289:ILE:HD12	3:A:325:PRO:HB2	2.03	0.40

There are no symmetry-related clashes.

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	680/698 (97%)	648 (95%)	25 (4%)	7 (1%)	15	17
4	B	103/108 (95%)	99 (96%)	4 (4%)	0	100	100
All	All	783/806 (97%)	747 (95%)	29 (4%)	7 (1%)	17	20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	156	ASP
3	A	312	PRO
3	A	585	GLN
3	A	310	ARG
3	A	359	LYS
3	A	576	SER
3	A	653	HIS

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	564/579 (97%)	543 (96%)	21 (4%)	34	48
4	B	85/87 (98%)	78 (92%)	7 (8%)	11	14
All	All	649/666 (97%)	621 (96%)	28 (4%)	29	40

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	142	ASP
3	A	156	ASP
3	A	171	ASN
3	A	181	LEU
3	A	232	PHE
3	A	237	LYS
3	A	308	GLU
3	A	312	PRO
3	A	332	VAL
3	A	343	GLN
3	A	366	ASP
3	A	391	MET
3	A	501	LEU
3	A	551	LEU
3	A	553	LYS
3	A	557	GLU
3	A	571	GLN
3	A	599	ARG
3	A	624	LEU
3	A	638	LEU
3	A	686	PHE
4	B	20	ASP
4	B	47	ASP
4	B	53	LEU
4	B	73	ARG
4	B	80	LEU
4	B	89	THR
4	B	99	LEU

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

Mol	Chain	Res	Type
3	A	266	GLN
3	A	276	HIS
3	A	343	GLN
3	A	347	GLN
3	A	570	GLN
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 (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	DDG	P	822	1,2	17,23,24	0.99	1 (5%)	15,33,36	1.09	1 (6%)
2	8OG	T	854	2	22,25,26	0.91	1 (4%)	30,37,40	1.91	5 (16%)

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	DDG	P	822	1,2	-	0/3/18/19	0/3/3/3
2	8OG	T	854	2	-	4/7/21/22	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	854	8OG	C8-N7	-3.77	1.31	1.38
1	P	822	DDG	C8-N7	-2.16	1.31	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	854	8OG	C2'-C1'-N9	-6.88	107.87	116.01
2	T	854	8OG	N7-C8-N9	4.89	112.38	106.58
2	T	854	8OG	C5-N7-C8	-3.17	104.91	109.47
2	T	854	8OG	C4-C5-N7	2.54	110.96	106.08
1	P	822	DDG	O6-C6-C5	2.52	129.29	124.37
2	T	854	8OG	O8-C8-N9	-2.39	122.66	125.99

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	854	8OG	C2'-C1'-N9-C4
2	T	854	8OG	O4'-C1'-N9-C8
2	T	854	8OG	C3'-C4'-C5'-O5'
2	T	854	8OG	C2'-C1'-N9-C8

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	854	8OG	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 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
6	SO4	A	994	-	4,4,4	0.28	0	6,6,6	0.05	0
8	IPE	A	901	-	15,15,15	1.02	0	14,14,14	0.89	0
7	DCT	A	823	5	24,28,28	0.67	0	33,43,43	0.93	2 (6%)
6	SO4	A	995	-	4,4,4	0.33	0	6,6,6	0.15	0
9	MES	A	902	-	12,12,12	0.58	0	14,16,16	0.74	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
7	DCT	A	823	5	-	4/22/31/31	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MES	A	902	-	-	4/6/14/14	0/1/1/1
8	1PE	A	901	-	-	3/13/13/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	823	DCT	O2G-PG-O1G	2.29	119.65	110.68
7	A	823	DCT	PB-O3B-PG	-2.10	125.61	132.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	901	1PE	OH7-C16-C26-OH6
9	A	902	MES	C7-C8-S-O3S
9	A	902	MES	C8-C7-N4-C5
8	A	901	1PE	OH2-C12-C22-OH3
9	A	902	MES	C7-C8-S-O2S
8	A	901	1PE	C16-C26-OH6-C15
7	A	823	DCT	PB-O3A-PA-O2A
7	A	823	DCT	PG-O3B-PB-O2B
7	A	823	DCT	PB-O3A-PA-O1A
7	A	823	DCT	PG-O3B-PB-O1B
9	A	902	MES	C7-C8-S-O1S

