



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:42 am BST

PDB ID : 3PX6  
Title : Crystal Structure of Bacillus DNA Polymerase I Large Fragment Bound to DNA and ddCTP-dA Mismatch (tautomer) in Closed Conformation  
Authors : Wang, W.; Beese, L.S.  
Deposited on : 2010-12-09  
Resolution : 1.59 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](mailto: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.

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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 : 2.11  
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) : 2.11

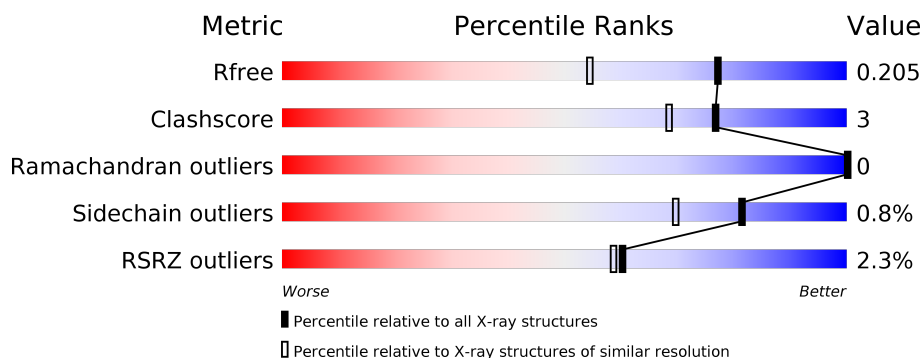
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.59 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	592	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div></div> </div> </div>
1	D	592	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div></div> </div> </div>
2	B	9	<div> <div></div> <div> <div>33%</div> <div>56%</div> <div>11%</div> </div> </div>
2	E	9	<div> <div></div> <div> <div>33%</div> <div>67%</div> </div> </div>
3	C	13	<div> <div>8%</div> <div> <div></div> <div>46%</div> <div>38%</div> <div>8%</div> <div>8%</div> </div> </div>
3	F	13	<div> <div>8%</div> <div> <div></div> <div>23%</div> <div>62%</div> <div>8%</div> <div>8%</div> </div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 21552 atoms, of which 10010 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	579	Total	C	H	N	O	S	0	5	0
			9410	2969	4740	810	874	17			
1	D	581	Total	C	H	N	O	S	0	15	0
			9513	3000	4794	818	884	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	598	ALA	ASP	ENGINEERED MUTATION	UNP Q5KWC1
A	710	TYR	PHE	ENGINEERED MUTATION	UNP Q5KWC1
A	823	HIS	ARG	SEE REMARK 999	UNP Q5KWC1
D	598	ALA	ASP	ENGINEERED MUTATION	UNP Q5KWC1
D	710	TYR	PHE	ENGINEERED MUTATION	UNP Q5KWC1
D	823	HIS	ARG	SEE REMARK 999	UNP Q5KWC1

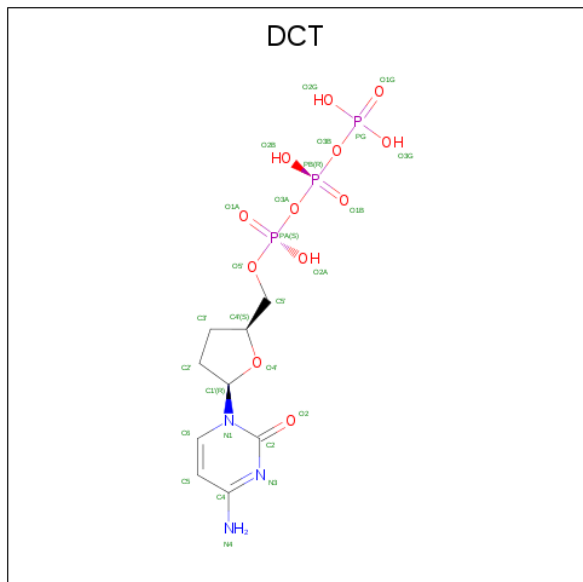
- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*CP\*TP\*GP\*AP\*CP\*TP\*CP\*(DOC))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	9	Total	C	H	N	O	P	0	0	0
			275	85	101	29	52	8			
2	E	9	Total	C	H	N	O	P	0	0	0
			275	85	101	29	52	8			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	12	Total	C	H	N	O	P	0	0	0
			383	119	133	52	68	11			
3	F	12	Total	C	H	N	O	P	0	0	0
			383	119	133	52	68	11			

- Molecule 4 is 2',3'-DIDEOXYCYTIDINE 5'-TRIPHOSPHATE (three-letter code: DCT) (formula:  $C_9H_{16}N_3O_{12}P_3$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	0	0
			29	9	2	3	12	3		
4	A	1	Total	C	H	N	O	P	0	0
			31	9	4	3	12	3		
4	D	1	Total	C	H	N	O	P	0	0
			29	9	2	3	12	3		

