



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:48 am BST

PDB ID : 9ICT  
Title : DNA POLYMERASE BETA (E.C.2.7.7.7)/DNA COMPLEX + 2'-DEOXY GUANOSINE-5'-TRIPHOSPHATE, SOAKED IN THE PRESENCE OF DGTP AND MNCL2  
Authors : Pelletier, H.; Sawaya, M.R.  
Deposited on : 1995-12-16  
Resolution : 3.00 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

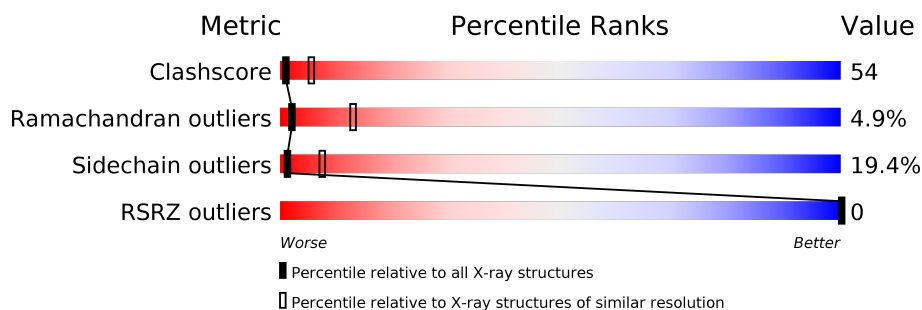
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	7	
2	P	6	
3	A	335	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3032 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\*CP\*TP\*GP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	7	Total	C	N	O	P	0	0	0
			122	58	20	38	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	6	Total	C	N	O	P	0	0	0
			126	59	25	36	6			

- 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			

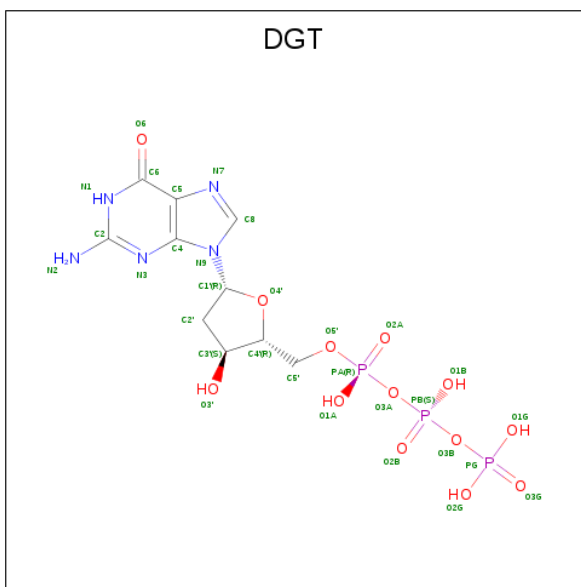
- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (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	O	P	0	0
			13	10	3		

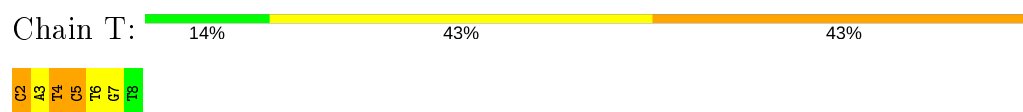
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	T	11	Total O 11 11	0	0
7	P	23	Total O 23 23	0	0
7	A	110	Total O 110 110	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.

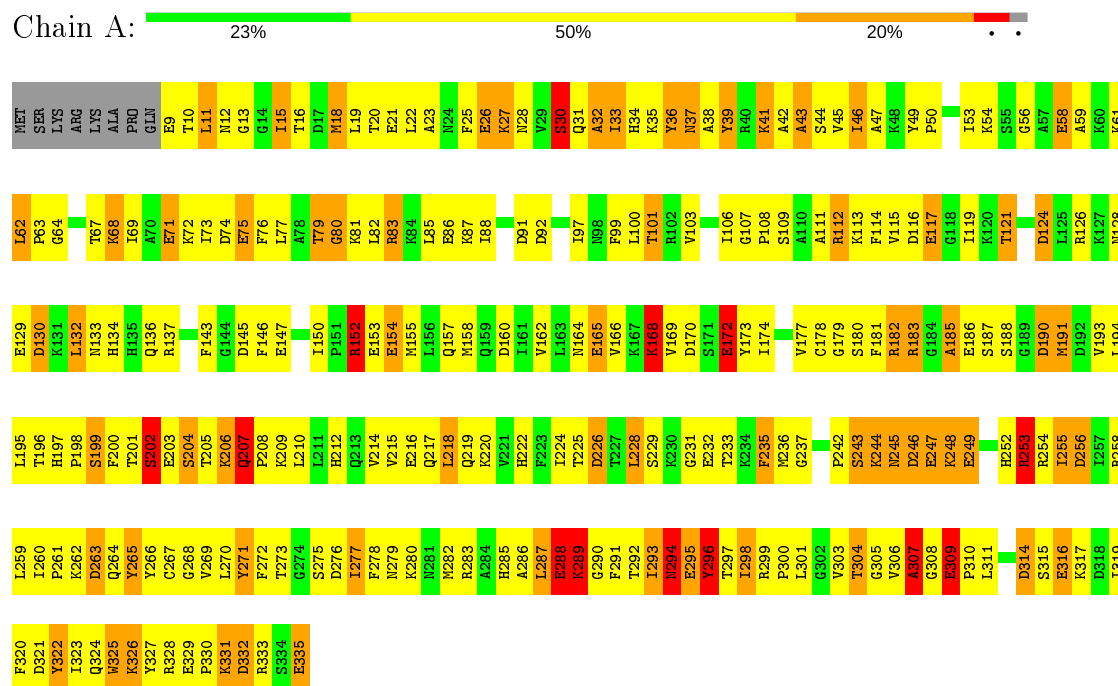
- Molecule 1: DNA (5'-D(\*CP\*AP\*TP\*CP\*TP\*GP\*T)-3')



