



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 01:28 pm BST

PDB ID : 8ICO  
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SEVEN BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF AZT-TP (1 MILLIMOLAR) AND MNCL2 (5 MILLIMOLAR)  
Authors : Pelletier, H.; Sawaya, M.R.  
Deposited on : 1995-12-15  
Resolution : 2.70 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.

---

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

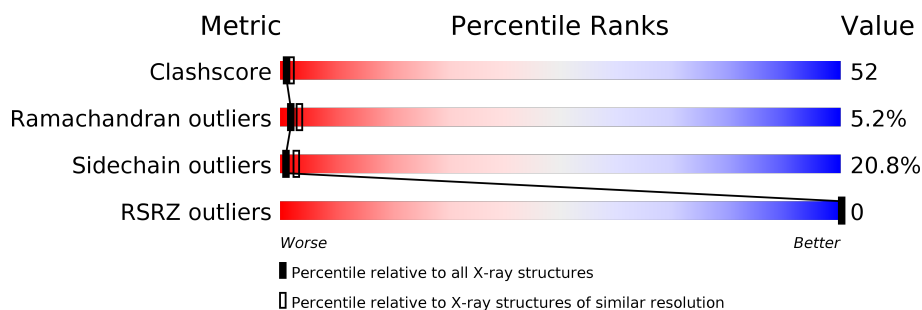
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	T	8	
2	P	7	
3	A	335	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3087 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called DNA (5'-D(\*CP\*AP\*TP\*TP\*AP\*GP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	8	Total	C	N	O	P	0	0	0
			145	69	27	42	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	P	0	0	0
			144	69	24	44	7			

- Molecule 3 is a protein called PROTEIN (DNA POLYMERASE BETA (E.C.2.7.7.7)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	327	Total	C	N	O	S	26	0	0
			2623	1657	458	499	9			

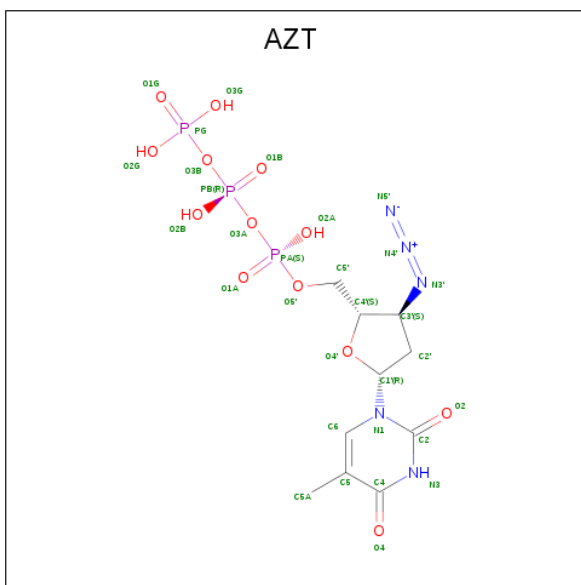
- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is 3'-AZIDO-3'-DEOXYTHYMIDINE-5'-TRIPHOSPHATE (three-letter code: AZT) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			30	10	4	13	3		

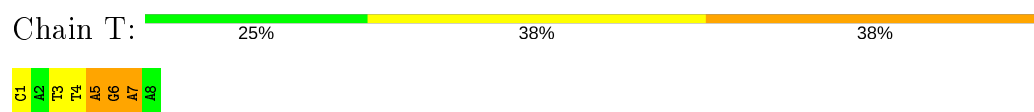
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	T	11	Total O 11 11	0	0
7	P	19	Total O 19 19	0	0
7	A	111	Total O 111 111	0	0

### 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 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.

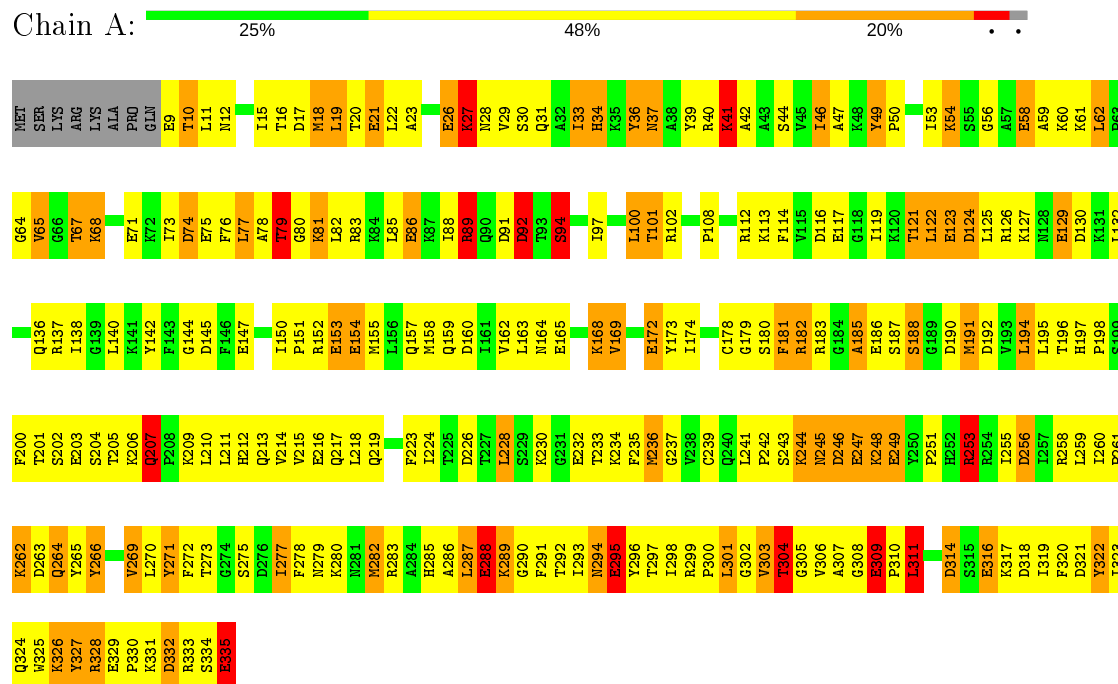
- Molecule 1: DNA (5'-D(\*CP\*AP\*TP\*TP\*AP\*GP\*AP\*A)-3')



- Molecule 2: DNA (5'-D(\*TP\*CP\*TP\*AP\*AP\*TP\*G)-3')



- Molecule 3: PROTEIN (DNA POLYMERASE BETA (E.C.2.7.7.7))



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.69 Å 57.63 Å 48.28 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 11.83 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.0 (20.00-2.70) 91.7 (11.83-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.70 Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, $R_{free}$	0.181 , (Not available) 0.173 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.1	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.16 , 108.6	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	0.95	EDS
Total number of atoms	3087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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: NA, MN, AZT