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

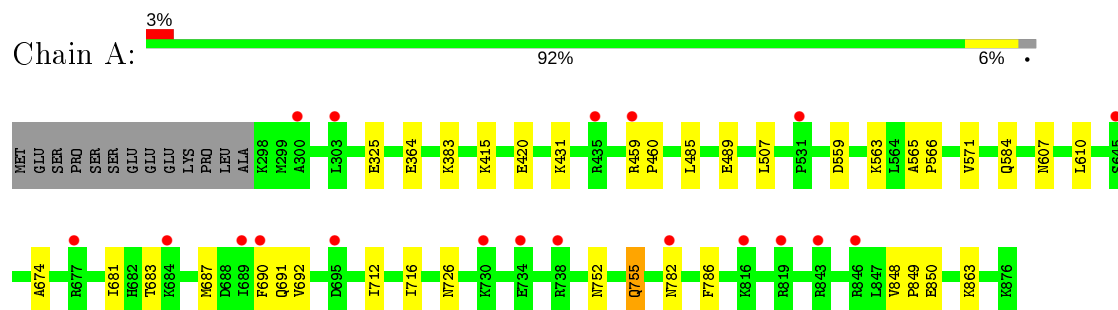
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	403	Total	O	0	0
			403	403		
7	D	611	Total	O	0	0
			611	611		
7	B	30	Total	O	0	0
			30	30		
7	C	62	Total	O	0	0
			62	62		
7	E	33	Total	O	0	0
			33	33		
7	F	63	Total	O	0	0
			63	63		

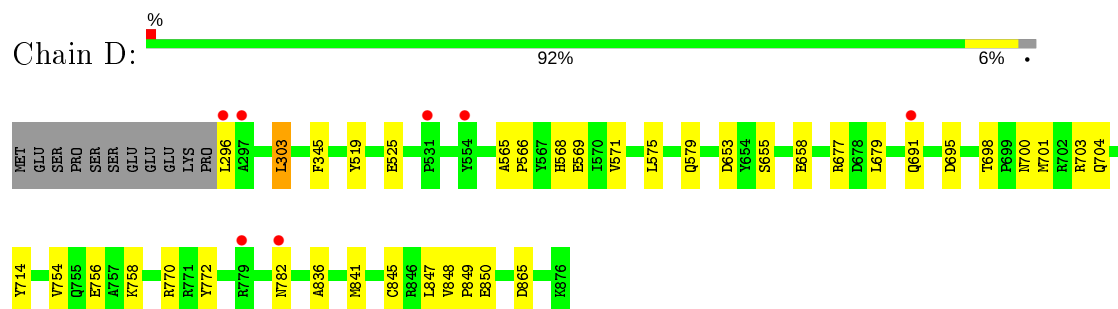
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: DNA polymerase I



#### • Molecule 1: DNA polymerase I



#### • Molecule 2: DNA (5'-D(\*CP\*CP\*TP\*GP\*AP\*CP\*TP\*CP\*(DOC))-3')

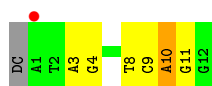


#### • Molecule 2: DNA (5'-D(\*CP\*CP\*TP\*GP\*AP\*CP\*TP\*CP\*(DOC))-3')



#### • Molecule 3: DNA (5'-D(\*C\*AP\*TP\*AP\*GP\*GP\*AP\*GP\*TP\*CP\*AP\*GP\*G)-3')





- Molecule 3: DNA (5'-D(\*C\*AP\*TP\*AP\*GP\*GP\*AP\*GP\*TP\*CP\*AP\*GP\*G)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.46 Å   108.28 Å   149.76 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	87.75 – 1.59 87.75 – 1.59	Depositor EDS
% Data completeness (in resolution range)	94.6 (87.75-1.59) 94.6 (87.75-1.59)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 1.59 Å)	Xtriage
Refinement program	PHENIX 1.7.1_743, REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.185 , 0.207 0.183 , 0.205	Depositor DCC
$R_{free}$ test set	8800 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 50.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	21552	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: DOC, DCT, MN, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.53	0/4769	0.63	0/6446
1	D	0.69	1/4862 (0.0%)	0.74	1/6570 (0.0%)
2	B	1.38	2/173 (1.2%)	2.04	9/264 (3.4%)
2	E	1.69	4/173 (2.3%)	2.25	12/264 (4.5%)
3	C	1.15	0/282	1.75	4/435 (0.9%)
3	F	1.48	3/282 (1.1%)	1.87	11/435 (2.5%)
All	All	0.72	10/10541 (0.1%)	0.89	37/14414 (0.3%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	25	DA	C3'-O3'	-7.32	1.34	1.44
2	E	26	DC	C3'-O3'	-6.20	1.35	1.44
3	F	4	DG	N7-C5	6.10	1.43	1.39
1	D	845	CYS	CB-SG	-5.77	1.72	1.81
3	F	7	DG	C2-N3	5.64	1.37	1.32
3	F	7	DG	C8-N7	5.59	1.34	1.30
2	E	27	DT	P-O5'	5.57	1.65	1.59
2	B	26	DC	C3'-O3'	-5.26	1.37	1.44
2	E	25	DA	N9-C4	5.10	1.41	1.37
2	B	27	DT	P-O5'	5.02	1.64	1.59

