



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:41 PM GMT

PDB ID : 3PV8
Title : Crystal Structure of Bacillus DNA Polymerase I Large Fragment Bound to
DNA and ddTTP-dA in Closed Conformation
Authors : Wang, W.; Beese, L.S.
Deposited on : 2010-12-06
Resolution : 1.52 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

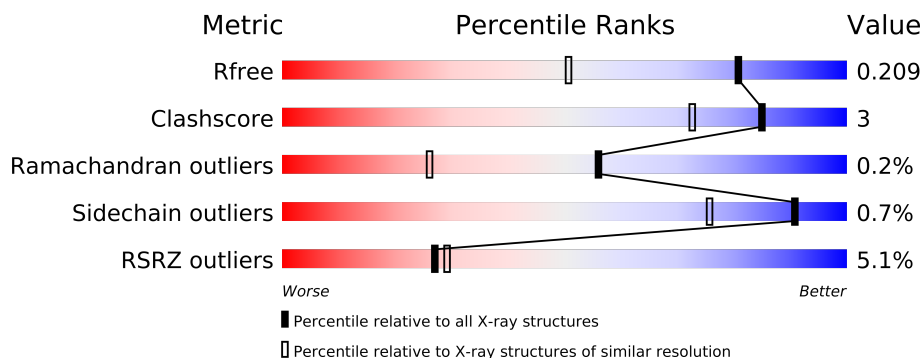
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.52 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}	66092	1879 (1.54-1.50)
Clashscore	79885	2184 (1.54-1.50)
Ramachandran outliers	78287	2123 (1.54-1.50)
Sidechain outliers	78261	2121 (1.54-1.50)
RSRZ outliers	66119	1880 (1.54-1.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	592	
1	D	592	
2	B	9	
2	E	9	
3	C	13	
3	F	13	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22076 atoms, of which 9986 are hydrogens and 0 are deuterium.

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	3	0
			9387	2962	4728	809	871	17			
1	D	579	Total	C	H	N	O	S	0	11	0
			9447	2980	4760	812	878	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*(2DT))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	9	Total	C	H	N	O	P	0	0	0
			277	86	102	28	53	8			
2	E	9	Total	C	H	N	O	P	0	0	0
			277	86	102	28	53	8			

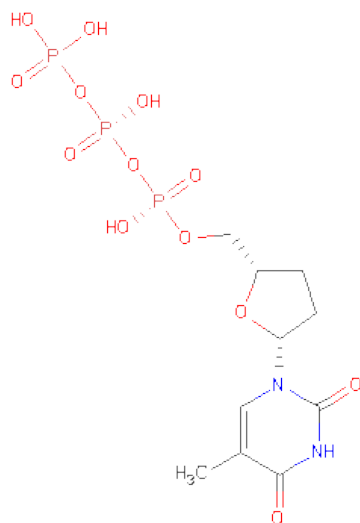
- Molecule 3 is a DNA chain called DNA (5'-D(*C*AP*TP*AP*AP*GP*AP*GP*TP*CP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	12	Total	C	H	N	O	P	0	0	0
			384	119	135	52	67	11			
3	F	12	Total	C	H	N	O	P	0	0	0
			384	119	135	52	67	11			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 40	C 10	H 12	N 2	O 13	P 3	0	0
5	D	1	Total 40	C 10	H 12	N 2	O 13	P 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	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.

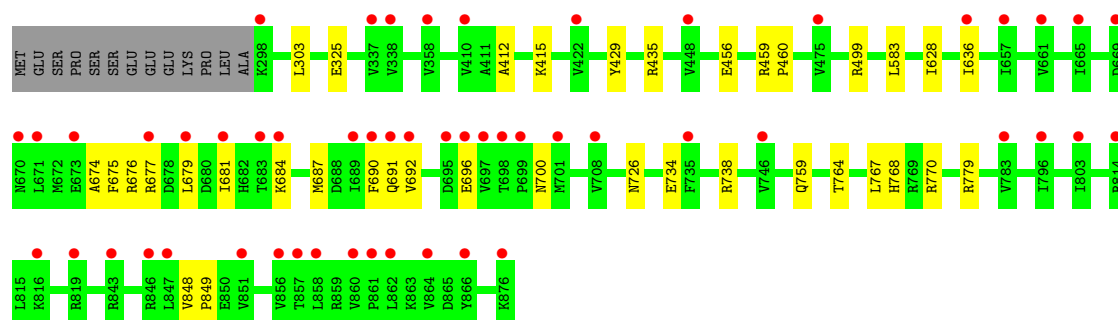
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	635	Total	O	0	0
			635	635		
7	D	913	Total	O	0	0
			913	913		
7	B	48	Total	O	0	0
			48	48		
7	C	85	Total	O	0	0
			85	85		
7	E	50	Total	O	0	0
			50	50		
7	F	92	Total	O	0	0
			92	92		