- Molecule 2: DNA (5'-D(\*CP\*AP\*GP\*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 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.54Å 57.72Å 48.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 15.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-3.00) 90.4 (15.80-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	4.30	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.82Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, $R_{free}$	0.157 , (Not available) 0.151 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.2	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 170.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3032	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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, DGT

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	2.13	5/135 (3.7%)	3.03	14/207 (6.8%)
2	P	2.47	5/141 (3.5%)	3.19	19/214 (8.9%)
3	A	1.29	26/2672 (1.0%)	1.73	52/3590 (1.4%)
All	All	1.42	36/2948 (1.2%)	1.92	85/4011 (2.1%)

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 (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	5	DT	N1-C2	13.96	1.49	1.38
2	P	5	DT	C1'-N1	10.68	1.63	1.49
2	P	5	DT	C3'-O3'	-7.60	1.34	1.44
3	A	203	GLU	CD-OE1	7.57	1.33	1.25
3	A	249	GLU	CD-OE2	7.00	1.33	1.25
3	A	129	GLU	CD-OE1	7.00	1.33	1.25
3	A	117	GLU	CD-OE2	6.89	1.33	1.25
2	P	5	DT	C4-C5	6.75	1.51	1.45
1	T	6	DT	C3'-O3'	-6.59	1.35	1.44
3	A	86	GLU	CD-OE1	6.59	1.32	1.25
3	A	71	GLU	CD-OE1	6.54	1.32	1.25
3	A	75	GLU	CD-OE1	6.48	1.32	1.25
3	A	309	GLU	CD-OE2	6.45	1.32	1.25
3	A	329	GLU	CD-OE2	6.40	1.32	1.25
3	A	271	TYR	CB-CG	-6.14	1.42	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	5	DC	C2-N3	6.08	1.40	1.35
3	A	21	GLU	CD-OE1	6.06	1.32	1.25
3	A	186	GLU	CD-OE1	5.96	1.32	1.25
3	A	295	GLU	CD-OE1	5.92	1.32	1.25
3	A	165	GLU	CD-OE2	5.88	1.32	1.25
3	A	26	GLU	CD-OE1	5.82	1.32	1.25
3	A	153	GLU	CD-OE2	5.74	1.31	1.25
3	A	288	GLU	CD-OE2	5.71	1.31	1.25
3	A	58	GLU	CD-OE1	5.68	1.31	1.25
3	A	335	GLU	CD-OE2	5.58	1.31	1.25
1	T	7	DG	N9-C4	-5.46	1.33	1.38
3	A	147	GLU	CD-OE2	5.34	1.31	1.25
3	A	316	GLU	CD-OE1	5.32	1.31	1.25
3	A	232	GLU	CD-OE2	5.30	1.31	1.25
3	A	9	GLU	CD-OE2	5.25	1.31	1.25
1	T	5	DC	C4-N4	5.24	1.38	1.33
3	A	247	GLU	CD-OE1	5.24	1.31	1.25
3	A	154	GLU	CD-OE2	5.14	1.31	1.25
3	A	172	GLU	CD-OE2	5.10	1.31	1.25
1	T	4	DT	N1-C2	5.05	1.42	1.38
2	P	3	DG	C5-C6	-5.03	1.37	1.42