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	T	2.12	6/162 (3.7%)	3.32	20/249 (8.0%)
2	P	2.47	8/160 (5.0%)	3.74	24/243 (9.9%)
3	A	1.27	29/2672 (1.1%)	1.73	66/3590 (1.8%)
All	All	1.42	43/2994 (1.4%)	2.04	110/4082 (2.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	2	0

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	1	DC	C3'-O3'	8.66	1.55	1.44
2	P	3	DT	C2'-C1'	-8.04	1.44	1.52
3	A	86	GLU	CD-OE1	7.59	1.33	1.25
3	A	58	GLU	CD-OE1	7.54	1.33	1.25
3	A	75	GLU	CD-OE1	7.50	1.33	1.25
3	A	147	GLU	CD-OE2	7.50	1.33	1.25
2	P	3	DT	N1-C2	7.44	1.44	1.38
2	P	3	DT	O4'-C1'	7.40	1.51	1.42
3	A	329	GLU	CD-OE2	7.26	1.33	1.25
3	A	117	GLU	CD-OE2	7.24	1.33	1.25
3	A	335	GLU	CD-OE2	7.13	1.33	1.25
3	A	71	GLU	CD-OE1	7.12	1.33	1.25
1	T	6	DG	C3'-O3'	-7.10	1.34	1.44
3	A	172	GLU	CD-OE2	7.08	1.33	1.25
3	A	249	GLU	CD-OE2	6.96	1.33	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	5	DA	N9-C4	6.95	1.42	1.37
1	T	3	DT	C3'-O3'	-6.82	1.35	1.44
1	T	5	DA	C5-C6	-6.68	1.35	1.41
3	A	288	GLU	CD-OE2	6.62	1.32	1.25
3	A	123	GLU	CD-OE1	6.62	1.32	1.25
3	A	295	GLU	CD-OE2	6.55	1.32	1.25
3	A	153	GLU	CD-OE2	6.53	1.32	1.25
3	A	129	GLU	CD-OE1	6.42	1.32	1.25
3	A	203	GLU	CD-OE1	6.37	1.32	1.25
3	A	216	GLU	CD-OE2	6.32	1.32	1.25
3	A	154	GLU	CD-OE2	6.25	1.32	1.25
2	P	3	DT	C1'-N1	6.19	1.57	1.49
3	A	309	GLU	CD-OE2	6.16	1.32	1.25
3	A	316	GLU	CD-OE1	6.05	1.32	1.25
3	A	232	GLU	CD-OE2	5.91	1.32	1.25
2	P	3	DT	C4'-C3'	-5.82	1.46	1.52
3	A	186	GLU	CD-OE1	5.81	1.32	1.25
1	T	5	DA	N7-C5	-5.73	1.35	1.39
2	P	1	DT	P-O5'	5.71	1.65	1.59
1	T	5	DA	N1-C2	5.56	1.39	1.34
3	A	247	GLU	CD-OE1	5.38	1.31	1.25
3	A	271	TYR	CB-CG	-5.35	1.43	1.51
3	A	9	GLU	CD-OE2	5.34	1.31	1.25
3	A	173	TYR	CB-CG	-5.25	1.43	1.51
3	A	26	GLU	CD-OE1	5.18	1.31	1.25
3	A	326	LYS	CE-NZ	-5.06	1.36	1.49
2	P	2	DC	C1'-N1	5.03	1.55	1.49
3	A	94	SER	CA-CB	-5.01	1.45	1.52