3 Residue-property plots

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

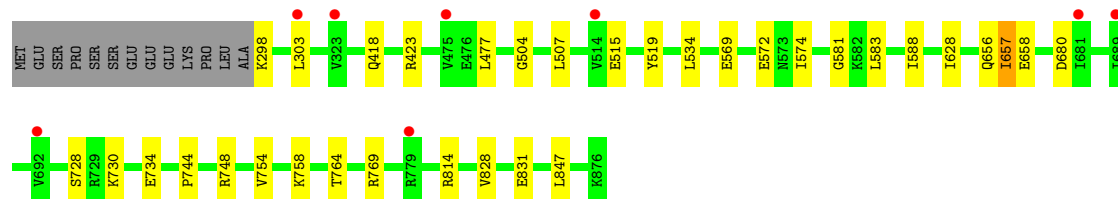
- Molecule 1: DNA polymerase I

Chain A: 



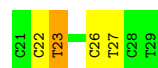
- Molecule 1: DNA polymerase I

Chain D: 



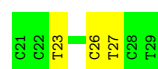
- Molecule 2: DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(2DT))-3')

Chain B: 



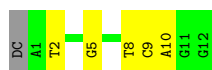
- Molecule 2: DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(2DT))-3')

Chain E: 



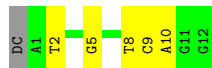
- Molecule 3: DNA (5'-D(*C*AP*TP*AP*AP*GP*AP*GP*TP*CP*AP*GP*G)-3')

Chain C: 



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

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.89Å 109.30Å 150.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.42 – 1.52 88.42 – 1.52	Depositor EDS
% Data completeness (in resolution range)	93.9 (88.42-1.52) 93.9 (88.42-1.52)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 1.52Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.185 , 0.211 0.184 , 0.209	Depositor DCC
R_{free} test set	10328 reflections (4.64%)	DCC
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 40.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 222669 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22076	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2DT, MG, D3T, 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	0.37	0/4755	0.52	0/6427
1	D	0.48	0/4815	0.61	0/6507
2	B	0.93	0/173	1.71	4/264 (1.5%)
2	E	1.08	0/173	1.79	6/264 (2.3%)
3	C	0.96	0/281	1.64	5/433 (1.2%)
3	F	0.97	0/281	1.56	6/433 (1.4%)
All	All	0.50	0/10478	0.75	21/14328 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	23	DT	O4'-C1'-N1	-9.41	101.42	108.00
2	E	26	DC	O4'-C1'-N1	9.12	114.39	108.00
3	C	8	DT	O4'-C1'-N1	-7.79	102.55	108.00
3	C	2	DT	O4'-C1'-N1	7.75	113.42	108.00
2	E	23	DT	O4'-C1'-N1	-7.44	102.79	108.00
3	F	8	DT	O4'-C1'-N1	-6.89	103.17	108.00
3	F	2	DT	O4'-C1'-N1	6.60	112.62	108.00
2	E	26	DC	O4'-C4'-C3'	6.30	109.78	106.00
2	E	27	DT	O5'-P-OP2	-6.28	100.05	105.70
2	E	27	DT	C4'-C3'-C2'	-6.18	97.54	103.10
3	C	2	DT	C1'-O4'-C4'	-5.56	104.54	110.10
3	C	5	DG	C8-N9-C4	-5.49	104.20	106.40
3	F	5	DG	O4'-C4'-C3'	-5.48	102.31	104.50
2	B	26	DC	O4'-C1'-N1	5.42	111.80	108.00
2	B	26	DC	O4'-C4'-C3'	5.39	109.23	106.00
3	F	2	DT	C1'-O4'-C4'	-5.34	104.76	110.10
3	F	2	DT	O4'-C1'-C2'	-5.24	101.71	105.90
2	B	27	DT	C4'-C3'-C2'	-5.24	98.39	103.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	DG	O4'-C4'-C3'	-5.15	102.44	104.50
3	F	2	DT	C6-C5-C7	-5.11	119.84	122.90
2	E	27	DT	OP1-P-OP2	5.08	127.22	119.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4659	4728	0	28	0
1	D	4687	4760	0	25	0
2	B	175	102	2	1	0
2	E	175	102	2	0	0
3	C	249	135	1	1	0
3	F	249	135	1	1	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	28	12	1	0	0
5	D	28	12	1	0	0
6	A	5	0	0	0	0
6	D	10	0	0	0	0
7	A	635	0	0	7	3
7	B	48	0	0	0	0
7	C	85	0	0	0	0
7	D	913	0	0	12	4
7	E	50	0	0	1	0
7	F	92	0	0	0	0
All	All	12090	9986	8	56	5

