



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:08 am BST

PDB ID : 4B9T  
Title : Structure of the high fidelity DNA polymerase I with an oxidative formamido pyrimidine-dG DNA lesion -dC basepair in the post-insertion site.  
Authors : Gehrke, T.H.; Lischke, U.; Arnold, S.; Schneider, S.; Carell, T.  
Deposited on : 2012-09-06  
Resolution : 2.65 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  
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

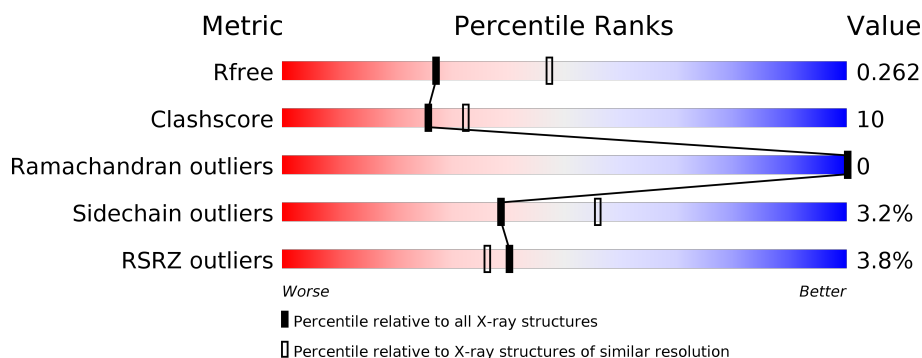
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	619	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>• 6%</div> </div> </div>
2	B	11	<div> <div>18%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
3	C	15	<div> <div>27%</div> <div> <div></div> <div>80%</div> <div>20%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5201 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 protein called DNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	580	Total	C	N	O	S	0	1	0
			4658	2959	810	872	17			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	MET	-	expression tag	UNP E1C9K5
A	259	ALA	-	expression tag	UNP E1C9K5
A	260	SER	-	expression tag	UNP E1C9K5
A	261	TRP	-	expression tag	UNP E1C9K5
A	262	SER	-	expression tag	UNP E1C9K5
A	263	HIS	-	expression tag	UNP E1C9K5
A	264	PRO	-	expression tag	UNP E1C9K5
A	265	GLN	-	expression tag	UNP E1C9K5
A	266	PHE	-	expression tag	UNP E1C9K5
A	267	GLU	-	expression tag	UNP E1C9K5
A	268	LYS	-	expression tag	UNP E1C9K5
A	269	GLY	-	expression tag	UNP E1C9K5
A	270	ALA	-	expression tag	UNP E1C9K5
A	271	SER	-	expression tag	UNP E1C9K5
A	272	THR	-	expression tag	UNP E1C9K5
A	273	SER	-	expression tag	UNP E1C9K5
A	274	LEU	-	expression tag	UNP E1C9K5
A	275	TYR	-	expression tag	UNP E1C9K5
A	276	LYS	-	expression tag	UNP E1C9K5
A	277	LYS	-	expression tag	UNP E1C9K5
A	278	ALA	-	expression tag	UNP E1C9K5
A	279	GLY	-	expression tag	UNP E1C9K5
A	280	SER	-	expression tag	UNP E1C9K5
A	281	ALA	-	expression tag	UNP E1C9K5
A	282	ALA	-	expression tag	UNP E1C9K5
A	283	ALA	-	expression tag	UNP E1C9K5
A	284	VAL	-	expression tag	UNP E1C9K5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	285	LEU	-	expression tag	UNP E1C9K5
A	286	GLU	-	expression tag	UNP E1C9K5
A	287	GLU	-	expression tag	UNP E1C9K5
A	288	ASN	-	expression tag	UNP E1C9K5
A	289	LEU	-	expression tag	UNP E1C9K5
A	290	TYR	-	expression tag	UNP E1C9K5
A	291	PHE	-	expression tag	UNP E1C9K5
A	292	GLN	-	expression tag	UNP E1C9K5
A	293	GLY	-	expression tag	UNP E1C9K5
A	294	SER	-	expression tag	UNP E1C9K5
A	295	PHE	-	expression tag	UNP E1C9K5
A	296	THR	-	expression tag	UNP E1C9K5