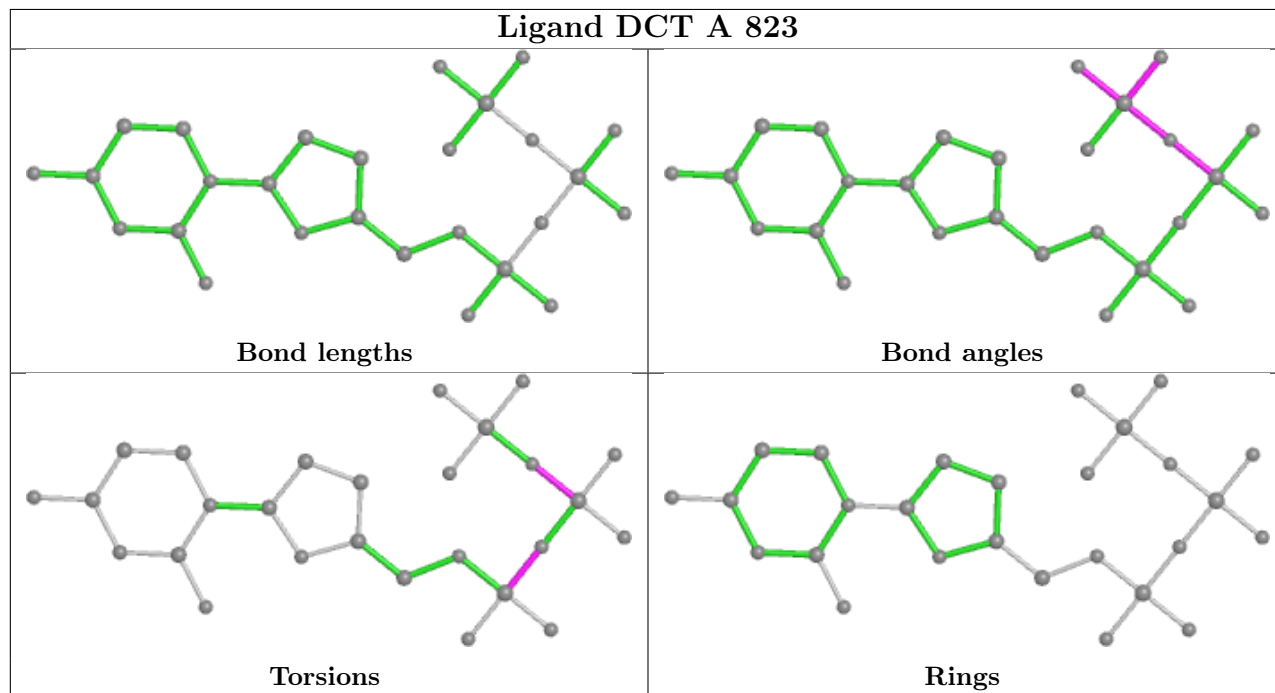
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	823	DCT	2	0
9	A	902	MES	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	12/22 (54%)	1.49	3 (25%) 0 0	29, 46, 97, 98	0
2	T	15/26 (57%)	1.06	3 (20%) 1 1	24, 39, 97, 100	0
3	A	686/698 (98%)	0.12	36 (5%) 27 34	16, 30, 64, 83	0
4	B	105/108 (97%)	0.27	3 (2%) 51 58	28, 45, 64, 67	0
All	All	818/854 (95%)	0.18	45 (5%) 25 31	16, 33, 66, 100	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	300	LYS	8.7
2	T	867	DG	6.6
1	P	811	DG	5.5
2	T	868	DT	5.4
1	P	810	DC	5.3
3	A	294	VAL	5.1
3	A	542	GLY	5.0
3	A	551	LEU	4.9
3	A	312	PRO	4.6
1	P	812	DG	4.1
3	A	584	GLN	3.9
3	A	577	SER	3.8
3	A	550	GLU	3.7
3	A	317	THR	3.6
3	A	358	ASP	3.6
4	B	73	ARG	3.6
3	A	298	PHE	3.6
3	A	301	PRO	3.5
3	A	511	ILE	3.4
3	A	151	GLY	3.3
3	A	166	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
3	A	156	ASP	3.2
3	A	311	GLU	3.1
3	A	352	VAL	3.0
4	B	20	ASP	2.9
3	A	318	ARG	2.9
3	A	361	ALA	2.8
3	A	501	LEU	2.7
3	A	585	GLN	2.7
2	T	866	DC	2.7
3	A	359	LYS	2.6
3	A	360	GLY	2.5
3	A	503	GLY	2.5
3	A	553	LYS	2.5
3	A	299	LYS	2.4
3	A	575	GLU	2.4
3	A	354	THR	2.3
3	A	571	GLN	2.3
3	A	541	VAL	2.3
3	A	505	ILE	2.3
3	A	555	PHE	2.2
3	A	284	PRO	2.2
3	A	152	GLU	2.2
3	A	310	ARG	2.2
4	B	103	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	8OG	T	854	23/24	0.91	0.14	38,42,51,53	0
1	DDG	P	822	21/22	0.97	0.17	24,28,29,32	0