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (56) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:572:GLU:HG3	7:D:1786:HOH:O	1.86	0.74
1:A:690:PHE:O	1:A:691:GLN:HB3	1.87	0.72
1:A:734:GLU:HG2	7:A:1648:HOH:O	1.90	0.71
1:A:499:ARG:NE	7:A:971:HOH:O	2.26	0.69
1:A:779:ARG:NH2	7:A:1609:HOH:O	2.26	0.68
1:A:325:GLU:OE2	1:A:435:ARG:NH1	2.24	0.66
1:D:583:LEU:HG	7:E:1397:HOH:O	1.96	0.66
1:A:848:VAL:HB	1:A:849:PRO:HD3	1.79	0.64
1:A:692:VAL:HB	1:A:696:GLU:HB3	1.82	0.61
1:A:499:ARG:CZ	7:A:971:HOH:O	2.47	0.61
1:A:738:ARG:HD3	7:A:1392:HOH:O	2.01	0.60
3:F:9:DC:H2"	3:F:10:DA:C8	2.37	0.60
1:D:504:GLY:HA2	1:D:588[B]:ILE:HD13	1.83	0.59
3:C:9:DC:H2"	3:C:10:DA:C8	2.40	0.57
1:D:828:VAL:HB	1:D:831[B]:GLU:CG	2.34	0.57
1:A:691:GLN:O	1:A:691:GLN:HG2	2.06	0.56
1:A:675:PHE:CE2	1:A:681:ILE:HD13	2.41	0.56
1:D:569:GLU:CD	7:D:1752:HOH:O	2.45	0.55
1:D:504:GLY:CA	1:D:588[B]:ILE:HD13	2.37	0.55
1:D:748:ARG:HD3	7:D:1288:HOH:O	2.07	0.54
1:D:507:LEU:HD23	1:D:588[B]:ILE:HD12	1.89	0.54
1:A:459:ARG:HB3	1:A:460:PRO:HD3	1.90	0.53
1:A:759:GLN:HG2	7:D:1616:HOH:O	2.09	0.53
1:A:764:THR:HG22	1:A:770:ARG:HG2	1.91	0.52
1:D:423:ARG:NH1	7:D:1766:HOH:O	2.43	0.51
1:D:734:GLU:HG3	7:D:889:HOH:O	2.10	0.51
1:D:814:ARG:NH1	7:D:1357:HOH:O	2.44	0.50
1:A:412:ALA:O	1:A:415:LYS:HG2	2.10	0.50
1:D:657:ILE:HG23	1:D:658:GLU:N	2.26	0.49
1:D:754:VAL:HG12	1:D:758:LYS:HE2	1.94	0.49
1:D:754:VAL:CG1	1:D:758:LYS:HE2	2.43	0.49
1:D:418:GLN:HA	7:D:1018:HOH:O	2.13	0.49
1:D:581:GLY:HA3	7:D:1196:HOH:O	2.13	0.48
1:A:303:LEU:HD23	7:A:1416:HOH:O	2.12	0.48
1:D:534:LEU:HD11	1:D:574:ILE:HD13	1.95	0.48
1:A:325:GLU:CD	1:A:325:GLU:H	2.17	0.47
1:A:674:ALA:HA	1:A:679:LEU:HD12	1.96	0.47
1:A:412:ALA:O	1:A:415:LYS:HE2	2.14	0.47
1:A:681:ILE:N	1:A:681:ILE:HD12	2.30	0.47
1:D:744:PRO:O	1:D:748:ARG:HG3	2.15	0.46
1:D:831[B]:GLU:CD	7:D:1822:HOH:O	2.54	0.45
1:A:684:LYS:HA	1:A:687:MET:HE3	1.97	0.45
1:D:847:LEU:HD23	1:D:847:LEU:C	2.37	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:298:LYS:N	7:D:1389:HOH:O	2.50	0.44
1:D:572:GLU:CD	7:D:1787:HOH:O	2.55	0.44
1:A:677:ARG:HD2	1:A:679:LEU:HD11	1.98	0.44
1:A:429:TYR:O	1:A:435:ARG:HA	2.18	0.44
1:A:687:MET:HB3	1:A:692:VAL:O	2.18	0.44
1:A:456:GLU:OE2	1:A:456:GLU:HA	2.18	0.43
1:D:515:GLU:HG2	1:D:519:TYR:CE2	2.54	0.43
1:D:764:THR:HA	1:D:769:ARG:O	2.19	0.43
1:D:656[A]:GLN:NE2	1:D:680:ASP:HA	2.34	0.42
1:A:767:LEU:O	1:A:768:HIS:HB2	2.19	0.42
2:B:22:DC:H2'	2:B:23:DT:H73	2.02	0.41
1:A:583:LEU:HD11	1:A:636:ILE:CG1	2.51	0.40
1:A:676:ARG:HD3	7:A:1746:HOH:O	2.21	0.40