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	P	0	0	0
			222	105	39	67	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			251	118	51	70	12			

- 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		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

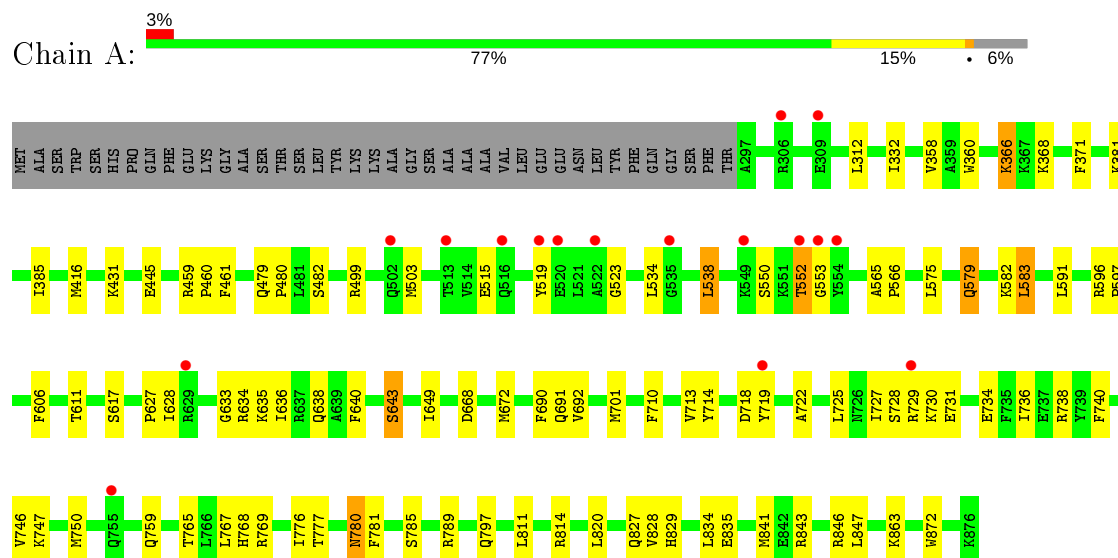
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	59	Total	O	0	0
			59	59		

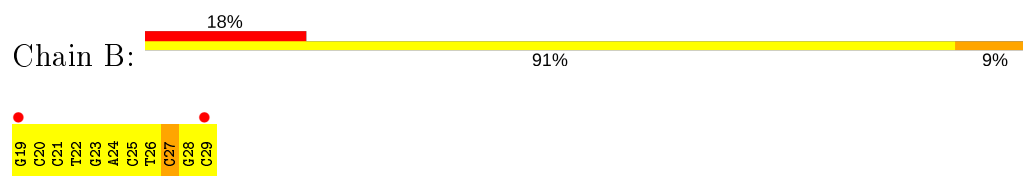
### 3 Residue-property plots [i](#)

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.

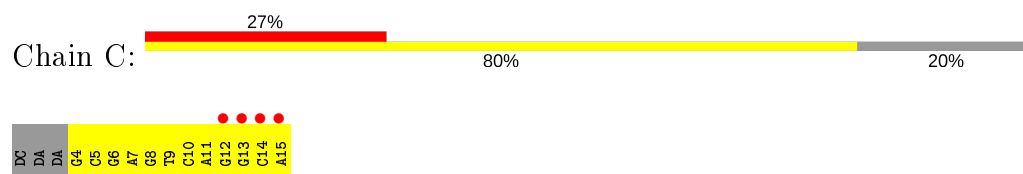
#### • Molecule 1: DNA POLYMERASE



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.38Å 93.78Å 105.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 2.65 45.33 – 2.65	Depositor EDS
% Data completeness (in resolution range)	94.4 (45.00-2.65) 94.4 (45.33-2.65)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.87 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.221 , 0.273 0.220 , 0.262	Depositor DCC
$R_{free}$ test set	1242 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.7	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5201	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FOX, 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	0.51	0/4744	0.60	0/6411
2	B	0.74	0/247	1.14	1/378 (0.3%)
3	C	0.72	0/256	1.06	0/393
All	All	0.54	0/5247	0.67	1/7182 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	27	DC	O4'-C4'-C3'	-5.09	102.47	104.50