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	5	DC	C2-N1-C1'	13.52	133.67	118.80
2	P	5	DT	C2-N1-C1'	13.18	139.29	118.20
2	P	5	DT	C6-N1-C1'	-13.16	100.66	120.40
1	T	6	DT	C6-N1-C1'	-12.56	101.57	120.40
2	P	6	DG	C8-N9-C1'	11.99	142.59	127.00
1	T	5	DC	C6-N1-C1'	-11.95	106.46	120.80
2	P	6	DG	C4-N9-C1'	-11.80	111.16	126.50
1	T	4	DT	C6-N1-C1'	-11.14	103.68	120.40
2	P	5	DT	N3-C2-O2	-10.74	115.86	122.30
1	T	4	DT	C2-N1-C1'	10.46	134.94	118.20
1	T	6	DT	C2-N1-C1'	10.11	134.37	118.20
2	P	2	DA	O4'-C4'-C3'	-9.31	100.41	106.00
2	P	3	DG	C8-N9-C1'	8.89	138.56	127.00
2	P	4	DA	O4'-C1'-N9	-8.86	101.80	108.00
3	A	92	ASP	CB-CG-OD2	-8.40	110.74	118.30
2	P	2	DA	C4'-C3'-C2'	-8.38	95.56	103.10
1	T	5	DC	N3-C4-C5	-8.37	118.55	121.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	7	DG	C4-N9-C1'	-8.34	115.67	126.50
2	P	4	DA	P-O3'-C3'	8.30	129.66	119.70
3	A	256	ASP	CB-CG-OD1	8.25	125.72	118.30
3	A	263	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	T	2	DC	C2-N1-C1'	7.94	127.54	118.80
3	A	152	ARG	N-CA-CB	7.90	124.82	110.60
3	A	271	TYR	CA-CB-CG	-7.83	98.53	113.40
3	A	271	TYR	CB-CG-CD1	-7.82	116.31	121.00
2	P	5	DT	O4'-C1'-N1	7.73	113.41	108.00
3	A	256	ASP	CB-CG-OD2	-7.67	111.40	118.30
3	A	116	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	T	2	DC	C6-N1-C1'	-7.51	111.78	120.80
1	T	7	DG	C8-N9-C1'	7.34	136.55	127.00
2	P	1	DC	C2-N1-C1'	7.23	126.75	118.80
3	A	263	ASP	CB-CG-OD1	7.21	124.79	118.30
2	P	3	DG	C4-N9-C1'	-7.20	117.14	126.50
3	A	199	SER	N-CA-CB	-7.06	99.92	110.50
3	A	74	ASP	CB-CG-OD1	6.92	124.53	118.30
3	A	126	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	T	5	DC	P-O3'-C3'	6.87	127.94	119.70
3	A	183	ARG	NE-CZ-NH1	6.83	123.72	120.30
3	A	124	ASP	CB-CG-OD1	6.82	124.44	118.30
3	A	265	TYR	CB-CG-CD2	6.82	125.09	121.00
2	P	1	DC	C6-N1-C1'	-6.73	112.72	120.80
3	A	190	ASP	CB-CG-OD1	6.73	124.35	118.30
3	A	39	TYR	CB-CG-CD1	-6.64	117.02	121.00
3	A	124	ASP	CB-CG-OD2	-6.50	112.45	118.30
3	A	170	ASP	CB-CG-OD2	-6.50	112.45	118.30
3	A	130	ASP	CB-CG-OD2	-6.48	112.47	118.30
3	A	74	ASP	CB-CG-OD2	-6.40	112.54	118.30
3	A	332	ASP	CB-CG-OD1	-6.37	112.56	118.30
3	A	190	ASP	CB-CG-OD2	-6.36	112.58	118.30
3	A	328	ARG	NE-CZ-NH2	-6.21	117.19	120.30
3	A	226	ASP	CB-CG-OD1	6.18	123.87	118.30
3	A	34	HIS	CA-CB-CG	-6.05	103.31	113.60
3	A	314	ASP	CB-CG-OD1	-6.04	112.86	118.30
2	P	3	DG	P-O3'-C3'	5.97	126.86	119.70
3	A	126	ARG	NE-CZ-NH1	5.92	123.26	120.30
3	A	326	LYS	CD-CE-NZ	5.91	125.30	111.70
3	A	332	ASP	CB-CG-OD2	5.90	123.61	118.30
3	A	92	ASP	CB-CG-OD1	5.75	123.47	118.30
3	A	83	ARG	NE-CZ-NH1	5.73	123.16	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	253	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	T	6	DT	C1'-O4'-C4'	-5.63	104.47	110.10
3	A	43	ALA	CB-CA-C	5.53	118.40	110.10
3	A	168	LYS	N-CA-CB	5.53	120.55	110.60
3	A	322	TYR	CB-CG-CD1	-5.50	117.70	121.00
3	A	265	TYR	CB-CG-CD1	-5.42	117.75	121.00
2	P	1	DC	P-O3'-C3'	5.36	126.13	119.70
3	A	307	ALA	CB-CA-C	5.34	118.12	110.10
3	A	296	TYR	CB-CA-C	-5.32	99.75	110.40
1	T	6	DT	C6-N1-C2	5.32	123.96	121.30
3	A	87	LYS	CB-CA-C	5.28	120.96	110.40
3	A	307	ALA	N-CA-CB	5.26	117.47	110.10
2	P	5	DT	N3-C4-O4	-5.26	116.74	119.90
2	P	3	DG	C8-N9-C4	-5.25	104.30	106.40
2	P	5	DT	C5-C6-N1	-5.25	120.55	123.70
3	A	91	ASP	CB-CG-OD1	-5.23	113.59	118.30
3	A	222	HIS	CB-CA-C	-5.18	100.03	110.40
3	A	294	ASN	N-CA-CB	5.17	119.90	110.60
3	A	30	SER	N-CA-C	-5.14	97.13	111.00
3	A	225	THR	CA-CB-CG2	-5.10	105.26	112.40
3	A	246	ASP	CB-CG-OD1	-5.09	113.72	118.30
3	A	243	SER	CB-CA-C	5.08	119.75	110.10
3	A	99	PHE	CA-CB-CG	-5.05	101.77	113.90
3	A	229	SER	N-CA-CB	5.05	118.08	110.50
3	A	229	SER	CB-CA-C	5.05	119.69	110.10
3	A	116	ASP	CB-CG-OD1	5.03	122.82	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	152	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	122	0	69	7	0
2	P	126	0	68	10	0
3	A	2623	0	2641	293	1
4	A	2	0	0	0	0
5	A	2	0	0	0	0
6	A	13	0	0	0	0
7	A	110	0	0	12	0
7	P	23	0	0	3	0
7	T	11	0	0	2	0
All	All	3032	0	2778	304	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 54.