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	3	DT	C6-N1-C1'	-18.42	92.77	120.40
2	P	3	DT	C2-N1-C1'	17.81	146.70	118.20
2	P	1	DT	C6-N1-C1'	-17.14	94.69	120.40
2	P	1	DT	C2-N1-C1'	17.03	145.45	118.20
1	T	7	DA	C4-N9-C1'	-16.60	96.41	126.30
1	T	7	DA	C8-N9-C1'	15.65	155.87	127.70
1	T	4	DT	C6-N1-C1'	-15.39	97.31	120.40
1	T	4	DT	C2-N1-C1'	12.74	138.59	118.20
2	P	6	DT	C6-N1-C1'	-12.25	102.02	120.40
2	P	6	DT	C2-N1-C1'	10.86	135.57	118.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	5	DA	N1-C6-N6	10.82	125.09	118.60
1	T	1	DC	P-O3'-C3'	10.35	132.12	119.70
1	T	6	DG	O4'-C1'-N9	10.07	115.05	108.00
2	P	3	DT	O4'-C1'-N1	9.76	114.83	108.00
2	P	3	DT	N3-C2-O2	-9.68	116.49	122.30
2	P	3	DT	N1-C1'-C2'	9.67	130.98	112.60
3	A	253	ARG	NE-CZ-NH1	9.31	124.96	120.30
2	P	2	DC	C2-N1-C1'	9.30	129.03	118.80
2	P	4	DA	C8-N9-C1'	-9.23	111.09	127.70
3	A	130	ASP	CB-CG-OD2	-9.07	110.14	118.30
2	P	4	DA	C4-N9-C1'	8.96	142.42	126.30
2	P	5	DA	C8-N9-C1'	-8.84	111.78	127.70
3	A	190	ASP	CB-CG-OD2	-8.54	110.61	118.30
2	P	5	DA	C4-N9-C1'	8.53	141.65	126.30
1	T	4	DT	C1'-O4'-C4'	-8.44	101.66	110.10
3	A	314	ASP	CB-CG-OD1	-8.22	110.91	118.30
3	A	263	ASP	CB-CG-OD2	-8.12	110.99	118.30
2	P	7	DG	C4-N9-C1'	-8.07	116.01	126.50
3	A	130	ASP	CB-CG-OD1	8.05	125.55	118.30
3	A	83	ARG	N-CA-CB	7.89	124.81	110.60
1	T	5	DA	C5-C6-N6	-7.76	117.50	123.70
3	A	124	ASP	CB-CG-OD2	-7.75	111.33	118.30
3	A	190	ASP	CB-CG-OD1	7.75	125.27	118.30
2	P	6	DT	O4'-C1'-N1	-7.69	102.62	108.00
1	T	5	DA	C6-C5-N7	-7.68	126.92	132.30
2	P	1	DT	O4'-C1'-N1	7.68	113.38	108.00
2	P	2	DC	O4'-C1'-N1	7.60	113.32	108.00
2	P	2	DC	C6-N1-C1'	-7.48	111.83	120.80
2	P	7	DG	C8-N9-C1'	7.48	136.72	127.00
3	A	256	ASP	CB-CG-OD2	-7.48	111.57	118.30
3	A	192	ASP	CB-CG-OD1	-7.45	111.60	118.30
3	A	89	ARG	NE-CZ-NH1	7.43	124.01	120.30
3	A	74	ASP	CB-CG-OD1	7.42	124.98	118.30
3	A	266	TYR	CA-CB-CG	-7.35	99.43	113.40
3	A	92	ASP	CB-CG-OD2	-7.32	111.71	118.30
3	A	326	LYS	CD-CE-NZ	6.85	127.45	111.70
1	T	4	DT	O4'-C1'-N1	6.78	112.74	108.00
1	T	3	DT	P-O5'-C5'	6.67	131.57	120.90
3	A	49	TYR	C-N-CD	-6.65	105.96	120.60
2	P	3	DT	O4'-C4'-C3'	6.55	109.93	106.00
3	A	311	LEU	C-N-CD	-6.54	106.22	120.60
3	A	92	ASP	CB-CG-OD1	6.53	124.17	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	39	TYR	CB-CG-CD1	-6.36	117.19	121.00
3	A	256	ASP	CB-CG-OD1	6.35	124.01	118.30
2	P	2	DC	C4'-C3'-C2'	-6.32	97.41	103.10
3	A	271	TYR	CB-CG-CD1	-6.30	117.22	121.00
3	A	192	ASP	CB-CA-C	-6.25	97.91	110.40
3	A	168	LYS	N-CA-CB	6.19	121.75	110.60
3	A	34	HIS	CA-CB-CG	-6.18	103.10	113.60
3	A	116	ASP	CB-CG-OD1	6.16	123.84	118.30
3	A	79	THR	CA-CB-CG2	-6.09	103.87	112.40
3	A	49	TYR	CA-CB-CG	6.05	124.89	113.40
1	T	5	DA	C4-C5-N7	5.95	113.68	110.70
3	A	116	ASP	CB-CG-OD2	-5.91	112.98	118.30
3	A	74	ASP	CB-CG-OD2	-5.87	113.01	118.30
2	P	3	DT	N1-C2-O2	5.82	127.76	123.10
3	A	253	ARG	NE-CZ-NH2	-5.75	117.42	120.30
3	A	304	THR	CA-CB-CG2	-5.67	104.46	112.40
3	A	39	TYR	CA-CB-CG	-5.67	102.64	113.40
3	A	322	TYR	CB-CG-CD1	-5.66	117.61	121.00
3	A	181	PHE	CB-CA-C	-5.66	99.09	110.40
3	A	332	ASP	CB-CG-OD1	-5.64	113.22	118.30
3	A	27	LYS	CB-CA-C	5.62	121.64	110.40
3	A	145	ASP	CB-CA-C	-5.62	99.16	110.40
3	A	91	ASP	CB-CG-OD1	-5.62	113.25	118.30
1	T	4	DT	C6-N1-C2	5.61	124.10	121.30
3	A	246	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	T	5	DA	C5-N7-C8	-5.57	101.12	103.90
3	A	195	LEU	N-CA-CB	-5.54	99.32	110.40
2	P	3	DT	C1'-O4'-C4'	-5.52	104.58	110.10
1	T	5	DA	C8-N9-C1'	5.47	137.56	127.70
3	A	124	ASP	CB-CG-OD1	5.46	123.22	118.30
3	A	89	ARG	NE-CZ-NH2	-5.46	117.57	120.30
3	A	246	ASP	CB-CG-OD2	5.42	123.18	118.30
3	A	36	TYR	CA-CB-CG	-5.42	103.11	113.40
3	A	266	TYR	CB-CG-CD1	-5.41	117.75	121.00
3	A	299	ARG	NE-CZ-NH1	5.41	123.00	120.30
3	A	17	ASP	CB-CG-OD2	5.40	123.16	118.30
3	A	116	ASP	CB-CA-C	5.38	121.17	110.40
3	A	41	LYS	N-CA-CB	5.35	120.23	110.60
3	A	116	ASP	N-CA-CB	5.33	120.20	110.60
1	T	4	DT	C5-C6-N1	-5.30	120.52	123.70
3	A	17	ASP	CB-CA-C	5.26	120.93	110.40
3	A	91	ASP	CB-CG-OD2	5.26	123.04	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	219	GLN	N-CA-CB	-5.26	101.14	110.60
3	A	314	ASP	CB-CG-OD2	5.25	123.03	118.30
3	A	102	ARG	CA-CB-CG	-5.25	101.85	113.40
3	A	157	GLN	N-CA-CB	5.24	120.04	110.60
1	T	1	DC	C2-N1-C1'	5.24	124.56	118.80
3	A	321	ASP	CB-CG-OD2	-5.20	113.62	118.30
3	A	335	GLU	N-CA-CB	5.19	119.94	110.60
3	A	318	ASP	CB-CG-OD2	-5.18	113.64	118.30
3	A	332	ASP	CB-CG-OD2	5.18	122.96	118.30
3	A	68	LYS	N-CA-CB	5.16	119.88	110.60
3	A	269	VAL	CA-CB-CG2	-5.14	103.19	110.90
1	T	1	DC	C6-N1-C1'	-5.11	114.66	120.80
3	A	207	GLN	C-N-CD	-5.09	109.41	120.60
3	A	142	TYR	CB-CA-C	-5.06	100.28	110.40
3	A	282	MET	CA-CB-CG	-5.06	104.70	113.30
1	T	7	DA	O4'-C1'-C2'	5.01	109.91	105.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	40	ARG	CA
3	A	246	ASP	CA

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	T	145	0	80	2	0
2	P	144	0	81	12	0
3	A	2623	0	2641	283	0
4	A	2	0	0	0	0
5	A	2	0	0	0	0
6	A	30	0	12	1	0
7	A	111	0	0	18	0
7	P	19	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	T	11	0	0	0	0
All	All	3087	0	2814	297	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 52.