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	23	DT	O4'-C1'-N1	-10.57	100.60	108.00
2	B	23	DT	O4'-C1'-N1	-9.00	101.70	108.00
2	E	26	DC	O4'-C1'-N1	8.22	113.76	108.00
2	E	27	DT	C6-N1-C2	-8.18	117.21	121.30
3	F	5	DG	N3-C4-N9	-8.04	121.18	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	26	DC	O4'-C4'-C3'	7.20	110.32	106.00
2	B	26	DC	O4'-C4'-C3'	7.19	110.32	106.00
2	B	27	DT	O4'-C4'-C3'	-7.00	101.70	104.50
3	C	8	DT	O4'-C1'-N1	-6.88	103.19	108.00
3	F	2	DT	O4'-C1'-N1	6.68	112.68	108.00
2	B	26	DC	N3-C4-N4	6.64	122.64	118.00
1	D	653	ASP	CB-CG-OD1	6.58	124.22	118.30
2	B	26	DC	C5-C4-N4	-6.54	115.62	120.20
3	F	8	DT	O4'-C1'-N1	-6.52	103.44	108.00
3	F	5	DG	C2-N3-C4	-6.19	108.81	111.90
2	E	28	DC	N3-C4-C5	-6.18	119.43	121.90
2	E	28	DC	C5-C4-N4	6.16	124.51	120.20
3	F	5	DG	O4'-C4'-C3'	-6.14	102.04	104.50
2	E	24	DG	C4-C5-N7	5.95	113.18	110.80
2	B	28	DC	N3-C2-O2	5.91	126.04	121.90
3	C	4	DG	N1-C2-N3	-5.79	120.42	123.90
3	F	9	DC	O4'-C1'-C2'	5.73	110.48	105.90
3	C	11	DG	N9-C4-C5	5.66	107.67	105.40
2	B	26	DC	O4'-C1'-N1	5.63	111.94	108.00
2	E	27	DT	N3-C4-C5	-5.47	111.92	115.20
2	B	28	DC	N1-C2-O2	-5.46	115.62	118.90
3	F	5	DG	N9-C4-C5	5.39	107.56	105.40
3	C	10	DA	O4'-C1'-N9	-5.38	104.23	108.00
3	F	4	DG	O5'-P-OP2	-5.38	100.86	105.70
3	F	6	DA	C6-N1-C2	-5.36	115.38	118.60
2	E	27	DT	OP1-P-OP2	5.32	127.57	119.60
2	B	22	DC	O4'-C1'-N1	-5.27	104.31	108.00
2	E	27	DT	C4-C5-C6	5.24	121.14	118.00
3	F	5	DG	N3-C4-C5	5.22	131.21	128.60
3	F	6	DA	C5-C6-N1	5.06	120.23	117.70
2	E	28	DC	O4'-C4'-C3'	-5.03	102.49	104.50
2	E	27	DT	C6-C5-C7	-5.00	119.90	122.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4670	4740	4722	30	0
1	D	4719	4794	4737	26	0
2	B	174	101	103	1	0
2	E	174	101	103	0	0
3	C	250	133	136	2	0
3	F	250	133	136	2	0
4	A	54	6	24	1	0
4	D	27	2	12	2	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	10	0	0	0	0
6	D	10	0	0	0	0
7	A	403	0	0	9	3
7	B	30	0	0	0	0
7	C	62	0	0	0	0
7	D	611	0	0	7	3
7	E	33	0	0	0	0
7	F	63	0	0	0	0
All	All	11542	10010	9973	61	3

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 3.