All (304) 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:31:GLN:NE2	3:A:112:ARG:HH12	1.45	1.13
2:P:1:DC:H2''	2:P:2:DA:H5''	1.33	1.05
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.43	0.97
3:A:23:ALA:HB2	3:A:39:TYR:HB2	1.44	0.97
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.01	0.96
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.49	0.94
3:A:31:GLN:HE21	3:A:112:ARG:HH12	0.94	0.94
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.67	0.92
3:A:178:CYS:SG	3:A:194:LEU:HD23	2.10	0.91
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.54	0.90
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.57	0.86
3:A:11:LEU:HD23	3:A:11:LEU:H	1.39	0.86
3:A:277:ILE:HG13	3:A:335:GLU:HB3	1.57	0.85
3:A:41:LYS:HE2	3:A:64:GLY:HA2	1.59	0.84
3:A:27:LYS:HG3	3:A:28:ASN:N	1.94	0.82
3:A:182:ARG:HG2	3:A:273:THR:HG23	1.60	0.82
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.10	0.82
3:A:197:HIS:ND1	3:A:199:SER:HB3	1.94	0.82
3:A:172:GLU:HG2	3:A:198:PRO:HG2	1.61	0.81
3:A:277:ILE:HG13	3:A:335:GLU:CB	2.11	0.81
3:A:182:ARG:HG2	3:A:273:THR:CG2	2.10	0.80
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.48	0.79
2:P:1:DC:C2'	2:P:2:DA:H5''	2.12	0.79
3:A:68:LYS:O	3:A:72:LYS:HE3	1.82	0.78
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.66	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.14	0.78
3:A:278:PHE:HB2	3:A:333:ARG:O	1.83	0.78
3:A:150:ILE:HG21	3:A:158:MET:CE	2.15	0.77
3:A:212:HIS:HB3	7:A:541:HOH:O	1.85	0.76
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.68	0.76
3:A:260:ILE:HG22	3:A:261:PRO:HD2	1.68	0.76
3:A:286:ALA:HA	3:A:323:ILE:HG21	1.67	0.76
3:A:32:ALA:HB1	3:A:35:LYS:HB2	1.66	0.75
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.69	0.75
3:A:155:MET:CE	3:A:188:SER:HB2	2.16	0.75
3:A:300:PRO:HD3	3:A:311:LEU:HD13	1.69	0.74
3:A:12:ASN:HB3	3:A:46:ILE:CD1	2.17	0.74
3:A:201:THR:HA	3:A:261:PRO:CB	2.17	0.74
3:A:271:TYR:HB2	7:A:592:HOH:O	1.88	0.74
3:A:68:LYS:HB2	3:A:68:LYS:NZ	2.02	0.73
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.18	0.73
3:A:62:LEU:HD12	3:A:63:PRO:HD2	1.71	0.72
3:A:41:LYS:HD3	3:A:42:ALA:N	2.04	0.71
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.20	0.71
3:A:330:PRO:CA	3:A:333:ARG:HG3	2.21	0.71
3:A:18:MET:CE	3:A:76:PHE:HB2	2.21	0.71
3:A:111:ALA:O	3:A:115:VAL:HG23	1.92	0.70
3:A:59:ALA:O	3:A:62:LEU:HB2	1.91	0.70
3:A:294:ASN:HB2	3:A:295:GLU:OE2	1.90	0.70
3:A:27:LYS:HB3	3:A:36:TYR:CD2	2.27	0.70
3:A:155:MET:HA	3:A:158:MET:HE3	1.74	0.69
3:A:31:GLN:N	7:A:641:HOH:O	2.25	0.69
3:A:12:ASN:HB3	3:A:46:ILE:HD11	1.74	0.69
3:A:113:LYS:O	3:A:117:GLU:HG3	1.93	0.69
3:A:133:ASN:O	3:A:137:ARG:HG3	1.92	0.69
3:A:23:ALA:CB	3:A:39:TYR:HB2	2.20	0.68
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.29	0.68
3:A:255:ILE:HG12	3:A:256:ASP:N	2.09	0.68
3:A:201:THR:HG23	3:A:204:SER:HB3	1.76	0.67
3:A:27:LYS:HB3	3:A:36:TYR:CG	2.30	0.67
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.28	0.67
1:T:3:DA:H2"	7:T:573:HOH:O	1.95	0.67
3:A:154:GLU:O	3:A:158:MET:HG3	1.94	0.66
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.24	0.66
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.23	0.66
3:A:278:PHE:CE2	3:A:333:ARG:HD3	2.31	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:319:ILE:O	3:A:322:TYR:HB2	1.95	0.66
2:P:3:DG:H1'	7:P:511:HOH:O	1.96	0.66
3:A:215:VAL:O	3:A:219:GLN:HG3	1.95	0.66
3:A:41:LYS:HD3	3:A:42:ALA:H	1.60	0.66
3:A:15:ILE:HG21	3:A:46:ILE:HD13	1.78	0.65