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	4658	0	4708	72	0
2	B	222	0	124	14	0
3	C	251	0	138	22	0
4	A	1	0	0	0	0
5	A	10	0	0	0	0
6	A	59	0	0	1	1
All	All	5201	0	4970	103	1



The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (103) 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:552:THR:OG1	2:B:24:DA:OP1	1.59	1.15
3:C:13:DG:H2''	3:C:14:DC:O5'	1.42	1.09
3:C:10:DC:H2''	3:C:11:DA:H5'	1.34	1.07
3:C:10:DC:H2''	3:C:11:DA:C5'	1.89	1.01
3:C:4:FOX:H2'1	3:C:5:DC:H5'	1.52	0.92
1:A:583:LEU:HD11	1:A:636:ILE:HD11	1.52	0.92
3:C:15:DA:H8	3:C:15:DA:OP2	1.56	0.87
3:C:15:DA:C8	3:C:15:DA:OP2	2.30	0.84
1:A:780:ASN:HD22	1:A:781:PHE:N	1.76	0.83
3:C:14:DC:C2'	3:C:15:DA:O5'	2.30	0.80
3:C:13:DG:C2'	3:C:14:DC:O5'	2.30	0.77
2:B:27:DC:H2'	2:B:28:DG:C8	2.19	0.77
1:A:728:SER:OG	1:A:731:GLU:HG3	1.83	0.77
1:A:691:GLN:OE1	1:A:738:ARG:NH2	2.23	0.72
1:A:575:LEU:O	1:A:579:GLN:HG2	1.93	0.68
1:A:611:THR:HG22	3:C:6:DG:H5''	1.74	0.68
1:A:729:ARG:HH12	1:A:730:LYS:HG2	1.57	0.68
3:C:14:DC:H2''	3:C:15:DA:O5'	1.93	0.68
1:A:366:LYS:O	1:A:368:LYS:NZ	2.27	0.68
3:C:10:DC:H2''	3:C:11:DA:H5''	1.74	0.67
3:C:8:DG:H2''	3:C:9:DT:O5'	1.95	0.67
3:C:12:DG:H2''	3:C:13:DG:OP2	1.96	0.66
1:A:827:GLN:HE22	1:A:829:HIS:N	1.94	0.66
1:A:729:ARG:NH1	1:A:730:LYS:HG2	2.11	0.65
1:A:360:TRP:CD1	1:A:366:LYS:HG2	2.32	0.64
3:C:13:DG:H2''	3:C:14:DC:C5'	2.27	0.64
1:A:552:THR:OG1	2:B:24:DA:P	2.55	0.62
1:A:550:SER:HB2	1:A:553:GLY:O	1.99	0.62
1:A:690:PHE:O	1:A:692:VAL:HG13	2.00	0.62
1:A:371:PHE:O	6:A:2012:HOH:O	2.16	0.59
1:A:714:TYR:OH	2:B:29:DC:H2'	2.02	0.59
1:A:780:ASN:HD22	1:A:780:ASN:C	2.02	0.59
1:A:583:LEU:CD1	1:A:636:ILE:HD11	2.30	0.59
1:A:731:GLU:O	1:A:734:GLU:HB2	2.02	0.59
2:B:19:DG:H2''	2:B:20:DC:H5'	1.85	0.58
1:A:785:SER:O	1:A:789:ARG:HG3	2.04	0.57
1:A:827:GLN:NE2	1:A:829:HIS:N	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:LEU:HD21	1:A:843:ARG:NH2	2.21	0.56
1:A:643:SER:HB3	1:A:835:GLU:OE2	2.05	0.56
1:A:591:LEU:HD21	1:A:640:PHE:CZ	2.41	0.56
2:B:20:DC:H2''	2:B:21:DC:O5'	2.05	0.55
1:A:565:ALA:HB3	1:A:566:PRO:HD3	1.88	0.55
1:A:718:ASP:OD1	1:A:719:TYR:N	2.39	0.55
1:A:780:ASN:ND2	1:A:780:ASN:C	2.58	0.55
3:C:15:DA:H8	3:C:15:DA:P	2.30	0.54
1:A:416:MET:HE3	1:A:461:PHE:CZ	2.43	0.53
1:A:746:VAL:O	1:A:750:MET:HG2	2.09	0.52
1:A:780:ASN:ND2	1:A:781:PHE:N	2.53	0.52
2:B:21:DC:H2''	2:B:22:DT:O5'	2.10	0.52