All (5) 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	Distance(Å)	Clash(Å)
7:A:1802:HOH:O	7:D:1799:HOH:O[2_755]	2.03	0.17
7:D:1388:HOH:O	7:D:1419:HOH:O[4_545]	2.05	0.15
7:A:1795:HOH:O	7:A:1798:HOH:O[3_755]	2.11	0.09
7:A:1747:HOH:O	7:D:1762:HOH:O[2_745]	2.15	0.05
7:D:1120:HOH:O	7:D:1183:HOH:O[4_445]	2.18	0.02

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	
1	A	580/592 (98%)	564 (97%)	15 (3%)	1 (0%)	56	26
1	D	588/592 (99%)	575 (98%)	12 (2%)	1 (0%)	56	26
All	All	1168/1184 (99%)	1139 (98%)	27 (2%)	2 (0%)	56	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	628	ILE
1	D	628	ILE

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	
1	A	498/507 (98%)	496 (100%)	2 (0%)	95	85
1	D	505/507 (100%)	500 (99%)	5 (1%)	85	64
All	All	1003/1014 (99%)	996 (99%)	7 (1%)	91	76

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	700	ASN
1	A	726	ASN
1	D	303	LEU
1	D	477	LEU
1	D	657	ILE
1	D	728	SER
1	D	730	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	704	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	2DT	B	29	3,2	18,20,21	0.95	2 (11%)	20,28,31	1.44	4 (20%)
2	2DT	E	29	3,2	18,20,21	0.86	2 (11%)	20,28,31	1.34	2 (10%)