All (61) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:ASN:O	1:A:755:GLN:HG3	1.77	0.85
1:D:850:GLU:HG2	7:D:1100:HOH:O	1.78	0.82
4:D:202:DCT:HN41	3:F:3:DA:H61	1.28	0.81
1:A:683:THR:HG22	1:A:687:MET:HE2	1.67	0.77
1:A:683:THR:HG22	1:A:687:MET:CE	2.24	0.68
1:D:754:VAL:HG12	1:D:758:LYS:HE2	1.76	0.67
4:A:201:DCT:HN41	3:C:3:DA:H61	1.43	0.66
1:D:700[A]:ASN:OD1	1:D:703:ARG:NH2	2.28	0.66
1:D:754:VAL:CG1	1:D:758:LYS:HE2	2.26	0.65
1:D:691:GLN:HG2	7:D:998:HOH:O	1.97	0.63
1:A:459:ARG:NE	7:A:919:HOH:O	2.30	0.63
1:A:690:PHE:O	1:A:692:VAL:HG13	1.99	0.63
1:D:698:THR:H	1:D:701:MET:HE3	1.66	0.60
1:A:415:LYS:NZ	7:A:1182:HOH:O	2.34	0.59
1:A:863:LYS:NZ	7:A:1166:HOH:O	2.36	0.58
1:A:565:ALA:HA	1:A:571:VAL:CG2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:GLU:HG2	7:A:1182:HOH:O	2.04	0.56
1:A:364:GLU:HG3	7:A:135:HOH:O	2.04	0.56
1:A:383:LYS:HE2	7:A:269:HOH:O	2.06	0.56
1:A:565:ALA:HA	1:A:571:VAL:HG21	1.89	0.54
1:D:565:ALA:HA	1:D:571:VAL:HG21	1.89	0.54
1:A:507:LEU:HD23	1:A:584[A]:GLN:OE1	2.07	0.54
1:D:568:HIS:O	1:D:571:VAL:HG22	2.08	0.53
1:D:698:THR:HG23	1:D:701:MET:HE3	1.91	0.53
1:D:519:TYR:CD2	1:D:525:GLU:HG2	2.46	0.51
1:A:607[B]:ASN:ND2	1:A:610:LEU:HD12	2.26	0.50
1:A:752:ASN:HA	1:A:755:GLN:HG2	1.93	0.50
1:A:325:GLU:CD	1:A:325:GLU:H	2.14	0.50
1:A:459:ARG:HB3	1:A:460:PRO:HD3	1.93	0.50
1:D:569:GLU:HA	7:D:1271:HOH:O	2.11	0.49
1:A:565:ALA:N	1:A:566:PRO:CD	2.75	0.49
1:A:752:ASN:HA	1:A:755:GLN:CG	2.42	0.49
1:D:565:ALA:HA	1:D:571:VAL:CG2	2.43	0.48
1:A:383:LYS:CE	7:A:269:HOH:O	2.61	0.48
1:D:847:LEU:HD23	1:D:847:LEU:C	2.35	0.47
1:D:296:LEU:N	7:D:1044:HOH:O	2.47	0.47
1:A:674:ALA:HB1	1:A:681:ILE:HD11	1.97	0.46
1:A:850:GLU:OE1	7:A:955:HOH:O	2.20	0.46
1:D:655[B]:SER:OG	1:D:865:ASP:OD2	2.32	0.46
1:A:712:ILE:HA	1:A:716:ILE:HG22	1.97	0.46
1:D:848:VAL:HB	1:D:849:PRO:HD3	1.97	0.46
1:A:690:PHE:O	1:A:691:GLN:C	2.55	0.45
1:A:782:ASN:O	1:A:786:PHE:HD2	2.00	0.45
1:D:565:ALA:N	1:D:566:PRO:CD	2.80	0.45
2:B:28:DC:H2'	2:B:29:DOC:H6	1.97	0.44
1:A:607[B]:ASN:CG	1:A:610:LEU:HB2	2.40	0.42
1:A:485:LEU:O	1:A:489:GLU:HG3	2.19	0.42
1:D:770:ARG:HD3	1:D:772:TYR:CZ	2.54	0.42
3:C:9:DC:H2'	3:C:10:DA:C8	2.55	0.42
1:A:420:GLU:CG	7:A:1182:HOH:O	2.67	0.41
1:D:303:LEU:HD13	1:D:345:PHE:HD2	1.83	0.41
1:D:575:LEU:O	1:D:579:GLN:HG3	2.21	0.41
1:A:563:LYS:NZ	1:A:726:ASN:OD1	2.54	0.41
1:D:296:LEU:CA	7:D:1044:HOH:O	2.68	0.41
1:D:850:GLU:CG	7:D:1100:HOH:O	2.50	0.41
1:D:677:ARG:HB2	1:D:679:LEU:HG	2.02	0.41
1:D:714:TYR:HB3	7:D:1221:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:836:ALA:HB3	1:D:841:MET:CE	2.51	0.40
3:F:9:DC:H2'	3:F:10:DA:C8	2.56	0.40
1:A:848:VAL:HB	1:A:849:PRO:HD3	2.03	0.40
1:D:658:GLU:CD	4:D:202:DCT:H2"	2.41	0.40

All (3) 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)
7:A:1118:HOH:O	7:D:1249:HOH:O[2_745]	1.89	0.31
7:A:1118:HOH:O	7:D:1251:HOH:O[2_745]	2.02	0.18
7:A:1191:HOH:O	7:D:1187:HOH:O[2_745]	2.13	0.07

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	582/592 (98%)	568 (98%)	14 (2%)	0	100	100
1	D	594/592 (100%)	579 (98%)	15 (2%)	0	100	100
All	All	1176/1184 (99%)	1147 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
1	A	500/507 (99%)	497 (99%)	3 (1%)	86	77
1	D	510/507 (101%)	505 (99%)	5 (1%)	76	61
All	All	1010/1014 (100%)	1002 (99%)	8 (1%)	81	70