All (297) 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)
3:A:151:PRO:HG2	3:A:154:GLU:HG3	1.28	1.08
3:A:155:MET:HA	3:A:158:MET:HE3	1.32	1.07
3:A:277:ILE:HG12	3:A:335:GLU:HA	1.36	1.03
3:A:245:ASN:H	3:A:245:ASN:HD22	1.04	1.01
3:A:245:ASN:N	3:A:245:ASN:HD22	1.55	0.96
3:A:18:MET:HE2	3:A:82:LEU:HD22	1.51	0.90
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.69	0.90
3:A:15:ILE:HD13	3:A:73:ILE:HG23	1.55	0.89
3:A:243:SER:HB3	3:A:249:GLU:HA	1.53	0.88
3:A:191:MET:HG2	3:A:255:ILE:HG13	1.55	0.87
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.37	0.87
3:A:210:LEU:HB3	3:A:259:LEU:HD21	1.57	0.87
3:A:29:VAL:HG21	3:A:94:SER:HB2	1.56	0.86
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.57	0.86
3:A:151:PRO:HG2	3:A:154:GLU:CG	2.09	0.83
3:A:150:ILE:HD13	3:A:253:ARG:HG2	1.60	0.82
3:A:172:GLU:HB3	3:A:197:HIS:NE2	1.95	0.81
2:P:6:DT:H2''	2:P:7:DG:H5'	1.63	0.80
3:A:245:ASN:ND2	3:A:245:ASN:N	2.29	0.80
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.27	0.80
3:A:277:ILE:HD13	3:A:277:ILE:H	1.47	0.80
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.17	0.80
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.81	0.79
3:A:245:ASN:H	3:A:245:ASN:ND2	1.83	0.77
3:A:11:LEU:HD23	3:A:11:LEU:H	1.48	0.77
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.14	0.77
3:A:259:LEU:O	3:A:260:ILE:HD13	1.85	0.76
2:P:1:DT:H2''	2:P:2:DC:H5'	1.67	0.76
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.66	0.76
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.69	0.75
2:P:6:DT:H2''	2:P:7:DG:C5'	2.18	0.73
3:A:73:ILE:O	3:A:77:LEU:HD22	1.89	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:306:VAL:HG22	7:A:650:HOH:O	1.88	0.73
3:A:255:ILE:HG12	3:A:256:ASP:N	2.02	0.73
3:A:108:PRO:O	3:A:112:ARG:HG3	1.88	0.72
3:A:172:GLU:HB3	3:A:197:HIS:CD2	2.26	0.71
3:A:291:PHE:HD1	3:A:300:PRO:HA	1.56	0.70
3:A:212:HIS:HB3	7:A:541:HOH:O	1.90	0.70
3:A:16:THR:O	3:A:20:THR:HG23	1.91	0.70
3:A:277:ILE:CG1	3:A:335:GLU:HA	2.17	0.70
3:A:243:SER:CB	3:A:249:GLU:HA	2.20	0.70
3:A:270:LEU:HD13	3:A:316:GLU:OE1	1.91	0.69
3:A:289:LYS:N	3:A:289:LYS:HD3	2.07	0.69
3:A:302:GLY:H	3:A:307:ALA:HB3	1.57	0.69
3:A:270:LEU:HD21	3:A:282:MET:CE	2.22	0.69
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.22	0.69
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.28	0.69
3:A:286:ALA:HB2	3:A:323:ILE:HG21	1.75	0.68
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.23	0.68
3:A:210:LEU:CB	3:A:259:LEU:HD21	2.23	0.68
3:A:182:ARG:NH1	3:A:182:ARG:HG2	2.05	0.68
3:A:121:THR:HG23	3:A:124:ASP:OD2	1.94	0.68
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.59	0.68
3:A:60:LYS:HA	3:A:65:VAL:CG2	2.25	0.67
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.76	0.67
3:A:68:LYS:HB2	3:A:68:LYS:NZ	2.09	0.67
3:A:253:ARG:HG3	3:A:253:ARG:HH11	1.59	0.67
3:A:294:ASN:HB2	3:A:295:GLU:OE1	1.95	0.67
3:A:125:LEU:HD22	3:A:132:LEU:HD21	1.77	0.67
3:A:278:PHE:CD2	3:A:333:ARG:HB3	2.30	0.67
3:A:60:LYS:HA	3:A:65:VAL:HG23	1.77	0.67
3:A:28:ASN:HD22	3:A:28:ASN:N	1.87	0.66
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.29	0.66
3:A:292:THR:O	3:A:298:ILE:HA	1.95	0.66
3:A:155:MET:HA	3:A:158:MET:CE	2.20	0.66
3:A:18:MET:HE1	3:A:82:LEU:HD13	1.78	0.65
3:A:41:LYS:HD3	3:A:42:ALA:N	2.10	0.65
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.78	0.64
3:A:279:ASN:O	3:A:283:ARG:HG3	1.97	0.64
3:A:262:LYS:O	3:A:262:LYS:HG3	1.95	0.64
3:A:18:MET:HE3	3:A:76:PHE:CD2	2.33	0.64
3:A:89:ARG:C	3:A:89:ARG:HD3	2.18	0.64
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.41	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.37	0.63
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.29	0.63
3:A:27:LYS:HB3	3:A:36:TYR:CG	2.34	0.63
3:A:31:GLN:HE21	3:A:112:ARG:NH2	1.96	0.63
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.14	0.63
3:A:31:GLN:HE21	3:A:112:ARG:CZ	2.12	0.62
3:A:121:THR:HG23	3:A:124:ASP:CG	2.19	0.62
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.35	0.62
3:A:323:ILE:O	3:A:324:GLN:HG2	1.99	0.62
3:A:79:THR:O	3:A:81:LYS:N	2.32	0.62
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.82	0.62
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.80	0.62
3:A:58:GLU:O	3:A:61:LYS:HG3	2.00	0.61
2:P:6:DT:H5'	2:P:6:DT:H6	1.64	0.61
3:A:125:LEU:CD2	3:A:132:LEU:HD21	2.30	0.61
3:A:180:SER:HB3	3:A:183:ARG:NH2	2.16	0.61
1:T:6:DG:H2''	1:T:7:DA:C8	2.35	0.61
3:A:163:LEU:N	3:A:163:LEU:HD23	2.15	0.61
3:A:28:ASN:ND2	3:A:28:ASN:N	2.45	0.61
3:A:119:ILE:HG23	3:A:124:ASP:CB	2.28	0.61