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	2DT	B	29	3,2	-	0/5/18/19	0/2/2/2
2	2DT	E	29	3,2	-	0/5/18/19	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	29	2DT	C6-C5	-2.44	1.33	1.40
2	E	29	2DT	C6-C5	-2.23	1.34	1.40
2	E	29	2DT	C6-N1	2.03	1.39	1.34
2	B	29	2DT	C6-N1	2.00	1.39	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	29	2DT	N3-C2-N1	-3.20	113.30	115.97
2	E	29	2DT	C4'-O4'-C1'	-3.12	108.75	110.05
2	E	29	2DT	C6-N1-C2	-2.81	121.61	122.41
2	B	29	2DT	C5-C6-N1	2.64	124.15	121.59
2	B	29	2DT	C6-N1-C2	-2.36	121.74	122.41
2	B	29	2DT	C5M-C5-C6	2.22	123.32	118.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 2 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	2	-	4,4,4	0.13	0	6,6,6	0.07	0
5	D3T	A	201	4	29,29,29	1.79	4 (13%)	40,45,45	2.66	8 (20%)
6	SO4	D	1	-	4,4,4	0.23	0	6,6,6	0.31	0
5	D3T	D	202	4	29,29,29	1.84	3 (10%)	40,45,45	1.62	6 (15%)
6	SO4	D	3	-	4,4,4	0.06	0	6,6,6	0.14	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
6	SO4	A	2	-	-	0/0/0/0	0/0/0/0
5	D3T	A	201	4	-	0/19/31/31	0/2/2/2
6	SO4	D	1	-	-	0/0/0/0	0/0/0/0
5	D3T	D	202	4	-	0/19/31/31	0/2/2/2
6	SO4	D	3	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	201	D3T	O4-C4	7.08	1.38	1.24
5	D	202	D3T	PB-O3B	-6.07	1.48	1.59
5	D	202	D3T	O4-C4	5.58	1.35	1.24
5	A	201	D3T	PB-O3B	-2.79	1.54	1.59
5	D	202	D3T	C3'-C2'	-2.78	1.45	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	201	D3T	C3'-C2'	-2.56	1.46	1.54
5	A	201	D3T	C2-N1	-2.53	1.35	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	201	D3T	C6-N1-C2	-12.60	118.83	122.41
5	A	201	D3T	N3-C2-N1	7.08	121.89	115.97
5	D	202	D3T	N3-C2-N1	4.69	119.89	115.97
5	A	201	D3T	O4'-C1'-N1	3.87	114.96	107.68
5	D	202	D3T	C2'-C1'-N1	-3.33	106.00	112.66
5	D	202	D3T	C6-N1-C2	-3.19	121.50	122.41
5	A	201	D3T	C2'-C1'-N1	-2.87	106.92	112.66
5	D	202	D3T	O4'-C1'-N1	2.84	113.02	107.68
5	A	201	D3T	PB-O3A-PA	-2.42	124.59	131.68
5	A	201	D3T	O2B-PB-O3B	2.29	116.02	105.14
5	D	202	D3T	C4-N3-C2	-2.25	120.78	125.39
5	A	201	D3T	C3'-C2'-C1'	2.18	105.21	102.80
5	A	201	D3T	O2B-PB-O3A	2.16	115.37	105.14
5	D	202	D3T	O2B-PB-O3B	2.08	115.01	105.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	579/592 (97%)	0.50	53 (9%) 9 9	13, 25, 44, 64	0
1	D	579/592 (97%)	0.06	8 (1%) 72 79	6, 16, 31, 43	0
2	B	9/9 (100%)	-0.49	0 100 100	14, 16, 27, 31	0
2	E	9/9 (100%)	-0.42	0 100 100	9, 14, 25, 32	0
3	C	12/13 (92%)	-0.27	0 100 100	13, 18, 39, 52	0
3	F	12/13 (92%)	-0.09	0 100 100	8, 13, 38, 52	0
All	All	1200/1228 (97%)	0.26	61 (5%) 27 29	6, 20, 39, 64	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	692	VAL	8.9
1	A	697	VAL	6.6
1	A	681	ILE	6.1
1	A	690	PHE	4.8
1	A	689	ILE	4.7
1	A	856	VAL	4.7
1	A	673	GLU	4.2
1	A	691	GLN	4.2
1	A	698	THR	4.0
1	A	862	LEU	3.8
1	A	866	TYR	3.6
1	A	783	VAL	3.5
1	A	819	ARG	3.5
1	A	298	LYS	3.5
1	A	448	VAL	3.5
1	A	699	PRO	3.3
1	A	857	THR	3.2
1	A	695	ASP	3.2
1	A	735	PHE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	851	VAL	3.1
1	A	677	ARG	3.0
1	A	661	VAL	2.9
1	A	864	VAL	2.9
1	A	796	ILE	2.9
1	D	689	ILE	2.9
1	A	816	LYS	2.8
1	A	858	LEU	2.8
1	A	847	LEU	2.8
1	A	422	VAL	2.7
1	D	323[A]	VAL	2.7
1	A	669	ASP	2.7
1	D	475	VAL	2.7
1	A	701	MET	2.6
1	A	670	ASN	2.5
1	A	684	LYS	2.5
1	A	475	VAL	2.5
1	A	679	LEU	2.5
1	D	303	LEU	2.5
1	A	846	ARG	2.5
1	A	683	THR	2.4
1	A	696	GLU	2.4
1	A	814	ARG	2.4
1	A	410	VAL	2.3
1	A	861	PRO	2.3
1	A	876	LYS	2.3
1	A	657	ILE	2.2
1	A	843	ARG	2.2
1	A	746	VAL	2.2
1	D	681	ILE	2.2
1	D	692	VAL	2.2
1	D	779	ARG	2.2
1	A	671	LEU	2.1
1	A	358	VAL	2.1
1	A	860	VAL	2.1
1	A	636	ILE	2.1
1	A	338	VAL	2.1
1	A	708	VAL	2.0
1	A	665	ILE	2.0
1	A	337	VAL	2.0
1	D	514	VAL	2.0
1	A	803	ILE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	2DT	E	29	19/20	0.09	-0.05	7,9,13,14	0
2	2DT	B	29	19/20	0.07	-0.60	12,15,19,22	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	SO4	D	3	5/5	0.16	1.86	34,42,47,47	0
5	D3T	D	202	28/28	0.08	-0.09	8,11,16,22	0
5	D3T	A	201	28/28	0.09	-0.33	15,19,27,27	0
6	SO4	D	1	5/5	0.08	-0.64	26,29,37,38	0
6	SO4	A	2	5/5	0.07	-0.78	29,42,50,53	0
4	MG	A	1	1/1	0.05	-2.10	23,23,23,23	0
4	MG	D	2	1/1	0.05	-2.34	14,14,14,14	0

6.5 Other polymers ⓘ

There are no such residues in this entry.