



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:21 pm BST

PDB ID : 3MR5  
Title : Human DNA polymerase eta - DNA ternary complex with a CPD 1bp upstream of the active site (TT3)  
Authors : Biertumpfel, C.; Zhao, Y.; Ramon-Maiques, S.; Gregory, M.T.; Lee, J.Y.; Yang, W.  
Deposited on : 2010-04-28  
Resolution : 1.80 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

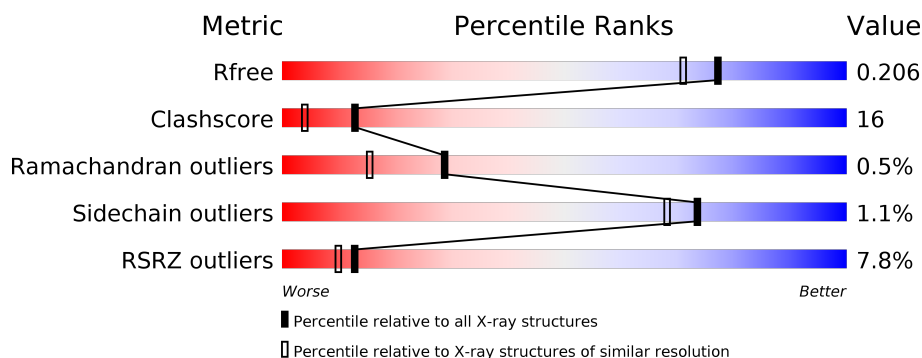
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	435	<div> <div>8%</div> <div>76%</div> <div>22%</div> <div>..</div> </div>
2	T	12	<div> <div>17%</div> <div>58%</div> <div>42%</div> </div>
3	P	9	<div> <div>100%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	440	-	-	X	-
6	GOL	A	442	-	-	X	-
6	GOL	A	443	-	-	X	-
6	GOL	T	15	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4347 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 eta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	20	0
			3474	2176	626	646	26			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q9Y253
A	-1	PRO	-	EXPRESSION TAG	UNP Q9Y253
A	0	HIS	-	EXPRESSION TAG	UNP Q9Y253

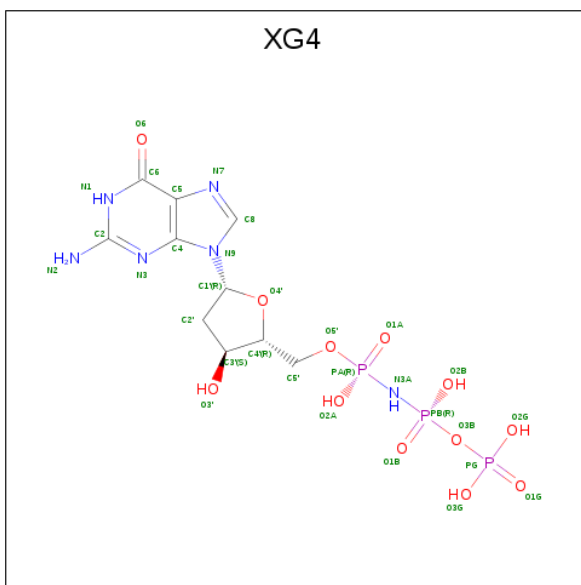
- Molecule 2 is a DNA chain called DNA (5'-D(\*TP\*AP\*AP\*CP\*(TTD)P\*AP\*TP\*GP\*AP\*CP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	12	Total	C	N	O	P	0	0	1
			231	108	42	69	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	P	0	0	1
			164	78	30	48	8			

- Molecule 4 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino}p hosphoryl]guanosine (three-letter code: XG4) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).

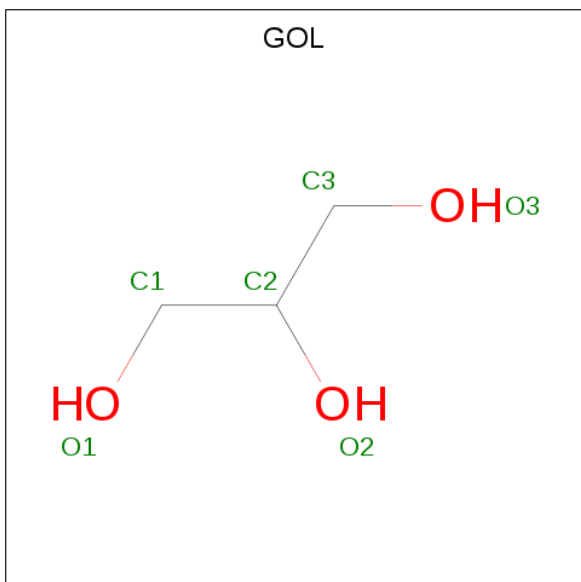


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	A	1	Total 12	C 6	N 5	O 1		0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mg 2 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	T	1	Total C O 6 3 3	0	0
6	T	1	Total C O 6 3 3	0	0
6	T	1	Total C O 6 3 3	0	0