6.3 Carbohydrates [i](#)

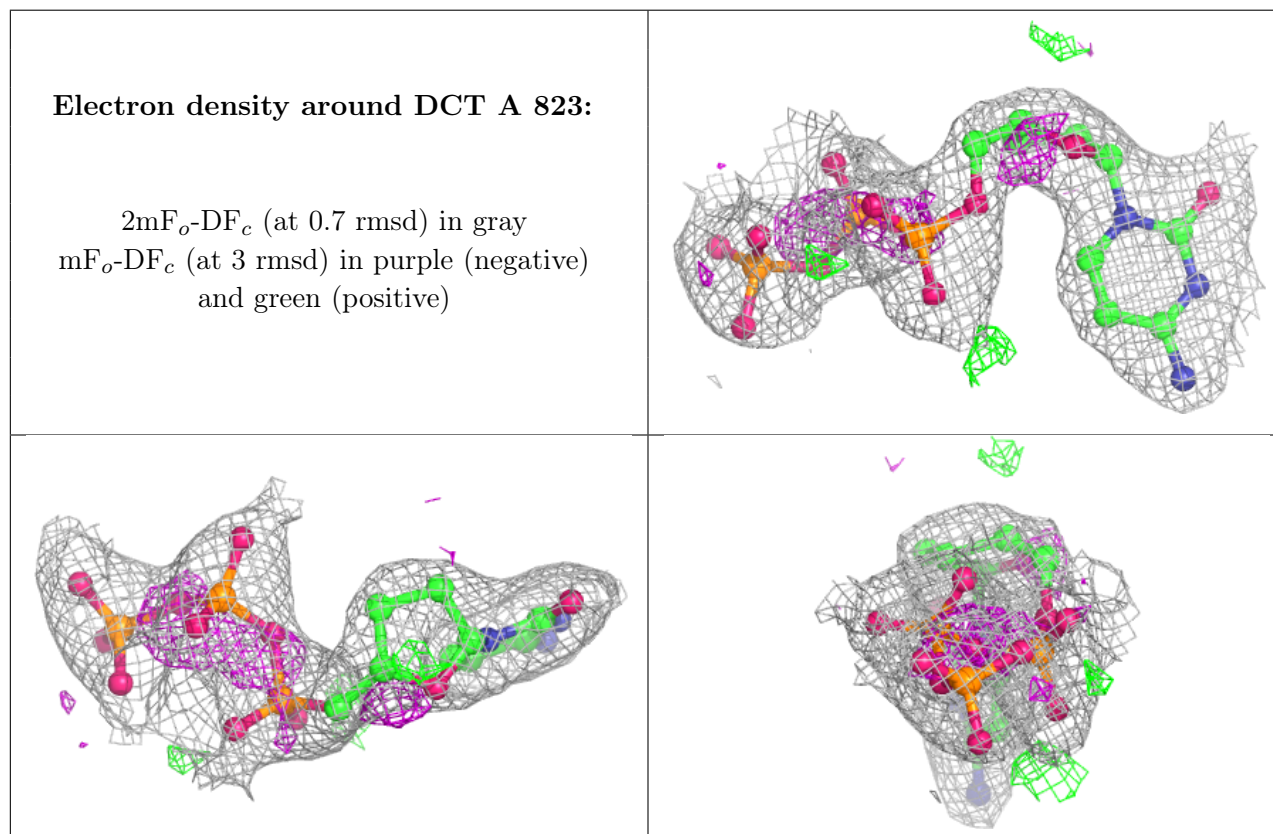
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	A	991	1/1	0.81	0.07	42,42,42,42	0
8	1PE	A	901	16/16	0.81	0.27	54,58,63,63	0
5	MG	A	992	1/1	0.92	0.10	33,33,33,33	0
7	DCT	A	823	27/27	0.94	0.14	28,35,37,39	0
6	SO4	A	994	5/5	0.95	0.16	63,64,65,65	0
6	SO4	A	995	5/5	0.95	0.17	65,66,66,67	0
5	MG	A	993	1/1	0.96	0.09	29,29,29,29	0
9	MES	A	902	12/12	0.96	0.20	46,48,49,50	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.