3:A:326:LYS:O	3:A:328:ARG:HG2	2.01	0.61
3:A:172:GLU:CG	3:A:198:PRO:HG2	2.31	0.61
3:A:31:GLN:HE21	3:A:112:ARG:HH22	1.48	0.60
3:A:218:LEU:HB3	3:A:224:ILE:HD12	1.83	0.60
3:A:264:GLN:NE2	3:A:296:TYR:HB3	2.17	0.60
3:A:317:LYS:O	3:A:320:PHE:N	2.34	0.60
3:A:330:PRO:HA	3:A:333:ARG:CG	2.31	0.60
3:A:248:LYS:HG2	3:A:248:LYS:O	2.01	0.60
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.37	0.60
3:A:306:VAL:HG23	3:A:307:ALA:N	2.18	0.59
3:A:282:MET:HE2	7:A:555:HOH:O	2.01	0.59
3:A:74:ASP:O	3:A:77:LEU:N	2.35	0.59
3:A:228:LEU:HB2	3:A:236:MET:O	2.03	0.59
3:A:165:GLU:HB3	3:A:217:GLN:HG2	1.84	0.59
1:T:5:DA:H2''	1:T:6:DG:O5'	2.00	0.59
3:A:82:LEU:HD23	3:A:85:LEU:HB2	1.84	0.59
3:A:291:PHE:CD1	3:A:300:PRO:HA	2.38	0.59
3:A:11:LEU:N	3:A:11:LEU:HD23	2.15	0.58
3:A:81:LYS:NZ	3:A:86:GLU:HB3	2.18	0.58
3:A:285:HIS:NE2	7:A:583:HOH:O	2.32	0.58
3:A:165:GLU:HB3	3:A:217:GLN:CG	2.34	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:18:MET:CE	3:A:76:PHE:HB2	2.33	0.57
3:A:172:GLU:HG3	3:A:198:PRO:HG2	1.85	0.57
3:A:270:LEU:HD21	3:A:282:MET:HE3	1.86	0.57
3:A:73:ILE:HG22	3:A:77:LEU:CD2	2.35	0.57
3:A:11:LEU:CD2	3:A:11:LEU:H	2.14	0.57
3:A:41:LYS:HD3	3:A:42:ALA:H	1.69	0.57
3:A:196:THR:OG1	3:A:197:HIS:N	2.38	0.57
3:A:270:LEU:HD21	3:A:282:MET:HE1	1.86	0.57
3:A:287:LEU:HD13	3:A:291:PHE:O	2.05	0.57
3:A:295:GLU:HA	7:A:592:HOH:O	2.05	0.57
3:A:180:SER:HB3	3:A:183:ARG:HH21	1.69	0.57
3:A:294:ASN:ND2	3:A:297:THR:H	2.02	0.57
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.40	0.56
3:A:277:ILE:HG13	3:A:335:GLU:CB	2.35	0.56
3:A:295:GLU:OE1	3:A:295:GLU:N	2.32	0.56
3:A:155:MET:CA	3:A:158:MET:HE3	2.21	0.55
3:A:42:ALA:O	3:A:46:ILE:HG23	2.06	0.55
3:A:282:MET:HB3	7:A:555:HOH:O	2.06	0.55
3:A:164:ASN:O	3:A:168:LYS:HG2	2.06	0.55
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.72	0.54
3:A:144:GLY:N	7:A:590:HOH:O	2.39	0.54
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.22	0.54
3:A:275:SER:HB2	7:A:661:HOH:O	2.08	0.54
3:A:33:ILE:O	3:A:37:ASN:N	2.40	0.54
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.42	0.54
3:A:287:LEU:HD12	3:A:287:LEU:O	2.08	0.54
3:A:302:GLY:H	3:A:307:ALA:CB	2.19	0.54
3:A:302:GLY:N	3:A:307:ALA:HB3	2.21	0.54
3:A:236:MET:HG2	3:A:256:ASP:OD1	2.07	0.54
3:A:311:LEU:HB3	3:A:322:TYR:HE2	1.72	0.54
3:A:278:PHE:HB2	3:A:333:ARG:O	2.08	0.54
3:A:298:ILE:HA	7:A:593:HOH:O	2.07	0.53
3:A:327:TYR:HD1	3:A:328:ARG:N	2.06	0.53
3:A:29:VAL:CG2	3:A:94:SER:HB2	2.35	0.53
3:A:123:GLU:O	3:A:127:LYS:HG2	2.09	0.53
3:A:288:GLU:C	3:A:290:GLY:H	2.11	0.53
3:A:15:ILE:HB	3:A:46:ILE:CD1	2.39	0.52
3:A:309:GLU:N	3:A:309:GLU:OE1	2.43	0.52
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.44	0.52
3:A:41:LYS:NZ	3:A:64:GLY:O	2.40	0.52
3:A:332:ASP:C	3:A:334:SER:H	2.12	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:12:ASN:HA	7:A:553:HOH:O	2.10	0.52
3:A:18:MET:CE	3:A:82:LEU:HD13	2.39	0.52
3:A:280:LYS:O	3:A:283:ARG:HB2	2.10	0.51
3:A:328:ARG:O	3:A:333:ARG:NE	2.29	0.51
3:A:129:GLU:HG2	3:A:137:ARG:HD3	1.93	0.51
3:A:150:ILE:O	3:A:187:SER:HA	2.11	0.51
3:A:18:MET:HE1	3:A:76:PHE:CB	2.41	0.50
3:A:15:ILE:CG2	3:A:46:ILE:HD13	2.42	0.50
3:A:15:ILE:HD13	3:A:73:ILE:CG2	2.36	0.50
3:A:291:PHE:O	3:A:301:LEU:HD22	2.11	0.50
3:A:56:GLY:N	3:A:74:ASP:OD1	2.39	0.50
3:A:200:PHE:HB2	7:A:625:HOH:O	2.10	0.50
3:A:303:VAL:C	3:A:305:GLY:H	2.13	0.50
3:A:16:THR:HG21	3:A:47:ALA:HB2	1.94	0.50
3:A:180:SER:CB	3:A:183:ARG:HH21	2.25	0.50
2:P:1:DT:C2'	2:P:2:DC:H5'	2.38	0.50
3:A:152:ARG:NH2	3:A:181:PHE:O	2.36	0.49
3:A:182:ARG:NH2	3:A:316:GLU:OE2	2.32	0.49
3:A:243:SER:O	3:A:244:LYS:O	2.29	0.49
3:A:79:THR:O	3:A:79:THR:OG1	2.30	0.49
3:A:152:ARG:HA	3:A:155:MET:HB2	1.94	0.49
3:A:288:GLU:O	3:A:290:GLY:N	2.44	0.49
3:A:194:LEU:N	3:A:194:LEU:HD13	2.27	0.49
3:A:272:PHE:HA	6:A:338:AZT:N4'	2.28	0.49
3:A:26:GLU:O	3:A:30:SER:O	2.30	0.49
3:A:165:GLU:HB2	3:A:218:LEU:HD11	1.94	0.49
3:A:295:GLU:H	3:A:295:GLU:CD	2.04	0.49
3:A:92:ASP:HB3	7:A:647:HOH:O	2.12	0.49
2:P:5:DA:C2'	2:P:6:DT:H72	2.43	0.48
3:A:18:MET:HG2	3:A:19:LEU:N	2.24	0.48
3:A:31:GLN:N	7:A:641:HOH:O	2.28	0.48
3:A:207:GLN:O	3:A:210:LEU:HB2	2.12	0.48
3:A:214:VAL:HG23	3:A:215:VAL:N	2.27	0.48
3:A:53:ILE:HG21	3:A:59:ALA:HB2	1.95	0.48
3:A:270:LEU:CD2	3:A:319:ILE:HD13	2.43	0.48
3:A:270:LEU:HD22	3:A:319:ILE:HD13	1.95	0.48
3:A:18:MET:O	3:A:21:GLU:HB2	2.13	0.48
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.28	0.48
3:A:31:GLN:HB2	3:A:112:ARG:NH1	2.29	0.48
3:A:162:VAL:HG13	3:A:218:LEU:HD21	1.96	0.47