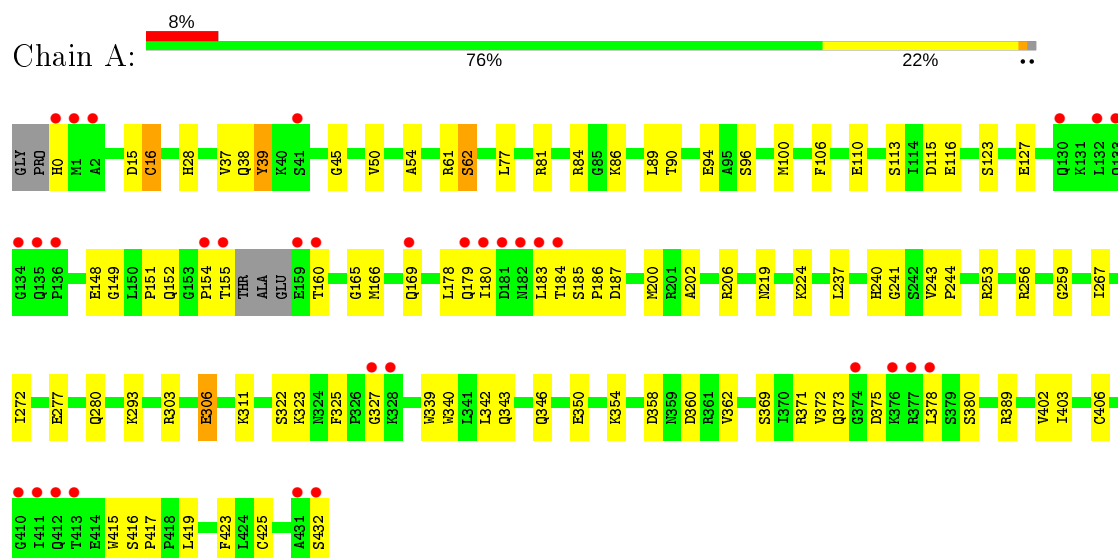
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	320	Total O 320 320	0	0
7	T	22	Total O 22 22	0	0
7	P	25	Total O 25 25	0	0

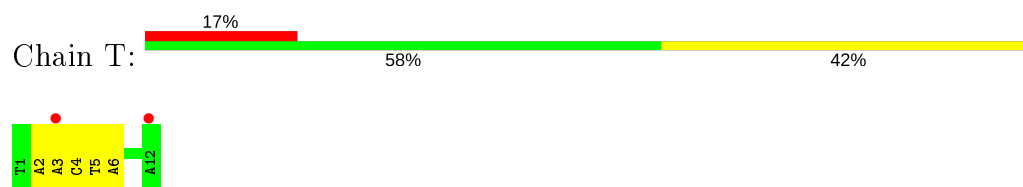
### 3 Residue-property plots [i](#)

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 eta



- Molecule 2: DNA (5'-D(\*TP\*AP\*AP\*CP\*(TTD)P\*AP\*TP\*GP\*AP\*CP\*GP\*A)-3')



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



There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.12Å 99.12Å 81.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.96 – 1.80 25.96 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (25.96-1.80) 99.4 (25.96-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 1.80Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.191 , 0.207 0.189 , 0.206	Depositor DCC
$R_{free}$ test set	3253 reflections (7.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.9	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 61.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.048 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4347	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: GOL, XG4, MG, TTD

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	0.34	0/3573	0.51	0/4822
2	T	0.43	0/213	0.81	0/326
3	P	0.32	0/183	0.73	0/281
All	All	0.34	0/3969	0.55	0/5429

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3474	0	3505	114	0
2	T	231	0	124	23	0
3	P	164	0	90	0	0
4	A	43	0	16	6	0
5	A	2	0	0	0	0
6	A	48	0	61	23	0
6	T	18	0	24	6	0
7	A	320	0	0	12	0
7	P	25	0	0	0	0
7	T	22	0	0	2	0
All	All	4347	0	3820	129	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 16.