3:A:80:GLY:O	3:A:81:LYS:HG2	1.96	0.65
3:A:293:ILE:HD13	3:A:298:ILE:CG1	2.26	0.65
2:P:2:DA:N7	7:P:598:HOH:O	2.30	0.65
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.45	0.65
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.30	0.65
3:A:162:VAL:O	3:A:166:VAL:HG23	1.97	0.65
3:A:33:ILE:O	3:A:37:ASN:HB2	1.97	0.64
2:P:2:DA:C8	2:P:2:DA:H5'	2.32	0.64
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.33	0.64
3:A:253:ARG:HH11	3:A:253:ARG:CG	2.11	0.63
3:A:41:LYS:O	3:A:45:VAL:HG13	1.99	0.63
3:A:268:GLY:O	3:A:271:TYR:HB3	1.98	0.63
3:A:11:LEU:CD2	3:A:11:LEU:H	2.09	0.63
3:A:155:MET:HE2	3:A:188:SER:HB2	1.80	0.63
3:A:296:TYR:HB2	3:A:297:THR:HG23	1.82	0.62
3:A:306:VAL:HG23	3:A:307:ALA:N	2.14	0.62
3:A:308:GLY:O	3:A:309:GLU:HB2	1.99	0.62
3:A:261:PRO:HG2	3:A:264:GLN:HG3	1.82	0.62
3:A:197:HIS:ND1	3:A:198:PRO:HD2	2.15	0.62
3:A:242:PRO:HG2	7:A:589:HOH:O	1.98	0.62
3:A:166:VAL:O	3:A:169:VAL:HG12	2.00	0.62
3:A:79:THR:O	3:A:81:LYS:N	2.31	0.62
3:A:259:LEU:O	3:A:260:ILE:HD13	2.00	0.61
3:A:245:ASN:N	3:A:245:ASN:HD22	1.99	0.61
3:A:286:ALA:O	3:A:291:PHE:HB2	2.00	0.60
3:A:12:ASN:HD21	3:A:53:ILE:H	1.49	0.60
3:A:172:GLU:HG2	3:A:198:PRO:CG	2.32	0.60
3:A:200:PHE:HB2	3:A:210:LEU:CD1	2.31	0.60
3:A:285:HIS:CE1	3:A:289:LYS:HE3	2.37	0.60
3:A:309:GLU:OE1	3:A:309:GLU:HA	2.00	0.60
3:A:327:TYR:HE1	3:A:333:ARG:NH2	2.00	0.59
3:A:326:LYS:O	3:A:326:LYS:HG3	2.00	0.59
3:A:288:GLU:O	3:A:290:GLY:N	2.34	0.59
3:A:103:VAL:HG22	3:A:143:PHE:CD2	2.37	0.59
3:A:286:ALA:HA	3:A:323:ILE:CG2	2.33	0.59
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.30	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:182:ARG:NH1	3:A:182:ARG:HG2	2.15	0.59
1:T:4:DT:H2"	1:T:5:DC:O5'	2.03	0.59
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.85	0.59
3:A:157:GLN:HE22	3:A:244:LYS:NZ	2.02	0.58
3:A:35:LYS:O	3:A:38:ALA:HB3	2.02	0.58
3:A:18:MET:HE3	3:A:76:PHE:CD1	2.38	0.58
3:A:330:PRO:O	3:A:333:ARG:HG3	2.03	0.58
3:A:121:THR:O	3:A:124:ASP:HB2	2.04	0.58
3:A:248:LYS:HG2	3:A:248:LYS:O	2.04	0.57
3:A:69:ILE:O	3:A:73:ILE:HG13	2.03	0.57
3:A:56:GLY:O	3:A:59:ALA:N	2.37	0.57
3:A:23:ALA:O	3:A:36:TYR:HD2	1.87	0.57
3:A:330:PRO:HA	3:A:333:ARG:CG	2.25	0.57
3:A:201:THR:HA	3:A:261:PRO:HB3	1.84	0.57
3:A:108:PRO:O	3:A:112:ARG:HG2	2.05	0.56
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.69	0.56
3:A:106:ILE:HG22	3:A:107:GLY:O	2.04	0.56
3:A:106:ILE:HG13	3:A:136:GLN:HG2	1.87	0.56
3:A:68:LYS:HB2	3:A:68:LYS:HZ1	1.70	0.56
3:A:97:ILE:O	3:A:101:THR:HB	2.05	0.56
3:A:75:GLU:O	3:A:79:THR:HG23	2.06	0.55
3:A:157:GLN:O	3:A:160:ASP:HB3	2.06	0.55
3:A:15:ILE:HD11	3:A:77:LEU:CD1	2.36	0.55
3:A:243:SER:CB	3:A:249:GLU:HA	2.37	0.55
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.88	0.55
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.89	0.54
3:A:124:ASP:O	3:A:128:ASN:ND2	2.38	0.54
3:A:41:LYS:NZ	3:A:64:GLY:O	2.31	0.54
3:A:79:THR:C	3:A:81:LYS:H	2.10	0.54
3:A:15:ILE:HG21	3:A:46:ILE:CD1	2.38	0.54
3:A:288:GLU:HA	3:A:288:GLU:OE1	1.89	0.54
3:A:325:TRP:HD1	7:A:583:HOH:O	1.90	0.53
3:A:174:ILE:HB	3:A:196:THR:HG22	1.89	0.53
3:A:155:MET:O	3:A:158:MET:HB2	2.08	0.53
3:A:182:ARG:HG2	3:A:273:THR:HG21	1.89	0.53
3:A:253:ARG:HG3	3:A:253:ARG:HH11	1.72	0.53
3:A:243:SER:OG	3:A:249:GLU:HA	2.08	0.53
3:A:191:MET:HG2	3:A:255:ILE:HG13	1.90	0.53
3:A:197:HIS:CE1	3:A:199:SER:HB3	2.44	0.53
3:A:182:ARG:CG	3:A:273:THR:HG23	2.38	0.52