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	431	LYS
1	A	559	ASP
1	A	755	GLN
1	D	303	LEU
1	D	695	ASP
1	D	704	GLN
1	D	756	GLU
1	D	782	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	DOC	B	29	3,2	14,19,20	1.01	1 (7%)	13,26,29	1.62	2 (15%)
2	DOC	E	29	3,2	14,19,20	1.04	2 (14%)	13,26,29	1.40	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	DOC	B	29	3,2	-	0/4/18/19	0/2/2/2
2	DOC	E	29	3,2	-	0/4/18/19	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	29	DOC	C2-N3	-2.49	1.33	1.38
2	E	29	DOC	C2-N3	-2.43	1.33	1.38
2	E	29	DOC	C6-C5	-2.35	1.32	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	29	DOC	C2-N3-C4	4.24	120.64	116.34
2	B	29	DOC	C2-N3-C4	3.23	119.62	116.34
2	B	29	DOC	C2'-C1'-N1	3.12	118.36	112.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	29	DOC	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DCT	A	203	-	22,28,28	0.95	1 (4%)	26,43,43	1.61	3 (11%)
4	DCT	D	202	5	22,28,28	0.87	0	26,43,43	1.77	7 (26%)
6	SO4	A	3	-	4,4,4	0.20	0	6,6,6	0.13	0
4	DCT	A	201	5	22,28,28	0.94	1 (4%)	26,43,43	1.73	5 (19%)
6	SO4	D	4	-	4,4,4	0.13	0	6,6,6	0.08	0
6	SO4	A	2	-	4,4,4	0.29	0	6,6,6	0.30	0
6	SO4	D	1	-	4,4,4	0.15	0	6,6,6	0.52	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
4	DCT	D	202	5	-	4/19/31/31	0/2/2/2
4	DCT	A	201	5	-	2/19/31/31	0/2/2/2
4	DCT	A	203	-	-	6/19/31/31	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	203	DCT	C4-N3	3.01	1.40	1.35
4	A	201	DCT	C6-N1	2.17	1.38	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	201	DCT	C2'-C1'-N1	-4.51	103.99	112.48
4	A	203	DCT	PB-O3B-PG	-4.48	117.47	132.83
4	A	203	DCT	PB-O3A-PA	-4.43	117.63	132.83
4	A	201	DCT	C4'-O4'-C1'	4.10	113.68	109.81
4	D	202	DCT	C2-N3-C4	3.91	120.31	116.34
4	D	202	DCT	C2'-C1'-N1	-3.57	105.76	112.48
4	D	202	DCT	C4'-O4'-C1'	3.57	113.17	109.81
4	A	201	DCT	PB-O3A-PA	-2.95	122.70	132.83
4	D	202	DCT	PB-O3A-PA	-2.49	124.28	132.83
4	A	201	DCT	C2-N3-C4	2.48	118.86	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	202	DCT	O4'-C4'-C5'	2.31	113.32	109.52
4	D	202	DCT	O2G-PG-O3B	2.25	112.16	104.64
4	A	201	DCT	O4'-C4'-C5'	2.22	113.17	109.52
4	A	203	DCT	C2'-C1'-N1	-2.09	108.55	112.48
4	D	202	DCT	O3B-PG-O1G	-2.05	99.83	111.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