All (129) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:3:DA:H4'	2:T:4:DC:OP1	1.46	1.08
1:A:372:VAL:HG22	1:A:380:SER:OG	1.57	1.04
1:A:303:ARG:HA	6:A:442:GOL:H2	1.41	1.01
1:A:354:LYS:HE3	1:A:358:ASP:OD2	1.61	1.00
1:A:293:LYS:HG2	4:A:444:XG4:H8	1.42	1.00
7:A:564:HOH:O	6:T:15:GOL:H31	1.70	0.90
1:A:184[B]:THR:HB	1:A:186:PRO:HD2	1.59	0.85
1:A:62[A]:SER:HA	2:T:3:DA:C6	2.13	0.83
1:A:293:LYS:HG2	4:A:444:XG4:C8	2.11	0.80
1:A:240:HIS:HB3	6:A:441:GOL:H31	1.67	0.75
1:A:62[B]:SER:OG	2:T:3:DA:N6	2.21	0.73
1:A:149:GLY:H	6:A:440:GOL:H11	1.54	0.73
1:A:149:GLY:N	6:A:440:GOL:H11	2.03	0.72
1:A:179[A]:GLN:OE1	1:A:185[A]:SER:HB2	1.87	0.72
1:A:61:ARG:HG3	2:T:3:DA:H61	1.54	0.72
1:A:39[B]:TYR:O	1:A:45:GLY:HA2	1.90	0.72
1:A:154:PRO:O	1:A:155:THR:CB	2.38	0.71
1:A:202:ALA:O	1:A:206[A]:ARG:HD3	1.92	0.69
1:A:362:VAL:HG13	1:A:432:SER:OG	1.92	0.69
1:A:183[B]:LEU:HD22	1:A:187:ASP:OD2	1.92	0.69
1:A:149:GLY:H	6:A:440:GOL:C1	2.07	0.68
1:A:148:GLU:HA	6:A:440:GOL:H12	1.74	0.68
1:A:62[B]:SER:HG	2:T:3:DA:H62	1.42	0.68
1:A:277:GLU:O	1:A:280[B]:GLN:HG3	1.91	0.68
2:T:5:TTD:H71	6:T:14:GOL:H12	1.76	0.67
1:A:148:GLU:CD	6:A:440:GOL:H32	2.13	0.67
1:A:224:LYS:HD2	1:A:256:ARG:HD3	1.77	0.67
1:A:224:LYS:HZ3	6:A:438:GOL:H11	1.61	0.66
1:A:389:ARG:HA	7:A:576:HOH:O	1.96	0.65
1:A:39[B]:TYR:O	1:A:45:GLY:CA	2.45	0.65
2:T:3:DA:C4'	2:T:4:DC:OP1	2.36	0.65
1:A:86:LYS:HE2	7:A:522:HOH:O	1.97	0.64
1:A:322:SER:HB3	1:A:423:PHE:HD2	1.62	0.64
2:T:6:DA:H1'	6:T:15:GOL:H2	1.82	0.62
2:T:6:DA:N7	6:T:14:GOL:O1	2.32	0.62
6:A:439:GOL:H12	7:A:618:HOH:O	1.99	0.62
1:A:160:THR:HB	1:A:169:GLN:OE1	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:HH22	1:A:350:GLU:CD	2.03	0.61
2:T:6:DA:H1'	6:T:15:GOL:C2	2.30	0.61
2:T:3:DA:H2''	2:T:4:DC:C6	2.34	0.61
1:A:372:VAL:HG22	1:A:380:SER:CB	2.31	0.61
2:T:3:DA:H2''	2:T:4:DC:H6	1.66	0.60
1:A:293:LYS:HE3	4:A:444:XG4:C1'	2.32	0.59
1:A:184[B]:THR:CB	1:A:186:PRO:HD2	2.30	0.59
1:A:62[B]:SER:HA	2:T:3:DA:C6	2.38	0.58
1:A:62[B]:SER:HG	2:T:3:DA:N6	2.00	0.58
1:A:224:LYS:NZ	6:A:438:GOL:H11	2.18	0.58
1:A:37[B]:VAL:CG2	1:A:77:LEU:HD22	2.35	0.57
1:A:149:GLY:O	1:A:152:GLN:HG3	2.04	0.57
1:A:84:ARG:NH2	1:A:350:GLU:CD	2.58	0.56
1:A:180[B]:ILE:HG22	1:A:180[B]:ILE:O	2.05	0.56
1:A:415:TRP:CD1	1:A:415:TRP:C	2.78	0.56
1:A:106:PHE:CG	1:A:200[B]:MET:HG2	2.41	0.55
1:A:322:SER:HB3	1:A:423:PHE:CD2	2.41	0.55
1:A:148:GLU:OE1	6:A:440:GOL:H32	2.07	0.55
1:A:323[B]:LYS:HG2	1:A:325:PHE:CZ	2.42	0.54
1:A:178[B]:LEU:HD23	1:A:183[B]:LEU:CD1	2.37	0.54
1:A:372:VAL:HG12	1:A:419:LEU:HD23	1.88	0.54
1:A:62[A]:SER:HA	2:T:3:DA:C5	2.43	0.53
1:A:259:GLY:HA3	6:A:443:GOL:O1	2.08	0.53
1:A:62[A]:SER:HB2	2:T:3:DA:N7	2.24	0.53
1:A:371:ARG:HD2	1:A:378:LEU:O	2.08	0.53
1:A:243:VAL:HG12	6:A:442:GOL:H31	1.90	0.53
1:A:303:ARG:CA	6:A:442:GOL:H2	2.26	0.53
2:T:6:DA:H2''	6:T:15:GOL:H11	1.91	0.53
1:A:244:PRO:HG3	6:A:442:GOL:H12	1.92	0.52
1:A:160:THR:CB	1:A:169:GLN:OE1	2.58	0.52
1:A:38:GLN:O	1:A:39[A]:TYR:HB2	2.08	0.52
1:A:372:VAL:HG23	1:A:375:ASP:HB2	1.92	0.52
1:A:327:GLY:O	1:A:373:GLN:NE2	2.39	0.52
1:A:148:GLU:OE2	6:A:440:GOL:H32	2.09	0.52
1:A:178[B]:LEU:HD23	1:A:183[B]:LEU:HD12	1.93	0.51
1:A:293:LYS:NZ	4:A:444:XG4:C1'	2.74	0.51
1:A:15:ASP:O	1:A:16:CYS:C	2.50	0.50
1:A:28:HIS:ND1	7:A:536:HOH:O	2.34	0.50
1:A:241:GLY:H	6:A:441:GOL:C3	2.24	0.50
1:A:61:ARG:CG	2:T:3:DA:H61	2.21	0.50
1:A:50:VAL:HG12	1:A:54:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LYS:HD3	6:A:443:GOL:O3	2.13	0.49
1:A:237:LEU:HD23	1:A:237:LEU:C	2.33	0.49
1:A:151:PRO:HD2	1:A:166:MET:CE	2.42	0.49
1:A:293:LYS:HE3	4:A:444:XG4:N9	2.27	0.49
1:A:28:HIS:CE1	7:A:536:HOH:O	2.66	0.49
2:T:2:DA:H4'	2:T:3:DA:H5'	1.95	0.49
1:A:267:ILE:HG23	1:A:272:ILE:O	2.12	0.49
1:A:342:LEU:O	1:A:346:GLN:HG3	2.13	0.49
1:A:81:ARG:HD3	7:A:661:HOH:O	2.12	0.49
1:A:89:LEU:HD11	7:T:300:HOH:O	2.13	0.48
1:A:0:HIS:HD2	7:A:759:HOH:O	1.96	0.48
1:A:62[A]:SER:CA	2:T:3:DA:C6	2.91	0.48
1:A:113:SER:OG	1:A:116:GLU:HG2	2.14	0.47
1:A:372:VAL:HG22	1:A:380:SER:HG	1.71	0.47
1:A:339:TRP:O	1:A:343:GLN:HG2	2.15	0.47
1:A:61:ARG:CG	2:T:3:DA:N6	2.78	0.47
1:A:61:ARG:CZ	7:A:610:HOH:O	2.62	0.47
1:A:416:SER:HA	1:A:417:PRO:C	2.35	0.47
1:A:0:HIS:CD2	7:A:759:HOH:O	2.68	0.47
1:A:293:LYS:CE	4:A:444:XG4:C1'	2.93	0.47
1:A:277:GLU:O	1:A:280[A]:GLN:HG2	2.15	0.47
1:A:224:LYS:CE	6:A:443:GOL:O3	2.64	0.46
1:A:148:GLU:HA	6:A:440:GOL:C1	2.45	0.46
1:A:89:LEU:CD1	7:T:300:HOH:O	2.63	0.46
1:A:90:THR:O	1:A:94:GLU:HG3	2.15	0.45
1:A:61:ARG:O	1:A:62[B]:SER:HB2	2.15	0.45
1:A:360:ASP:C	1:A:432:SER:OXT	2.54	0.45
1:A:184[B]:THR:HG21	6:A:441:GOL:O1	2.16	0.45
1:A:96:SER:O	1:A:100:MET:HG2	2.17	0.45
1:A:256:ARG:HA	6:A:443:GOL:H2	1.97	0.45
1:A:219:ASN:HB2	1:A:306:GLU:HG3	1.99	0.44
1:A:369:SER:HB3	1:A:423:PHE:HB3	2.00	0.44
1:A:323[B]:LYS:HD3	1:A:340:TRP:CZ3	2.52	0.44
1:A:84:ARG:NH2	1:A:350:GLU:OE2	2.51	0.44
1:A:185[B]:SER:HB3	1:A:186:PRO:HD3	1.99	0.44
2:T:3:DA:C2'	2:T:4:DC:C6	3.01	0.43
1:A:110:GLU:HB2	1:A:311:LYS:O	2.19	0.43
6:A:439:GOL:C1	7:A:618:HOH:O	2.62	0.43
1:A:180[B]:ILE:O	1:A:180[B]:ILE:CG2	2.66	0.43
1:A:39[A]:TYR:O	1:A:45:GLY:HA3	2.19	0.43
2:T:5:TTD:H6T	2:T:5:TTD:H2R1	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:VAL:CG1	1:A:54:ALA:HB3	2.49	0.42
1:A:165:GLY:O	1:A:169:GLN:HG3	2.19	0.42
1:A:123:SER:O	1:A:127:GLU:HG3	2.20	0.42
1:A:423:PHE:CZ	1:A:425:CYS:HB2	2.53	0.42
1:A:253:ARG:HG2	7:A:513:HOH:O	2.19	0.42
1:A:37[B]:VAL:HG23	1:A:77:LEU:HD22	2.02	0.41
1:A:39[B]:TYR:O	1:A:45:GLY:HA3	2.20	0.41
1:A:402:VAL:HG23	1:A:403:ILE:HG23	2.02	0.41
1:A:37[B]:VAL:HG21	1:A:77:LEU:HD22	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
1	A	446/435 (102%)	439 (98%)	4 (1%)	3 (1%)	22 10