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.95	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:234:LYS:HD3	7:A:617:HOH:O	2.14	0.47
3:A:122:LEU:CD2	3:A:126:ARG:NH2	2.78	0.47
3:A:303:VAL:HG22	3:A:303:VAL:O	2.14	0.47
3:A:180:SER:HB2	3:A:185:ALA:HB2	1.96	0.47
3:A:280:LYS:O	3:A:283:ARG:N	2.48	0.47
3:A:271:TYR:HB2	7:A:592:HOH:O	2.14	0.47
3:A:85:LEU:HA	3:A:85:LEU:HD12	1.74	0.47
3:A:154:GLU:O	3:A:158:MET:HG3	2.14	0.47
3:A:200:PHE:HE2	3:A:261:PRO:HD3	1.79	0.47
3:A:286:ALA:HA	3:A:323:ILE:CG2	2.45	0.46
3:A:49:TYR:CB	3:A:50:PRO:HD2	2.23	0.46
3:A:12:ASN:HD21	3:A:53:ILE:H	1.63	0.46
3:A:140:LEU:O	3:A:140:LEU:HD12	2.15	0.46
3:A:15:ILE:O	3:A:19:LEU:HD22	2.15	0.46
3:A:316:GLU:O	3:A:320:PHE:HD2	1.98	0.46
2:P:5:DA:H1'	2:P:6:DT:H5''	1.98	0.46
3:A:172:GLU:HG2	3:A:198:PRO:HG2	1.97	0.46
2:P:6:DT:H2''	2:P:7:DG:H5''	1.97	0.46
3:A:59:ALA:O	3:A:62:LEU:HB2	2.15	0.46
3:A:150:ILE:HG21	3:A:158:MET:CE	2.45	0.46
3:A:277:ILE:HG13	3:A:335:GLU:HB2	1.96	0.46
3:A:30:SER:HB3	7:A:561:HOH:O	2.16	0.46
3:A:159:GLN:HG2	3:A:160:ASP:N	2.30	0.46
3:A:97:ILE:O	3:A:101:THR:HB	2.16	0.46
3:A:150:ILE:HG13	3:A:188:SER:O	2.16	0.46
3:A:292:THR:O	3:A:293:ILE:HD13	2.15	0.46
3:A:68:LYS:HB2	3:A:68:LYS:HZ2	1.77	0.45
3:A:54:LYS:HD2	3:A:54:LYS:HA	1.48	0.45
3:A:302:GLY:N	3:A:307:ALA:CB	2.79	0.45
3:A:241:LEU:HA	3:A:242:PRO:HD3	1.71	0.45
3:A:259:LEU:C	3:A:260:ILE:HD13	2.37	0.45
3:A:27:LYS:HB3	3:A:36:TYR:CD1	2.51	0.45
3:A:113:LYS:HG2	3:A:114:PHE:N	2.31	0.45
3:A:123:GLU:HG3	7:A:623:HOH:O	2.16	0.45
3:A:210:LEU:HB3	3:A:259:LEU:CD2	2.38	0.45
3:A:23:ALA:O	3:A:26:GLU:N	2.49	0.45
3:A:182:ARG:NH1	3:A:273:THR:CG2	2.79	0.45
3:A:214:VAL:CG2	3:A:215:VAL:N	2.79	0.44
2:P:6:DT:C6	2:P:6:DT:H5'	2.49	0.44
3:A:298:ILE:HG23	3:A:298:ILE:O	2.18	0.44
3:A:183:ARG:HB2	3:A:183:ARG:HE	1.49	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:121:THR:OG1	3:A:123:GLU:N	2.51	0.44
3:A:194:LEU:HD11	3:A:258:ARG:HD3	1.99	0.44
3:A:81:LYS:HZ2	3:A:86:GLU:HB3	1.81	0.43
3:A:179:GLY:O	3:A:182:ARG:HB3	2.18	0.43
3:A:183:ARG:HD3	3:A:273:THR:O	2.19	0.43
3:A:62:LEU:HA	3:A:62:LEU:HD12	1.52	0.43
3:A:150:ILE:N	3:A:188:SER:O	2.43	0.43
3:A:251:PRO:HG2	3:A:253:ARG:NH2	2.33	0.43
3:A:264:GLN:HE21	3:A:264:GLN:HB3	1.42	0.43
3:A:46:ILE:HG13	3:A:47:ALA:N	2.30	0.43
2:P:7:DG:C8	2:P:7:DG:H5'	2.54	0.43
3:A:218:LEU:CB	3:A:224:ILE:HD12	2.48	0.43
3:A:285:HIS:CD2	3:A:323:ILE:HD12	2.53	0.43
3:A:182:ARG:HH11	3:A:273:THR:CG2	2.31	0.43
3:A:18:MET:HE3	3:A:76:PHE:CG	2.54	0.43
3:A:114:PHE:HB3	3:A:119:ILE:HB	1.99	0.42
3:A:11:LEU:N	3:A:11:LEU:CD2	2.78	0.42
3:A:159:GLN:O	3:A:163:LEU:HG	2.19	0.42
3:A:287:LEU:HA	3:A:287:LEU:HD13	1.38	0.42
3:A:213:GLN:HB2	3:A:213:GLN:HE21	1.47	0.42
3:A:243:SER:HB3	3:A:249:GLU:CA	2.37	0.42
3:A:258:ARG:NH1	7:A:658:HOH:O	2.33	0.42
2:P:2:DC:H2'	2:P:2:DC:O5'	2.19	0.42
3:A:182:ARG:HH11	3:A:273:THR:HG21	1.84	0.42
3:A:316:GLU:CD	3:A:333:ARG:HH22	2.21	0.42
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.54	0.42
3:A:60:LYS:HE3	3:A:67:THR:N	2.34	0.42
3:A:165:GLU:O	3:A:169:VAL:HG12	2.20	0.42
3:A:152:ARG:HH11	3:A:152:ARG:HD3	1.65	0.41
3:A:183:ARG:HH11	3:A:275:SER:HA	1.85	0.41
2:P:2:DC:H2'	2:P:2:DC:H6	1.69	0.41
3:A:223:PHE:O	3:A:239:CYS:HA	2.20	0.41
3:A:81:LYS:HZ3	3:A:86:GLU:HB3	1.82	0.41
3:A:260:ILE:HD12	3:A:260:ILE:HG23	1.63	0.41
3:A:260:ILE:HG22	3:A:261:PRO:N	2.35	0.41
3:A:11:LEU:O	3:A:12:ASN:ND2	2.54	0.41
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.64	0.41
3:A:308:GLY:O	3:A:309:GLU:HB2	2.20	0.41
3:A:41:LYS:HE2	3:A:64:GLY:HA2	2.01	0.41
3:A:211:LEU:O	3:A:211:LEU:HD12	2.21	0.41
3:A:253:ARG:HH11	3:A:253:ARG:CG	2.31	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:266:TYR:HA	3:A:269:VAL:HB	2.02	0.41
3:A:26:GLU:HB2	3:A:36:TYR:HB2	2.02	0.41
3:A:291:PHE:HB3	3:A:292:THR:H	1.48	0.41
3:A:322:TYR:C	3:A:324:GLN:H	2.24	0.41
3:A:200:PHE:CE2	3:A:261:PRO:N	2.89	0.41
3:A:286:ALA:CA	3:A:323:ILE:HG21	2.51	0.41
3:A:34:HIS:O	3:A:37:ASN:N	2.54	0.41
3:A:88:ILE:HG22	3:A:89:ARG:N	2.36	0.41
3:A:200:PHE:CE2	3:A:261:PRO:HD3	2.56	0.41
3:A:178:CYS:SG	3:A:194:LEU:CD2	3.08	0.40
3:A:27:LYS:HD2	3:A:28:ASN:ND2	2.37	0.40
3:A:277:ILE:CG1	3:A:335:GLU:CB	3.00	0.40
3:A:136:GLN:HB2	3:A:136:GLN:HE21	1.57	0.40
3:A:209:LYS:HA	3:A:209:LYS:HD3	1.94	0.40
3:A:259:LEU:HA	3:A:259:LEU:HD12	1.88	0.40
3:A:279:ASN:HD22	3:A:279:ASN:HA	1.50	0.40
3:A:79:THR:H	3:A:79:THR:HG23	1.32	0.40
3:A:174:ILE:HG21	3:A:174:ILE:HD13	1.73	0.40
3:A:301:LEU:HD12	3:A:301:LEU:HA	1.58	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	325/335 (97%)	265 (82%)	43 (13%)	17 (5%)	<b>2</b> <b>3</b>