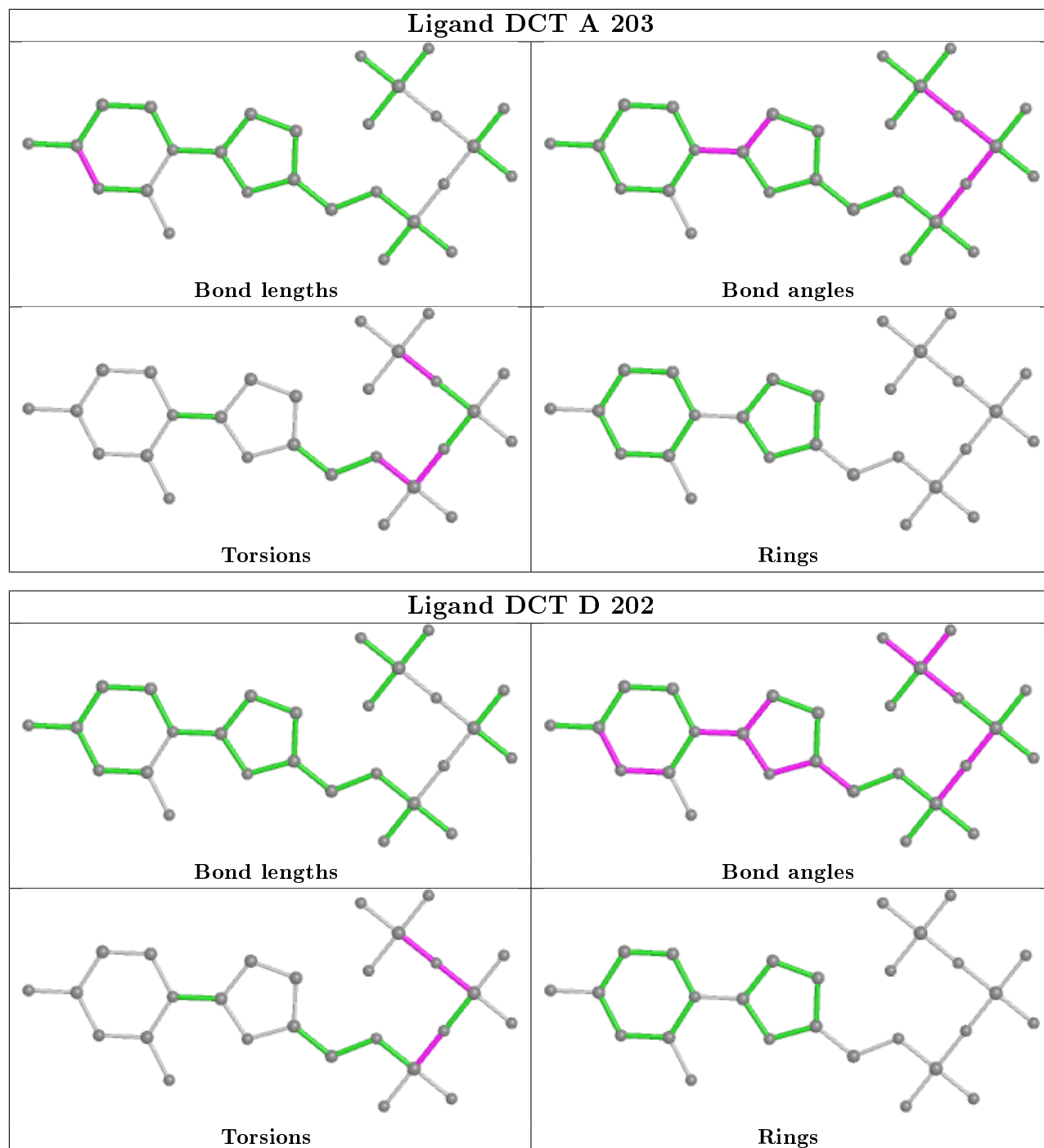
Mol	Chain	Res	Type	Atoms
4	A	203	DCT	C5'-O5'-PA-O2A
4	A	203	DCT	PB-O3B-PG-O2G
4	A	203	DCT	PB-O3B-PG-O3G
4	A	203	DCT	C5'-O5'-PA-O3A
4	A	203	DCT	PB-O3A-PA-O2A
4	D	202	DCT	PG-O3B-PB-O2B
4	A	201	DCT	PG-O3B-PB-O2B
4	A	203	DCT	C5'-O5'-PA-O1A
4	A	201	DCT	PB-O3A-PA-O1A
4	D	202	DCT	PB-O3B-PG-O1G
4	D	202	DCT	PB-O3A-PA-O1A
4	D	202	DCT	PG-O3B-PB-O1B

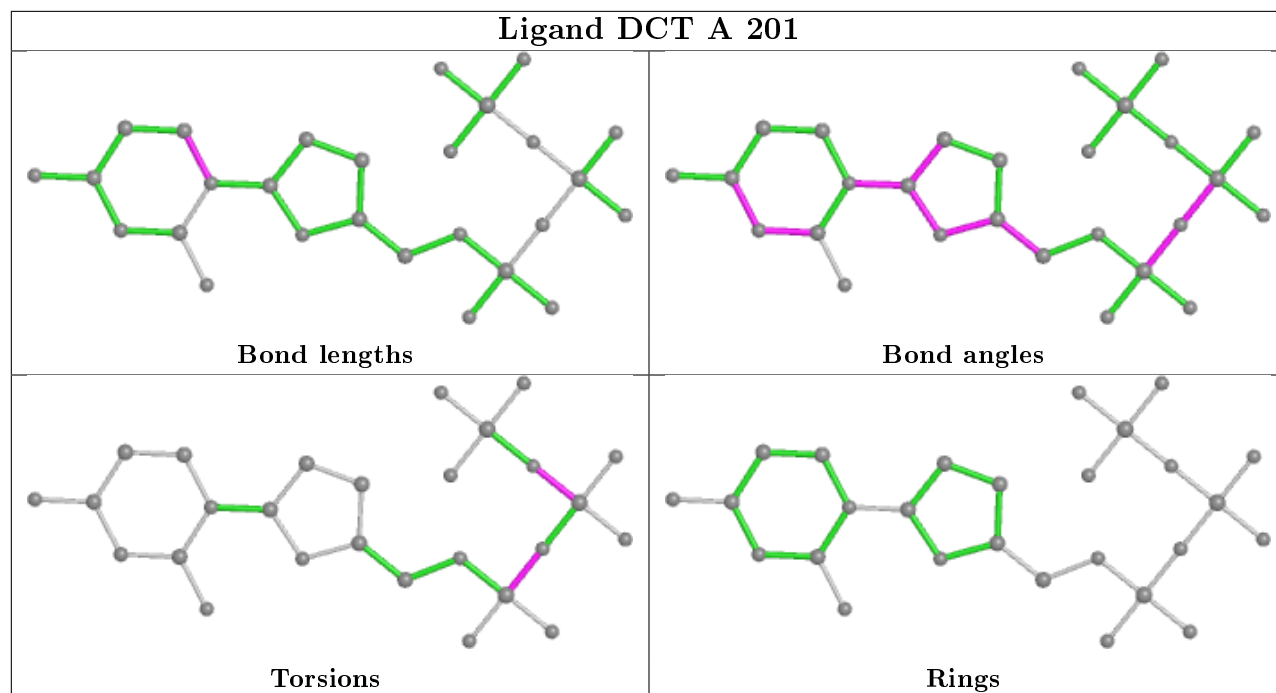
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	202	DCT	2	0
4	A	201	DCT	1	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	579/592 (97%)	0.06	19 (3%) 46 43	16, 29, 48, 58	0
1	D	581/592 (98%)	0.12	7 (1%) 79 78	10, 20, 38, 50	0
2	B	8/9 (88%)	-0.33	0 100 100	18, 23, 43, 52	0
2	E	8/9 (88%)	-0.29	0 100 100	15, 23, 40, 50	0
3	C	12/13 (92%)	-0.08	1 (8%) 11 10	16, 22, 50, 67	0
3	F	12/13 (92%)	0.11	1 (8%) 11 10	14, 19, 48, 64	0
All	All	1200/1228 (97%)	0.08	28 (2%) 60 59	10, 25, 45, 67	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	816	LYS	4.3
1	A	690	PHE	4.1
1	A	689	ILE	4.1
1	A	819	ARG	4.0
1	A	531	PRO	3.7
1	A	303	LEU	3.3
1	A	695	ASP	3.3
3	C	1	DA	3.3
1	A	843	ARG	3.3
1	D	779	ARG	3.1
1	D	531	PRO	3.1
1	D	691	GLN	3.0
1	D	296	LEU	2.6
1	A	846	ARG	2.5
1	A	459	ARG	2.5
1	A	677	ARG	2.5
1	D	554	TYR	2.5
1	A	730	LYS	2.4
1	A	734	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	738	ARG	2.2
1	D	782	ASN	2.2
1	A	300	ALA	2.2
1	A	435	ARG	2.2
3	F	1	DA	2.2
1	A	684	LYS	2.1
1	A	645	SER	2.1
1	A	782	ASN	2.1
1	D	297	ALA	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	DOC	B	29	18/19	0.96	0.07	17,19,23,26	0
2	DOC	E	29	18/19	0.98	0.09	11,13,18,20	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