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39[A]	TYR
1	A	39[B]	TYR
1	A	16	CYS

### 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	382/372 (103%)	377 (99%)	5 (1%)	69 62

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62[A]	SER
1	A	62[B]	SER
1	A	115	ASP
1	A	306	GLU
1	A	406	CYS

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	294	ASN

### 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	$\# Z  > 2$
2	TTD	T	5	3,2	42,45,46	2.45	12 (28%)	62,74,77	3.56	27 (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
2	TTD	T	5	3,2	-	4/22/109/110	0/5/6/6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	5	TTD	C5T-C6T	6.97	1.63	1.55
2	T	5	TTD	C1R-N1T	6.41	1.54	1.45
2	T	5	TTD	C1'-N1	5.77	1.53	1.45
2	T	5	TTD	C5A-C5	4.34	1.62	1.53
2	T	5	TTD	O2-C2	-4.26	1.15	1.23
2	T	5	TTD	C5-C4	-4.24	1.43	1.51
2	T	5	TTD	O2T-C2T	-3.57	1.16	1.23
2	T	5	TTD	C6T-N1T	3.49	1.52	1.46
2	T	5	TTD	C5-C6	3.29	1.58	1.55
2	T	5	TTD	C4-N3	2.78	1.41	1.37
2	T	5	TTD	O4-C4	-2.31	1.18	1.22
2	T	5	TTD	C6-N1	2.04	1.49	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	5	TTD	O4-C4-C5	-10.81	114.25	122.88
2	T	5	TTD	C5-C6-N1	10.33	130.09	115.61
2	T	5	TTD	C5T-C6T-N1T	-9.94	101.68	115.61
2	T	5	TTD	O4R-C1R-N1T	7.95	118.08	108.65
2	T	5	TTD	O4T-C4T-C5T	-7.30	117.05	122.88
2	T	5	TTD	C5-C5T-C4T	-6.03	93.33	113.21
2	T	5	TTD	C2R-C1R-N1T	5.74	123.34	115.59
2	T	5	TTD	N3T-C2T-N1T	-5.37	111.12	116.69
2	T	5	TTD	C5M-C5T-C4T	4.86	116.59	108.22
2	T	5	TTD	C5-C4-N3	4.85	120.29	116.06
2	T	5	TTD	C5A-C5-C4	4.67	116.26	108.22
2	T	5	TTD	C5-C5T-C6T	4.20	93.60	88.38
2	T	5	TTD	C5A-C5-C6	-4.01	101.85	114.16
2	T	5	TTD	C5T-C6T-C6	-3.76	83.11	89.28
2	T	5	TTD	C5T-C5-C4	3.55	124.92	113.21
2	T	5	TTD	C4-N3-C2	3.24	131.65	126.67
2	T	5	TTD	O2T-C2T-N3T	3.12	127.31	121.50
2	T	5	TTD	O4-C4-N3	3.11	125.46	120.50
2	T	5	TTD	O4R-C1R-C2R	-3.09	100.41	106.25
2	T	5	TTD	C6-C5-C4	-3.00	105.95	114.50
2	T	5	TTD	C5-C6-C6T	2.99	94.19	89.28
2	T	5	TTD	C6T-C5T-C4T	2.80	122.49	114.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	5	TTD	O4T-C4T-N3T	2.79	124.95	120.50
2	T	5	TTD	C5T-C5-C6	-2.42	85.37	88.38
2	T	5	TTD	C4T-N3T-C2T	2.29	130.18	126.67
2	T	5	TTD	O4'-C1'-C2'	-2.12	102.24	106.25
2	T	5	TTD	O2T-C2T-N1T	-2.03	120.34	123.49