3:C:7:DA:H2''	3:C:8:DG:O5'	2.10	0.52
1:A:713:VAL:O	1:A:797:GLN:NE2	2.44	0.51
3:C:8:DG:C8	3:C:9:DT:H72	2.46	0.51
1:A:740:PHE:CD1	1:A:747:LYS:HB2	2.46	0.50
1:A:827:GLN:NE2	1:A:829:HIS:H	2.10	0.49
3:C:12:DG:C2'	3:C:13:DG:OP2	2.59	0.49
1:A:503:MET:HE1	1:A:635:LYS:O	2.12	0.49
1:A:668:ASP:O	1:A:672:MET:HG3	2.12	0.48
2:B:22:DT:H2'	2:B:23:DG:C8	2.48	0.48
2:B:28:DG:H2'	2:B:29:DC:C6	2.47	0.48
1:A:358:VAL:HG13	1:A:385:ILE:HG23	1.93	0.48
3:C:14:DC:H2'	3:C:15:DA:O5'	2.09	0.48
1:A:841:MET:HE2	1:A:841:MET:HA	1.95	0.48
1:A:828:VAL:HG12	1:A:828:VAL:O	2.14	0.48
1:A:627:PRO:HB2	1:A:633:GLY:O	2.14	0.47
1:A:722:ALA:HB1	1:A:727:ILE:O	2.15	0.47
2:B:22:DT:C2'	2:B:23:DG:C8	2.98	0.47
1:A:479:GLN:HB2	1:A:480:PRO:HD3	1.95	0.47
1:A:767:LEU:O	1:A:768:HIS:HB2	2.14	0.47
3:C:8:DG:H2'	3:C:9:DT:H72	1.96	0.47
1:A:710:PHE:CE2	1:A:714:TYR:CE2	3.03	0.47
2:B:19:DG:C2'	2:B:20:DC:H5'	2.45	0.46
1:A:416:MET:HE1	1:A:461:PHE:HE2	1.80	0.46
1:A:416:MET:CE	1:A:461:PHE:CE2	2.98	0.46
1:A:591:LEU:HD21	1:A:640:PHE:HZ	1.79	0.46
1:A:582:LYS:NZ	2:B:26:DT:O2	2.32	0.46
1:A:728:SER:HG	1:A:731:GLU:HG3	1.80	0.46
1:A:606:PHE:HA	1:A:617:SER:O	2.16	0.46
1:A:827:GLN:HE22	1:A:829:HIS:CA	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:ILE:HD12	1:A:634:ARG:HG3	1.98	0.45
1:A:519:TYR:O	1:A:523:GLY:N	2.50	0.45
1:A:725:LEU:O	1:A:727:ILE:HG23	2.17	0.45
1:A:780:ASN:HD22	1:A:781:PHE:H	1.60	0.45
1:A:814:ARG:NH2	1:A:847:LEU:CD1	2.80	0.44
3:C:8:DG:H2'	3:C:9:DT:C7	2.47	0.44
1:A:416:MET:CE	1:A:461:PHE:HE2	2.31	0.43
1:A:459:ARG:HB3	1:A:460:PRO:HD3	1.98	0.43
1:A:738:ARG:HD2	1:A:738:ARG:HA	1.75	0.43
1:A:765:THR:OG1	1:A:769:ARG:HB3	2.18	0.43
1:A:534:LEU:HG	1:A:538:LEU:HD22	1.99	0.43
1:A:692:VAL:HG21	1:A:701:MET:CE	2.49	0.43
1:A:312:LEU:HD22	1:A:360:TRP:CB	2.49	0.43
1:A:515:GLU:HG2	1:A:519:TYR:CE2	2.54	0.43
3:C:6:DG:H2''	3:C:7:DA:O5'	2.19	0.42
1:A:499:ARG:NH2	1:A:638:GLN:OE1	2.53	0.42
1:A:736:ILE:HG22	1:A:740:PHE:CE2	2.54	0.42
2:B:25:DC:C5	2:B:26:DT:H73	2.54	0.42
1:A:811:LEU:HD21	1:A:834:LEU:HD21	2.02	0.41
2:B:25:DC:H2''	2:B:26:DT:O5'	2.19	0.41
1:A:776:ILE:HA	1:A:776:ILE:HD12	1.75	0.41
1:A:649:ILE:HG21	1:A:872:TRP:HA	2.03	0.41
1:A:579:GLN:H	1:A:579:GLN:HG2	1.64	0.40
1:A:596:ARG:HA	1:A:597:PRO:HD3	1.98	0.40
1:A:827:GLN:HE22	1:A:829:HIS:H	1.63	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2056:HOH:O	6:A:2058:HOH:O[3_554]	2.01	0.19