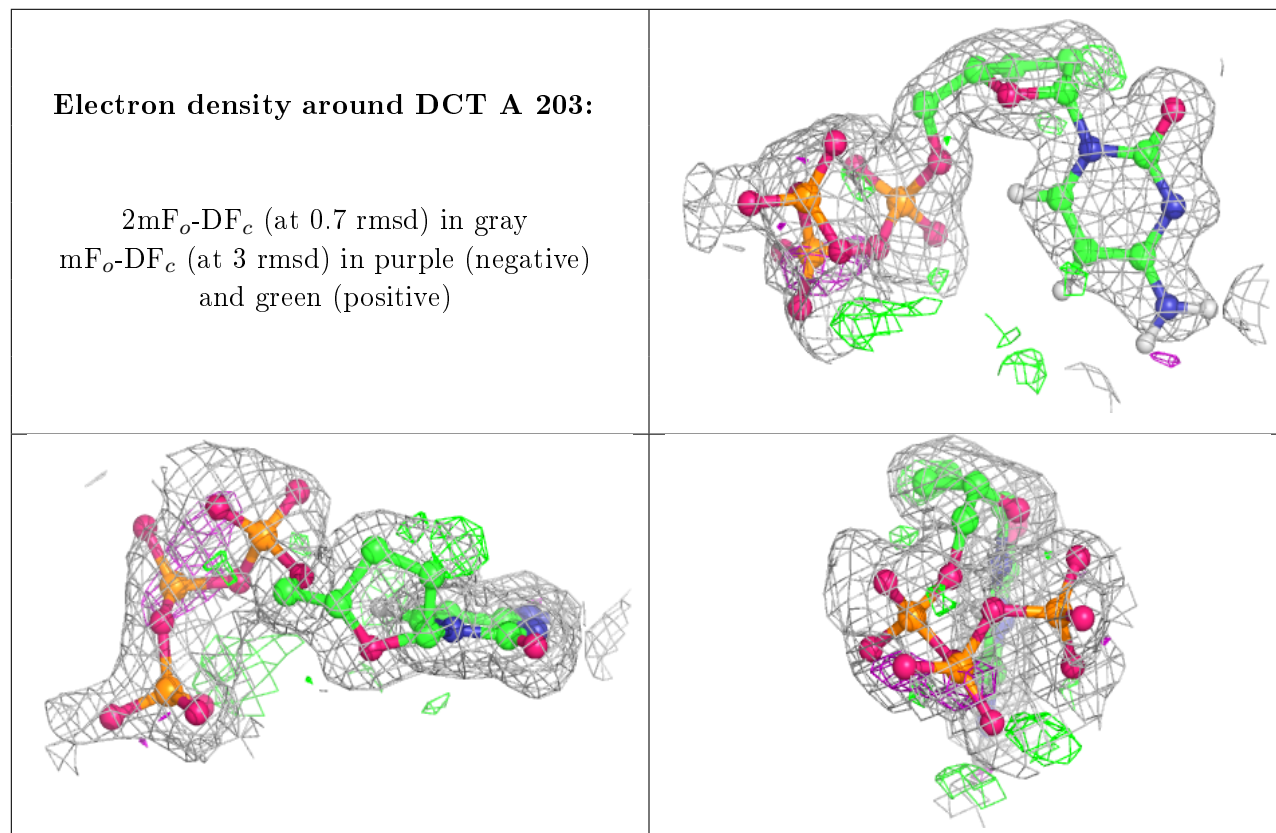
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	SO4	D	4	5/5	0.80	0.16	67,74,76,85	0
6	SO4	A	3	5/5	0.88	0.20	34,37,52,72	0
4	DCT	A	203	27/27	0.89	0.11	21,28,63,75	0
6	SO4	A	2	5/5	0.96	0.18	32,36,36,42	0
4	DCT	A	201	27/27	0.97	0.07	17,21,25,29	0
4	DCT	D	202	27/27	0.99	0.09	13,16,20,21	0
5	MN	A	1	1/1	0.99	0.06	22,22,22,22	0