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	5	TTD	C2'-C1'-N1-C6
2	T	5	TTD	C2'-C1'-N1-C2
2	T	5	TTD	O4'-C1'-N1-C2
2	T	5	TTD	O4'-C1'-N1-C6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	5	TTD	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	GOL	T	13	-	5,5,5	0.38	0	5,5,5	0.56	0
6	GOL	A	440	-	5,5,5	1.59	1 (20%)	5,5,5	1.66	1 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	A	437	-	5,5,5	0.48	0	5,5,5	0.59	0
6	GOL	T	14	-	5,5,5	1.98	1 (20%)	5,5,5	1.74	1 (20%)
6	GOL	A	439	-	5,5,5	0.29	0	5,5,5	0.41	0
6	GOL	A	442	-	5,5,5	1.53	2 (40%)	5,5,5	1.46	2 (40%)
6	GOL	A	443	-	5,5,5	0.15	0	5,5,5	0.47	0
4	XG4	A	444	-	10,13,33	1.34	2 (20%)	10,19,52	2.45	5 (50%)
4	XG4	A	433	5	29,33,33	4.43	13 (44%)	35,52,52	1.98	10 (28%)
6	GOL	T	15	-	5,5,5	0.35	0	5,5,5	0.31	0
6	GOL	A	441	-	5,5,5	1.11	1 (20%)	5,5,5	2.21	2 (40%)
6	GOL	A	436	-	5,5,5	0.52	0	5,5,5	0.50	0
6	GOL	A	438	-	5,5,5	1.57	2 (40%)	5,5,5	1.35	1 (20%)

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	GOL	T	13	-	-	0/4/4/4	-
6	GOL	A	440	-	-	2/4/4/4	-
6	GOL	A	437	-	-	0/4/4/4	-
6	GOL	T	14	-	-	2/4/4/4	-
6	GOL	A	439	-	-	0/4/4/4	-
6	GOL	A	442	-	-	0/4/4/4	-
6	GOL	A	443	-	-	0/4/4/4	-
4	XG4	A	444	-	-	-	0/2/2/3
4	XG4	A	433	5	-	5/15/34/34	0/3/3/3
6	GOL	T	15	-	-	0/4/4/4	-
6	GOL	A	441	-	-	2/4/4/4	-
6	GOL	A	436	-	-	0/4/4/4	-
6	GOL	A	438	-	-	0/4/4/4	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	433	XG4	PB-O1B	-12.94	1.25	1.46
4	A	433	XG4	PB-O2B	-10.46	1.28	1.56
4	A	433	XG4	PA-O1A	-9.31	1.31	1.46
4	A	433	XG4	PA-O2A	-6.61	1.39	1.56
4	A	433	XG4	PG-O3G	-5.22	1.34	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	433	XG4	PG-O2G	-5.15	1.35	1.54
4	A	433	XG4	PG-O1G	-5.12	1.34	1.50
4	A	433	XG4	PB-O3B	-4.20	1.53	1.59
6	T	14	GOL	C3-C2	3.96	1.68	1.51
4	A	433	XG4	O4'-C1'	-3.83	1.33	1.42
4	A	433	XG4	O3'-C3'	-3.38	1.36	1.43
4	A	433	XG4	O4'-C4'	-3.31	1.37	1.45
6	A	440	GOL	C3-C2	3.07	1.64	1.51
6	A	438	GOL	C1-C2	-2.52	1.41	1.51
6	A	441	GOL	O1-C1	-2.41	1.32	1.42
4	A	433	XG4	C6-N1	2.37	1.37	1.33
6	A	442	GOL	O3-C3	-2.30	1.32	1.42
6	A	442	GOL	C1-C2	-2.25	1.42	1.51
6	A	438	GOL	O3-C3	-2.23	1.33	1.42
4	A	444	XG4	C8-N7	-2.22	1.30	1.34
4	A	444	XG4	C6-N1	2.11	1.36	1.33
4	A	433	XG4	C2-N2	2.04	1.38	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	444	XG4	C2-N3-C4	4.23	120.19	115.36
4	A	433	XG4	C2-N3-C4	4.21	120.17	115.36
4	A	433	XG4	O1B-PB-N3A	-4.12	105.71	111.77
4	A	444	XG4	N3-C2-N1	-3.91	122.00	127.22
4	A	433	XG4	N3-C2-N1	-3.83	122.12	127.22
4	A	433	XG4	O2A-PA-O1A	3.69	117.67	109.92
6	A	441	GOL	C3-C2-C1	-3.66	97.49	111.70
4	A	433	XG4	C5-C6-N1	-3.07	119.23	123.43
4	A	433	XG4	C6-C5-C4	-3.04	117.90	120.80
4	A	444	XG4	C5-C6-N1	-2.96	119.39	123.43
6	A	440	GOL	O2-C2-C1	2.94	122.09	109.12
6	T	14	GOL	O2-C2-C1	2.91	121.94	109.12
6	A	441	GOL	O2-C2-C3	2.67	120.89	109.12
4	A	433	XG4	C6-N1-C2	2.64	120.13	115.93
4	A	444	XG4	C6-C5-C4	-2.61	118.31	120.80
4	A	433	XG4	C2'-C1'-N9	-2.56	108.36	114.27
4	A	444	XG4	C6-N1-C2	2.48	119.86	115.93
4	A	433	XG4	O5'-C5'-C4'	2.34	117.06	108.99
4	A	433	XG4	O3'-C3'-C2'	2.30	119.13	110.90
6	A	438	GOL	C3-C2-C1	-2.28	102.84	111.70
6	A	442	GOL	C3-C2-C1	-2.23	103.04	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	442	GOL	O3-C3-C2	2.01	119.84	110.20