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	185	ALA
3	A	204	SER

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
3	A	205	THR
3	A	206	LYS
3	A	244	LYS
3	A	246	ASP
3	A	289	LYS
3	A	10	THR
3	A	309	GLU
3	A	310	PRO
3	A	202	SER
3	A	247	GLU
3	A	265	TYR
3	A	304	THR
3	A	78	ALA
3	A	80	GLY
3	A	207	GLN

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	288/295 (98%)	228 (79%)	60 (21%)	<b>1</b> <b>3</b>

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	THR
3	A	18	MET
3	A	19	LEU
3	A	21	GLU
3	A	22	LEU
3	A	27	LYS
3	A	33	ILE
3	A	37	ASN
3	A	40	ARG
3	A	41	LYS
3	A	44	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	A	46	ILE
3	A	54	LYS
3	A	62	LEU
3	A	65	VAL
3	A	67	THR
3	A	77	LEU
3	A	79	THR
3	A	81	LYS
3	A	89	ARG
3	A	92	ASP
3	A	94	SER
3	A	100	LEU
3	A	101	THR
3	A	121	THR
3	A	122	LEU
3	A	138	ILE
3	A	153	GLU
3	A	169	VAL
3	A	182	ARG
3	A	188	SER
3	A	191	MET
3	A	194	LEU
3	A	201	THR
3	A	226	ASP
3	A	228	LEU
3	A	230	LYS
3	A	233	THR
3	A	236	MET
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	262	LYS
3	A	264	GLN
3	A	277	ILE
3	A	287	LEU
3	A	288	GLU
3	A	294	ASN
3	A	295	GLU
3	A	301	LEU
3	A	303	VAL
3	A	304	THR
3	A	309	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	A	311	LEU
3	A	314	ASP
3	A	325	TRP
3	A	327	TYR
3	A	328	ARG
3	A	331	LYS
3	A	335	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	28	ASN
3	A	31	GLN
3	A	133	ASN
3	A	136	GLN
3	A	157	GLN
3	A	213	GLN
3	A	217	GLN
3	A	245	ASN
3	A	264	GLN
3	A	279	ASN
3	A	294	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	AZT	A	338	4	23,31,32	1.47	3 (13%)	30,48,49	3.73	9 (30%)

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	AZT	A	338	4	-	10/19/36/37	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	338	AZT	O4-C4	4.66	1.36	1.24
6	A	338	AZT	C3'-N3'	-3.53	1.38	1.48
6	A	338	AZT	C4-N3	2.10	1.36	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	338	AZT	C3'-N3'-N4'	16.24	174.19	115.99
6	A	338	AZT	C6-N1-C1'	-7.78	101.77	119.24
6	A	338	AZT	C4-N3-C2	7.01	121.06	115.14
6	A	338	AZT	C4'-C3'-N3'	2.69	119.04	111.64
6	A	338	AZT	C5-C6-N1	-2.56	119.44	122.19
6	A	338	AZT	C5A-C5-C4	-2.43	117.02	121.37
6	A	338	AZT	C5A-C5-C6	2.36	123.66	118.68
6	A	338	AZT	O3G-PG-O3B	-2.19	97.27	104.64
6	A	338	AZT	O2G-PG-O1G	2.10	118.92	110.68

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	338	AZT	C5'-O5'-PA-O1A
6	A	338	AZT	C5'-O5'-PA-O2A
6	A	338	AZT	O4'-C1'-N1-C6
6	A	338	AZT	C3'-C4'-C5'-O5'
6	A	338	AZT	O4'-C4'-C5'-O5'
6	A	338	AZT	PB-O3B-PG-O1G
6	A	338	AZT	PB-O3B-PG-O2G
6	A	338	AZT	PB-O3B-PG-O3G
6	A	338	AZT	C5'-O5'-PA-O3A
6	A	338	AZT	PA-O3A-PB-O2B