3:A:166:VAL:HG12	3:A:173:TYR:CB	2.39	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:254:ARG:NH1	3:A:255:ILE:N	2.57	0.52
3:A:286:ALA:HB1	3:A:293:ILE:CD1	2.31	0.52
3:A:152:ARG:O	3:A:155:MET:HB2	2.10	0.52
3:A:262:LYS:HG3	3:A:262:LYS:O	2.10	0.52
3:A:316:GLU:O	3:A:320:PHE:HD2	1.93	0.52
3:A:330:PRO:C	3:A:333:ARG:HG3	2.30	0.52
3:A:182:ARG:HH11	3:A:273:THR:CG2	2.23	0.52
3:A:297:THR:HG22	7:A:626:HOH:O	2.08	0.51
3:A:164:ASN:O	3:A:168:LYS:HG2	2.10	0.51
3:A:243:SER:HB3	3:A:249:GLU:HA	1.93	0.51
3:A:254:ARG:HH11	3:A:255:ILE:N	2.09	0.51
3:A:15:ILE:HG22	3:A:16:THR:N	2.22	0.51
3:A:133:ASN:H	3:A:136:GLN:NE2	2.09	0.50
3:A:254:ARG:NH1	3:A:255:ILE:H	2.09	0.50
3:A:288:GLU:C	3:A:290:GLY:H	2.15	0.50
3:A:30:SER:HB3	7:A:561:HOH:O	2.10	0.50
3:A:132:LEU:HD23	3:A:132:LEU:N	2.26	0.50
3:A:157:GLN:HE22	3:A:244:LYS:HZ1	1.58	0.50
3:A:259:LEU:HD12	3:A:260:ILE:H	1.76	0.50
3:A:195:LEU:O	3:A:260:ILE:N	2.44	0.50
3:A:254:ARG:HH11	3:A:255:ILE:H	1.58	0.50
3:A:132:LEU:HB3	3:A:136:GLN:HB3	1.94	0.50
3:A:289:LYS:HD2	3:A:324:GLN:OE1	2.12	0.50
2:P:5:DT:P	3:A:109:SER:HB3	2.52	0.49
3:A:150:ILE:HG21	3:A:158:MET:HE2	1.91	0.49
3:A:201:THR:HA	3:A:261:PRO:HB2	1.93	0.49
3:A:56:GLY:O	3:A:59:ALA:HB3	2.12	0.49
2:P:5:DT:H1'	7:P:565:HOH:O	2.11	0.49
3:A:292:THR:HG21	3:A:299:ARG:HH21	1.78	0.49
3:A:265:TYR:O	3:A:269:VAL:HG23	2.13	0.49
3:A:321:ASP:O	3:A:324:GLN:N	2.44	0.49
3:A:43:ALA:O	3:A:47:ALA:HB2	2.13	0.49
3:A:177:VAL:HG22	3:A:193:VAL:HG22	1.95	0.49
3:A:208:PRO:O	3:A:212:HIS:HD2	1.96	0.49
3:A:31:GLN:O	3:A:33:ILE:N	2.46	0.49
3:A:58:GLU:O	3:A:61:LYS:HB2	2.12	0.49
3:A:68:LYS:O	3:A:71:GLU:HB3	2.13	0.49
3:A:196:THR:HG23	3:A:197:HIS:N	2.27	0.48
3:A:295:GLU:H	3:A:295:GLU:CD	2.16	0.48
3:A:205:THR:O	3:A:205:THR:HG23	2.13	0.48
3:A:103:VAL:HG22	3:A:143:PHE:HD2	1.78	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:207:GLN:O	3:A:210:LEU:HB2	2.13	0.48
3:A:16:THR:O	3:A:20:THR:HG23	2.14	0.48
3:A:266:TYR:HA	3:A:269:VAL:HB	1.94	0.48
3:A:289:LYS:HG3	3:A:323:ILE:O	2.13	0.48
3:A:32:ALA:O	3:A:36:TYR:HB3	2.14	0.48
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.28	0.48
3:A:279:ASN:O	3:A:283:ARG:HG3	2.13	0.48
3:A:237:GLY:O	3:A:254:ARG:NH1	2.47	0.48
3:A:145:ASP:CG	3:A:252:HIS:H	2.17	0.48
3:A:292:THR:O	3:A:298:ILE:HA	2.13	0.48
3:A:150:ILE:O	3:A:187:SER:HA	2.13	0.48
3:A:12:ASN:ND2	3:A:53:ILE:H	2.11	0.47
3:A:261:PRO:HG2	3:A:264:GLN:CG	2.44	0.47
3:A:114:PHE:HB3	3:A:119:ILE:HB	1.95	0.47
3:A:26:GLU:OE1	3:A:32:ALA:HB3	2.14	0.47
3:A:282:MET:HG2	7:A:555:HOH:O	2.14	0.47
3:A:298:ILE:HG23	3:A:311:LEU:HB2	1.97	0.47
3:A:315:SER:OG	3:A:316:GLU:N	2.48	0.47
3:A:267:CYS:O	3:A:271:TYR:HB2	2.14	0.47
3:A:287:LEU:HA	3:A:287:LEU:HD13	1.59	0.47
2:P:5:DT:H5"	3:A:107:GLY:N	2.30	0.46
3:A:216:GLU:O	3:A:220:LYS:N	2.43	0.46
3:A:303:VAL:C	3:A:305:GLY:H	2.18	0.46
2:P:2:DA:H5'	2:P:2:DA:H2'	1.57	0.46
3:A:103:VAL:HG22	3:A:143:PHE:CE2	2.51	0.46
3:A:72:LYS:HG2	3:A:82:LEU:HD11	1.97	0.46
3:A:155:MET:HE3	3:A:188:SER:HB2	1.96	0.46
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.50	0.46
3:A:279:ASN:O	3:A:283:ARG:N	2.46	0.46
3:A:11:LEU:N	3:A:11:LEU:CD2	2.78	0.46
3:A:206:LYS:O	3:A:207:GLN:HB2	2.16	0.46
3:A:26:GLU:OE1	3:A:26:GLU:HA	2.15	0.46
3:A:209:LYS:HA	3:A:209:LYS:HD3	1.47	0.45
3:A:49:TYR:CE2	3:A:53:ILE:HG12	2.51	0.45
3:A:287:LEU:HA	3:A:291:PHE:O	2.15	0.45
3:A:152:ARG:NH2	3:A:181:PHE:O	2.49	0.45
3:A:244:LYS:CB	3:A:245:ASN:HD22	2.29	0.45
3:A:218:LEU:HB2	3:A:224:ILE:HD12	1.98	0.45
3:A:157:GLN:NE2	3:A:244:LYS:NZ	2.65	0.45