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	433	XG4	PB-N3A-PA-O1A
6	T	14	GOL	O2-C2-C3-O3
6	A	440	GOL	O1-C1-C2-O2
6	A	440	GOL	O2-C2-C3-O3
4	A	433	XG4	PB-O3B-PG-O1G
6	T	14	GOL	O1-C1-C2-O2
6	A	441	GOL	O1-C1-C2-O2
4	A	433	XG4	PB-N3A-PA-O5'
6	A	441	GOL	O2-C2-C3-O3
4	A	433	XG4	PB-O3B-PG-O2G
4	A	433	XG4	PB-O3B-PG-O3G

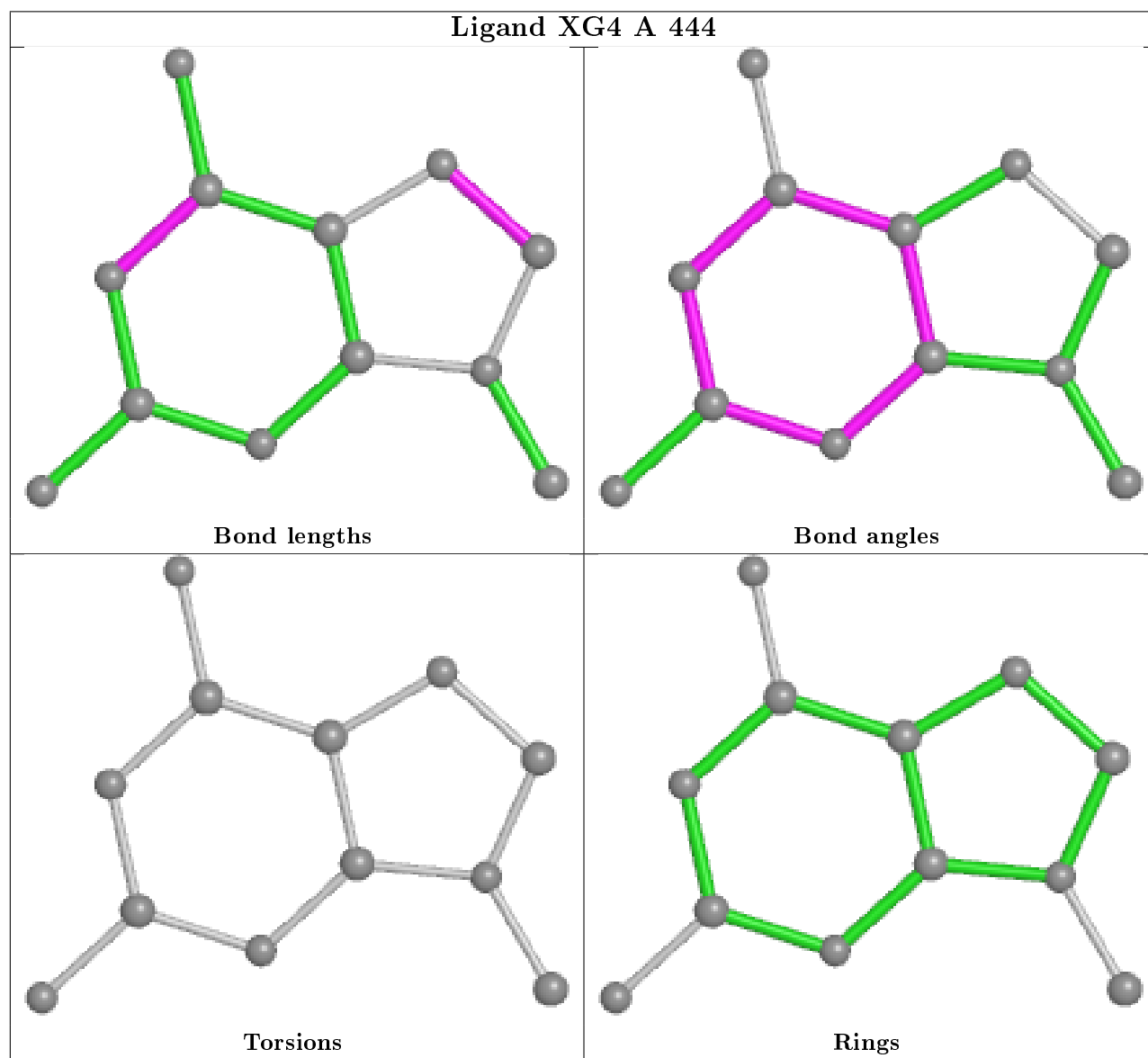
There are no ring outliers.