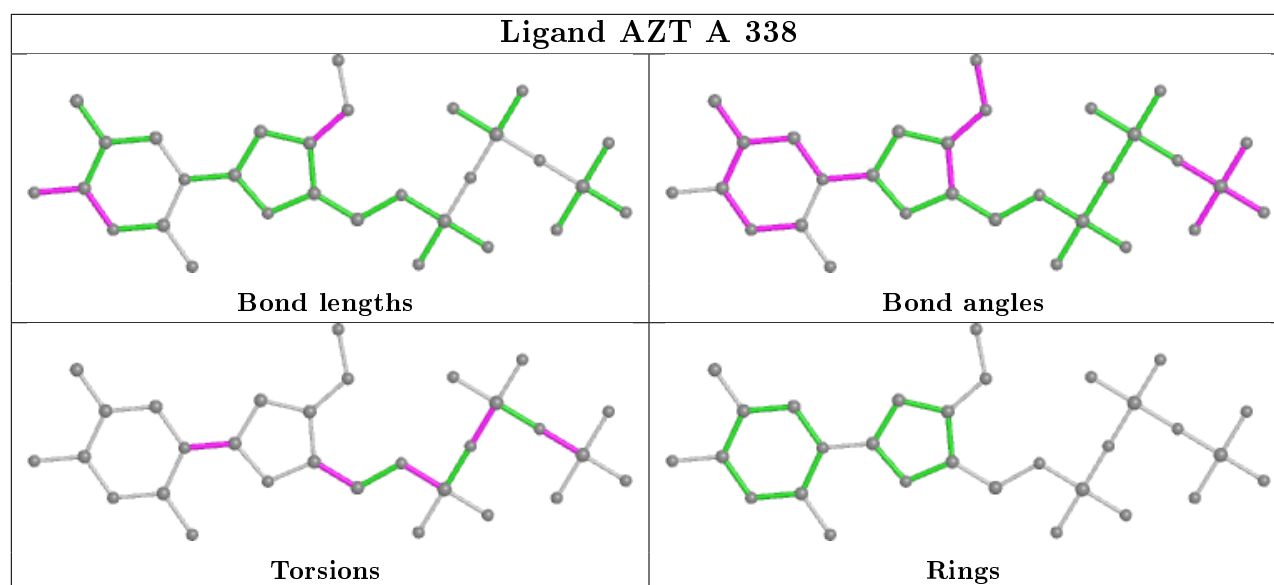
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	338	AZT	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	T	8/8 (100%)	-0.75	0 100 100	21, 46, 100, 100	0
2	P	7/7 (100%)	-1.42	0 100 100	20, 34, 44, 54	0
3	A	324/335 (96%)	-1.12	0 100 100	7, 36, 85, 100	0
All	All	339/350 (96%)	-1.12	0 100 100	7, 36, 87, 100	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

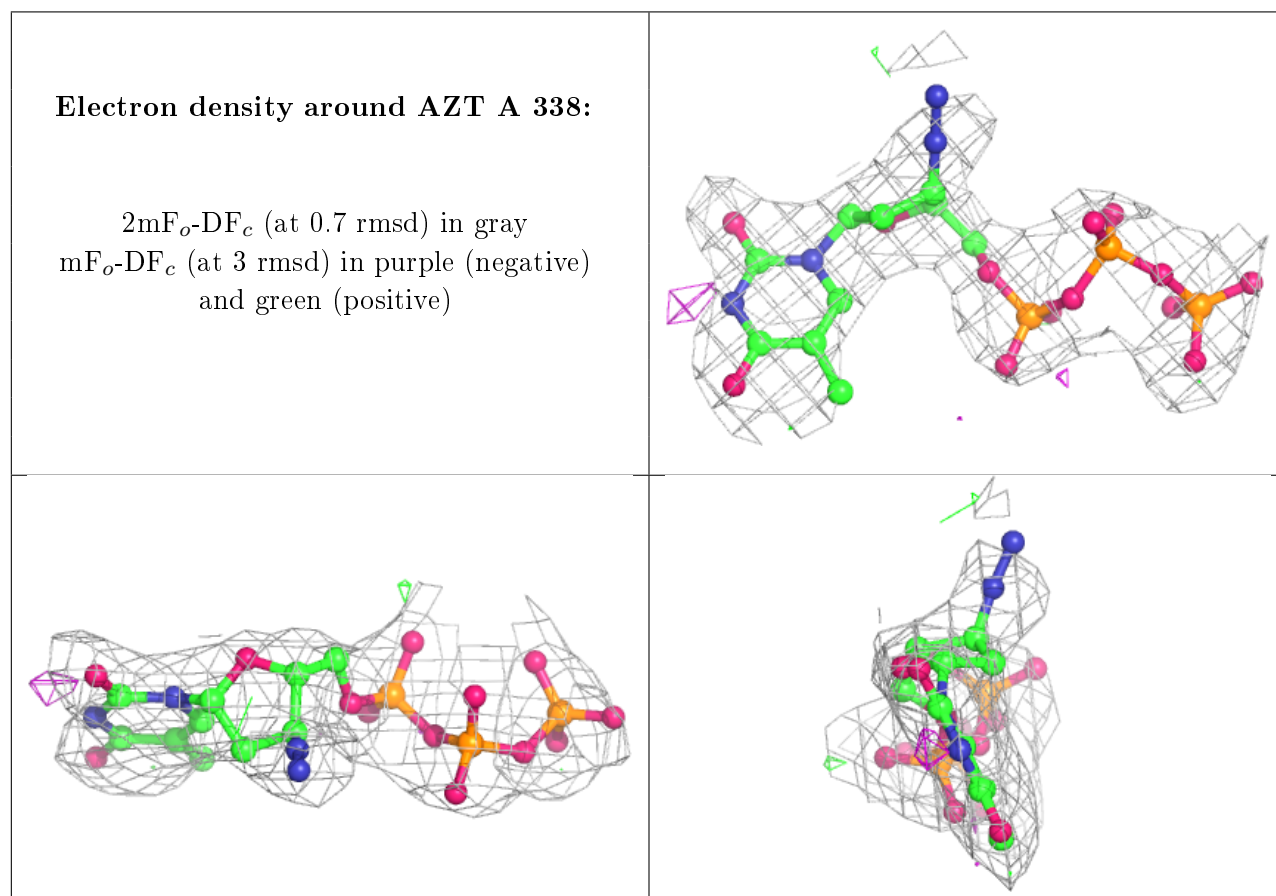
There are no carbohydrates in this entry.

### 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	NA	A	342	1/1	0.90	0.17	65,65,65,65	0
4	MN	A	340	1/1	0.90	0.20	30,30,30,30	1
6	AZT	A	338	30/31	0.94	0.14	59,70,96,100	0
5	NA	A	341	1/1	0.98	0.06	23,23,23,23	0
4	MN	A	339	1/1	0.98	0.07	30,30,30,30	1

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.