3:A:217:GLN:HA	3:A:217:GLN:NE2	2.31	0.45
3:A:298:ILE:HG21	3:A:322:TYR:HD2	1.82	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:165:GLU:HB2	3:A:218:LEU:HD11	1.99	0.45
3:A:303:VAL:O	3:A:305:GLY:N	2.50	0.45
3:A:85:LEU:HA	3:A:85:LEU:HD12	1.82	0.45
3:A:201:THR:CG2	3:A:204:SER:HB3	2.45	0.45
3:A:292:THR:CG2	3:A:299:ARG:HH21	2.30	0.45
3:A:37:ASN:HA	3:A:37:ASN:HD22	1.63	0.45
3:A:200:PHE:O	3:A:262:LYS:N	2.46	0.44
3:A:36:TYR:CD1	3:A:37:ASN:N	2.85	0.44
3:A:236:MET:HG2	3:A:254:ARG:HH22	1.83	0.44
3:A:277:ILE:HG13	3:A:335:GLU:HB2	1.97	0.44
1:T:4:DT:H5''	3:A:231:GLY:HA3	1.98	0.44
3:A:23:ALA:HA	3:A:39:TYR:CD2	2.52	0.44
3:A:300:PRO:HG3	3:A:311:LEU:HD11	2.00	0.44
3:A:218:LEU:CB	3:A:224:ILE:HD12	2.47	0.44
3:A:228:LEU:HA	3:A:228:LEU:HD12	1.35	0.44
3:A:331:LYS:HD2	3:A:332:ASP:N	2.33	0.44
2:P:5:DT:P	3:A:107:GLY:HA3	2.57	0.44
3:A:179:GLY:O	3:A:182:ARG:HB3	2.17	0.44
3:A:182:ARG:NH2	3:A:316:GLU:OE2	2.43	0.44
3:A:150:ILE:O	3:A:188:SER:N	2.48	0.44
3:A:317:LYS:HG3	7:A:501:HOH:O	2.17	0.44
3:A:59:ALA:O	3:A:62:LEU:N	2.37	0.43
3:A:183:ARG:HG3	3:A:273:THR:HG22	2.01	0.43
3:A:44:SER:O	3:A:47:ALA:HB3	2.18	0.43
3:A:194:LEU:HA	3:A:194:LEU:HD13	1.61	0.43
3:A:299:ARG:HA	3:A:300:PRO:HD3	1.88	0.43
1:T:4:DT:H5'	7:T:617:HOH:O	2.18	0.43
3:A:197:HIS:CE1	3:A:198:PRO:HD2	2.53	0.43
3:A:273:THR:O	3:A:273:THR:HG22	2.18	0.43
3:A:146:PHE:HA	3:A:146:PHE:HD1	1.58	0.43
3:A:301:LEU:HD12	3:A:301:LEU:HA	1.71	0.43
3:A:270:LEU:HD12	7:A:584:HOH:O	2.17	0.43
3:A:275:SER:OG	3:A:277:ILE:HG12	2.18	0.43
3:A:133:ASN:HD22	3:A:134:HIS:N	2.16	0.43
3:A:202:SER:HB2	3:A:263:ASP:OD1	2.19	0.43
3:A:182:ARG:NH1	3:A:273:THR:CG2	2.82	0.43
3:A:294:ASN:HD22	3:A:294:ASN:C	2.22	0.43
3:A:88:ILE:HD13	3:A:88:ILE:HG21	1.71	0.43
3:A:18:MET:HE2	3:A:82:LEU:HD22	2.01	0.43
3:A:205:THR:O	3:A:206:LYS:O	2.36	0.43
3:A:272:PHE:HD1	7:A:587:HOH:O	2.02	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:267:CYS:SG	3:A:297:THR:HA	2.59	0.43
3:A:18:MET:HE3	3:A:76:PHE:CG	2.54	0.42
1:T:2:DC:H2'	1:T:2:DC:H6	1.50	0.42
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.70	0.42
3:A:26:GLU:HA	3:A:30:SER:OG	2.18	0.42
3:A:299:ARG:HB3	3:A:300:PRO:HD2	2.02	0.42
3:A:295:GLU:HG2	3:A:296:TYR:CE1	2.55	0.42
1:T:4:DT:P	3:A:231:GLY:HA3	2.59	0.42
3:A:254:ARG:HA	3:A:254:ARG:HD2	1.84	0.42
3:A:260:ILE:HG22	3:A:261:PRO:CD	2.45	0.42
3:A:276:ASP:OD1	3:A:276:ASP:N	2.52	0.42
3:A:180:SER:HB2	3:A:185:ALA:CB	2.49	0.42
3:A:172:GLU:CG	3:A:198:PRO:CG	2.97	0.42
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.35	0.42
3:A:73:ILE:HG22	3:A:77:LEU:HD13	2.02	0.42
3:A:82:LEU:HD23	3:A:85:LEU:HB2	2.01	0.42
3:A:182:ARG:NH1	3:A:182:ARG:CG	2.80	0.41
3:A:218:LEU:HD12	3:A:218:LEU:HA	1.67	0.41
3:A:280:LYS:O	3:A:283:ARG:N	2.53	0.41
3:A:264:GLN:HB3	3:A:296:TYR:O	2.21	0.41
3:A:68:LYS:NZ	3:A:68:LYS:CB	2.79	0.41
1:T:4:DT:C5'	3:A:231:GLY:HA3	2.51	0.41
3:A:264:GLN:HA	7:A:508:HOH:O	2.21	0.41
3:A:300:PRO:HG3	3:A:311:LEU:CD1	2.51	0.41
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.33	0.41
3:A:12:ASN:CB	3:A:46:ILE:HD12	2.50	0.41
3:A:166:VAL:CG1	3:A:173:TYR:HB3	2.51	0.41
3:A:311:LEU:HA	3:A:311:LEU:HD12	1.80	0.41
3:A:197:HIS:CG	3:A:198:PRO:CD	3.00	0.41
3:A:15:ILE:CG2	3:A:46:ILE:CD1	2.98	0.41
3:A:298:ILE:HG21	3:A:322:TYR:CD2	2.55	0.40
3:A:235:PHE:C	3:A:235:PHE:CD1	2.95	0.40
3:A:207:GLN:OE1	3:A:210:LEU:HG	2.21	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)
3:A:83:ARG:NH1	3:A:117:GLU:CB[3_558]	1.89	0.31