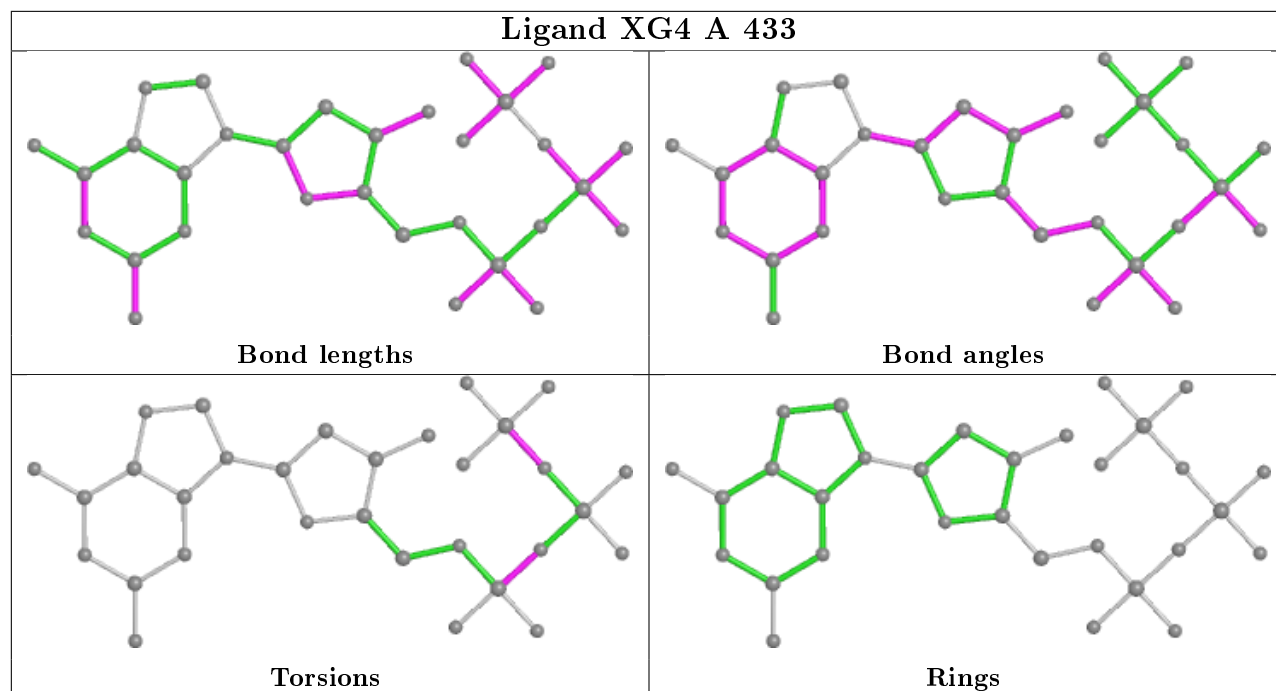
9 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	440	GOL	8	0
6	T	14	GOL	2	0
6	A	439	GOL	2	0
6	A	442	GOL	4	0
6	A	443	GOL	4	0
4	A	444	XG4	6	0
6	T	15	GOL	4	0
6	A	441	GOL	3	0
6	A	438	GOL	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, 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	430/435 (98%)	0.13	33 (7%) <span>13</span> <span>10</span>	9, 21, 50, 62	0
2	T	11/12 (91%)	0.32	2 (18%) <span>1</span> <span>0</span>	24, 28, 69, 73	0
3	P	9/9 (100%)	-0.44	0 <span>100</span> <span>100</span>	21, 28, 41, 53	0
All	All	450/456 (98%)	0.13	35 (7%) <span>13</span> <span>10</span>	9, 22, 52, 73	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	GLY	6.8
1	A	132	LEU	6.2
1	A	160	THR	5.8
1	A	180[A]	ILE	5.7
1	A	410	GLY	5.5
1	A	2	ALA	4.8
1	A	154	PRO	4.3
1	A	179[A]	GLN	4.2
1	A	181[A]	ASP	3.7
1	A	378	LEU	3.7
1	A	431	ALA	3.7
1	A	133	GLN	3.7
1	A	183[A]	LEU	3.6
1	A	0	HIS	3.6
1	A	376	LYS	3.4
1	A	377	ARG	3.4
1	A	135	GLN	3.3
1	A	159	GLU	3.3
1	A	411	ILE	3.3
1	A	374	GLY	3.2
2	T	3	DA	3.1
1	A	328	LYS	3.0
1	A	155	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	130	GLN	2.8
1	A	432	SER	2.6
1	A	412	GLN	2.5
1	A	182[A]	ASN	2.5
1	A	41	SER	2.4
1	A	1	MET	2.4
1	A	413	THR	2.3
1	A	327	GLY	2.3
1	A	184[A]	THR	2.2
1	A	136	PRO	2.2
2	T	12	DA	2.1
1	A	169	GLN	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	TTD	T	5	40/41	0.93	0.12	19,22,25,28	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	GOL	A	437	6/6	0.45	0.31	56,57,57,58	0
6	GOL	T	13	6/6	0.55	0.24	62,63,64,64	0
6	GOL	A	440	6/6	0.60	0.36	54,55,56,56	0
6	GOL	A	441	6/6	0.61	0.29	42,48,50,53	0
4	XG4	A	444	12/31	0.68	0.29	67,67,68,68	0