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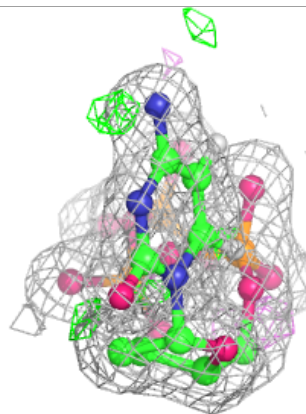
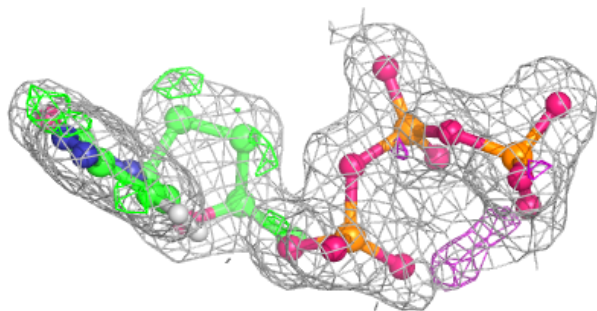
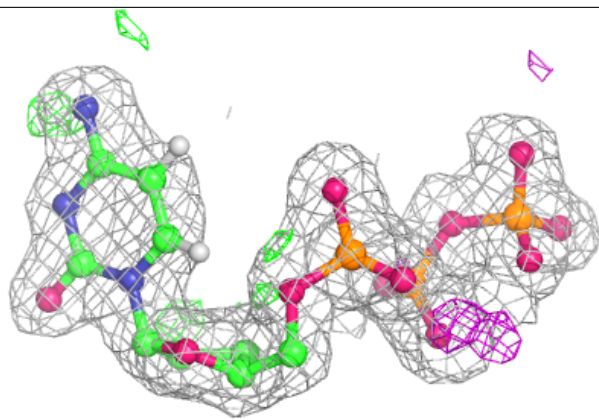
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	D	1	5/5	0.99	0.09	26,28,33,40	0
5	MN	D	2	1/1	1.00	0.09	14,14,14,14	0

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.

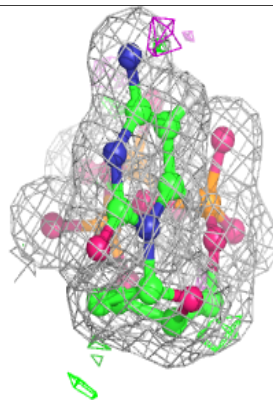
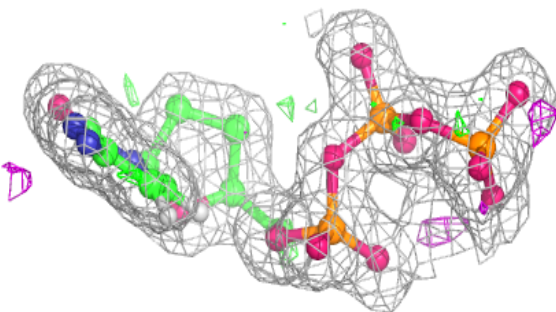
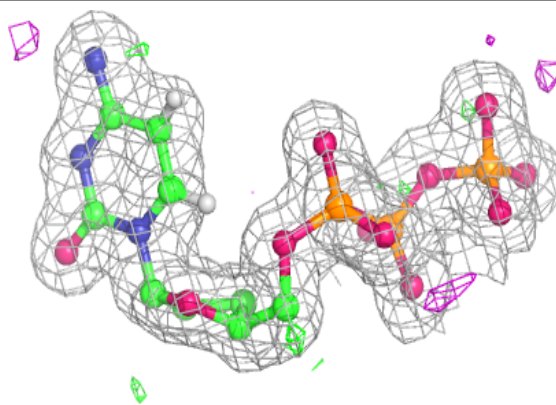


**Electron density around DCT A 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around DCT D 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.