## 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	579/619 (94%)	563 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	496/526 (94%)	480 (97%)	16 (3%)	39	56

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	ILE
1	A	366	LYS
1	A	381	LYS
1	A	431	LYS
1	A	445	GLU
1	A	482	SER
1	A	538	LEU
1	A	552	THR
1	A	579	GLN
1	A	583	LEU
1	A	643	SER
1	A	759	GLN
1	A	777	THR
1	A	780	ASN
1	A	846	ARG
1	A	863	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	780	ASN
1	A	827	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
3	FOX	C	4	3,2	20,24,25	1.62	2 (10%)	23,33,36	2.64	10 (43%)

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
3	FOX	C	4	3,2	-	5/10/24/25	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	FOX	C6'-C1'	-5.25	1.43	1.53
3	C	4	FOX	C6'-C4'	-3.86	1.43	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	FOX	O8-C8-N7	-8.01	115.58	125.80
3	C	4	FOX	C4'-C6'-C1'	4.63	111.39	103.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	FOX	N1-C2-N3	-3.58	119.81	125.42
3	C	4	FOX	C2-N3-C4	3.12	121.53	114.54
3	C	4	FOX	C6-N1-C2	3.08	120.83	115.93
3	C	4	FOX	C6-C5-N7	3.01	123.54	117.67
3	C	4	FOX	C6-C5-C4	2.76	117.02	114.57
3	C	4	FOX	C2'-C1'-N9	-2.31	106.51	112.44
3	C	4	FOX	C5-N7-C8	2.08	126.78	123.68
3	C	4	FOX	N2-C2-N3	2.04	120.43	117.25

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	4	FOX	C6'-C4'-C5'-O5'
3	C	4	FOX	C4-C5-N7-C8
3	C	4	FOX	C6-C5-N7-C8
3	C	4	FOX	O8-C8-N7-C5
3	C	4	FOX	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4	FOX	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	A	1878	-	4,4,4	0.16	0	6,6,6	0.32	0
5	SO4	A	1879	-	4,4,4	0.52	0	6,6,6	1.00	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	A	1879	SO4	O4-S-O3	2.25	118.68	109.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	580/619 (93%)	0.15	17 (2%) 51 48	44, 57, 88, 104	0
2	B	11/11 (100%)	1.36	2 (18%) 1 1	83, 108, 122, 130	0
3	C	11/15 (73%)	1.58	4 (36%) 0 0	94, 100, 197, 225	0
All	All	602/645 (93%)	0.20	23 (3%) 40 36	44, 58, 94, 225	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	552	THR	5.3
3	C	15	DA	4.3
2	B	19	DG	4.0
3	C	13	DG	3.8
1	A	519	TYR	3.0
1	A	554	TYR	2.9
2	B	29	DC	2.8
1	A	535	GLY	2.6
1	A	516	GLN	2.6
1	A	522	ALA	2.5
1	A	719	TYR	2.5
1	A	520	GLU	2.5
1	A	502	GLN	2.5
1	A	755	GLN	2.4
1	A	629	ARG	2.3
1	A	513	THR	2.3
3	C	14	DC	2.3
1	A	306	ARG	2.2
3	C	12	DG	2.2
1	A	553	GLY	2.2
1	A	549	LYS	2.1
1	A	729	ARG	2.1
1	A	309	GLU	2.1



## 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
3	FOX	C	4	23/24	0.75	0.31	138,144,166,173	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
5	SO4	A	1879	5/5	0.89	0.31	124,124,124,124	0
4	MG	A	1877	1/1	0.91	0.17	48,48,48,48	0
5	SO4	A	1878	5/5	0.93	0.43	133,134,135,136	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.