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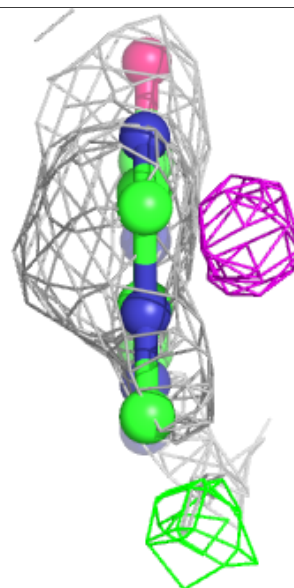
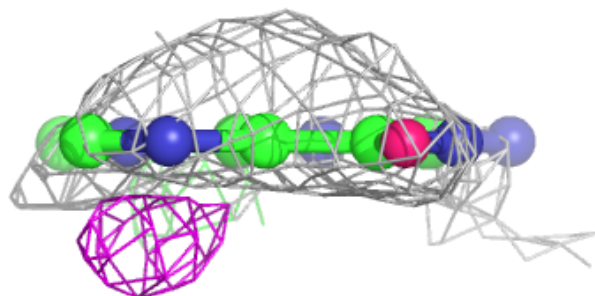
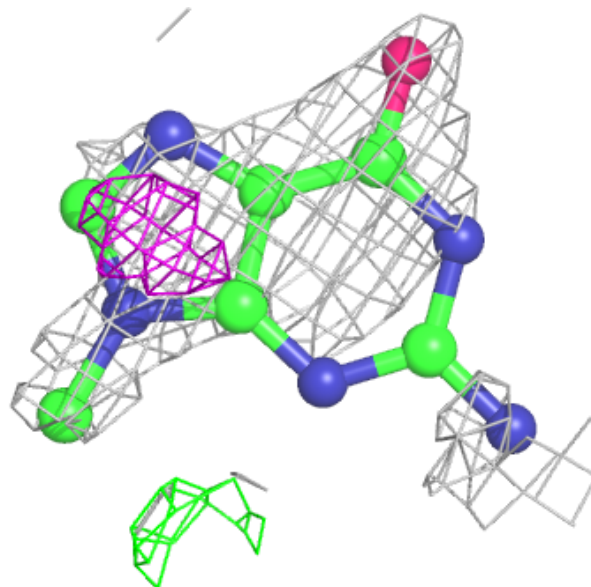
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	T	15	6/6	0.73	0.28	41,45,46,47	0
6	GOL	A	442	6/6	0.75	0.27	32,38,39,42	0
6	GOL	A	439	6/6	0.76	0.20	48,49,49,49	0
6	GOL	A	438	6/6	0.78	0.24	37,44,46,48	0
6	GOL	A	443	6/6	0.78	0.33	53,54,55,56	0
6	GOL	T	14	6/6	0.81	0.22	50,51,52,52	0
6	GOL	A	436	6/6	0.86	0.17	17,22,23,27	0
4	XG4	A	433	31/31	0.98	0.08	10,12,18,20	0
5	MG	A	434	1/1	0.99	0.05	13,13,13,13	0
5	MG	A	435	1/1	1.00	0.09	13,13,13,13	0

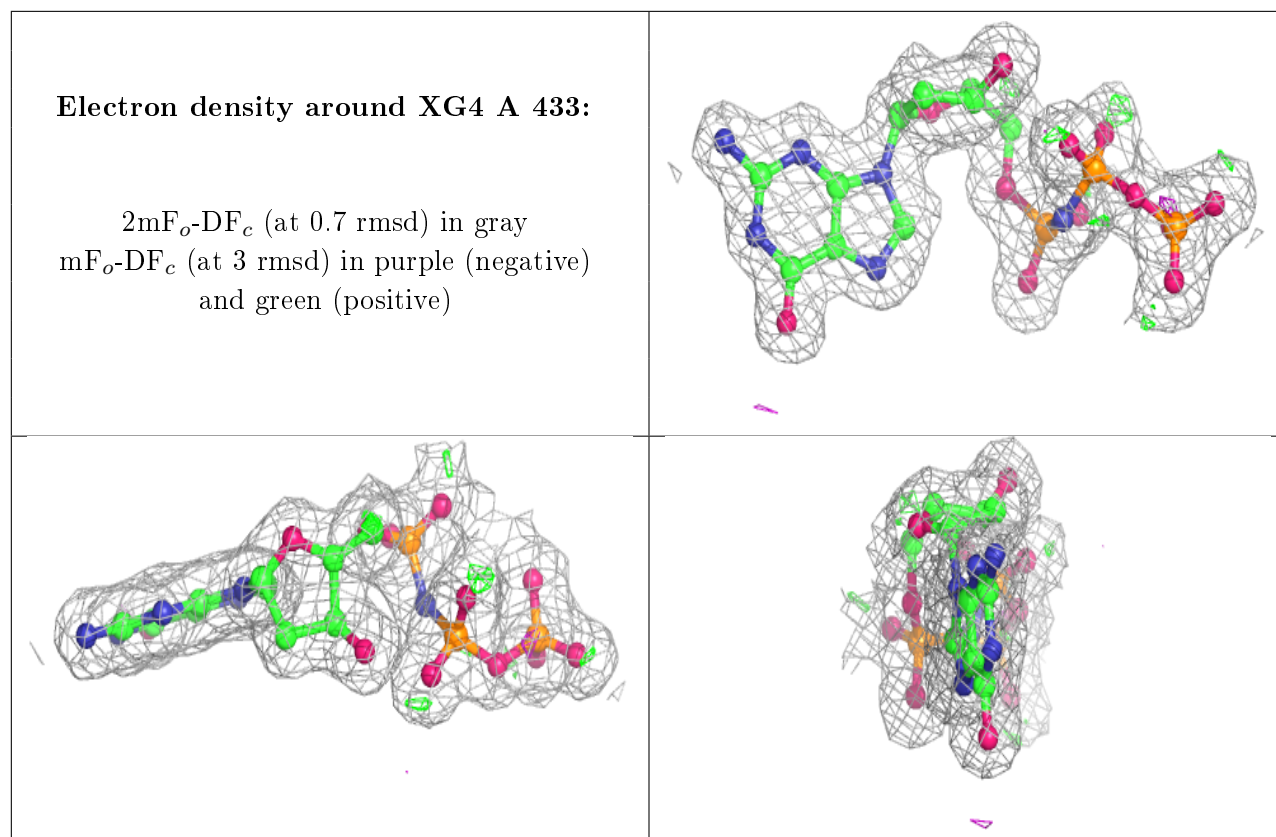
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around XG4 A 444:**

$2mF_o-DF_c$  (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.