## 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	
3	A	325/335 (97%)	275 (85%)	34 (10%)	16 (5%)	2	13

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	32	ALA
3	A	80	GLY
3	A	185	ALA
3	A	202	SER
3	A	206	LYS
3	A	207	GLN
3	A	244	LYS
3	A	246	ASP
3	A	247	GLU
3	A	289	LYS
3	A	307	ALA
3	A	309	GLU
3	A	10	THR
3	A	304	THR
3	A	310	PRO
3	A	13	GLY

### 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.

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
-----	-------	----------	-----------	----------	-------------

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	288/295 (98%)	232 (81%)	56 (19%)	<b>1</b> <b>7</b>

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	11	LEU
3	A	15	ILE
3	A	18	MET
3	A	19	LEU
3	A	22	LEU
3	A	25	PHE
3	A	27	LYS
3	A	30	SER
3	A	33	ILE
3	A	36	TYR
3	A	37	ASN
3	A	41	LYS
3	A	46	ILE
3	A	54	LYS
3	A	62	LEU
3	A	67	THR
3	A	68	LYS
3	A	79	THR
3	A	101	THR
3	A	112	ARG
3	A	121	THR
3	A	130	ASP
3	A	132	LEU
3	A	152	ARG
3	A	168	LYS
3	A	172	GLU
3	A	182	ARG
3	A	190	ASP
3	A	191	MET
3	A	202	SER
3	A	204	SER
3	A	207	GLN
3	A	214	VAL
3	A	218	LEU
3	A	226	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	A	228	LEU
3	A	233	THR
3	A	235	PHE
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE
3	A	258	ARG
3	A	277	ILE
3	A	287	LEU
3	A	288	GLU
3	A	289	LYS
3	A	293	ILE
3	A	294	ASN
3	A	296	TYR
3	A	298	ILE
3	A	304	THR
3	A	309	GLU
3	A	314	ASP
3	A	325	TRP
3	A	331	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	28	ASN
3	A	31	GLN
3	A	37	ASN
3	A	90	GLN
3	A	98	ASN
3	A	133	ASN
3	A	134	HIS
3	A	136	GLN
3	A	157	GLN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	219	GLN
3	A	245	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	DGT	A	338	4	8,12,33	1.50	1 (12%)	15,20,52	1.38	3 (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	DGT	A	338	4	-	3/12/12/34	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	338	DGT	PG-O3G	2.66	1.59	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	338	DGT	O2G-PG-O1G	2.92	118.78	107.64
6	A	338	DGT	O3B-PG-O3G	-2.35	98.15	111.19
6	A	338	DGT	O1A-PA-O2A	2.09	118.85	110.68

There are no chirality outliers.

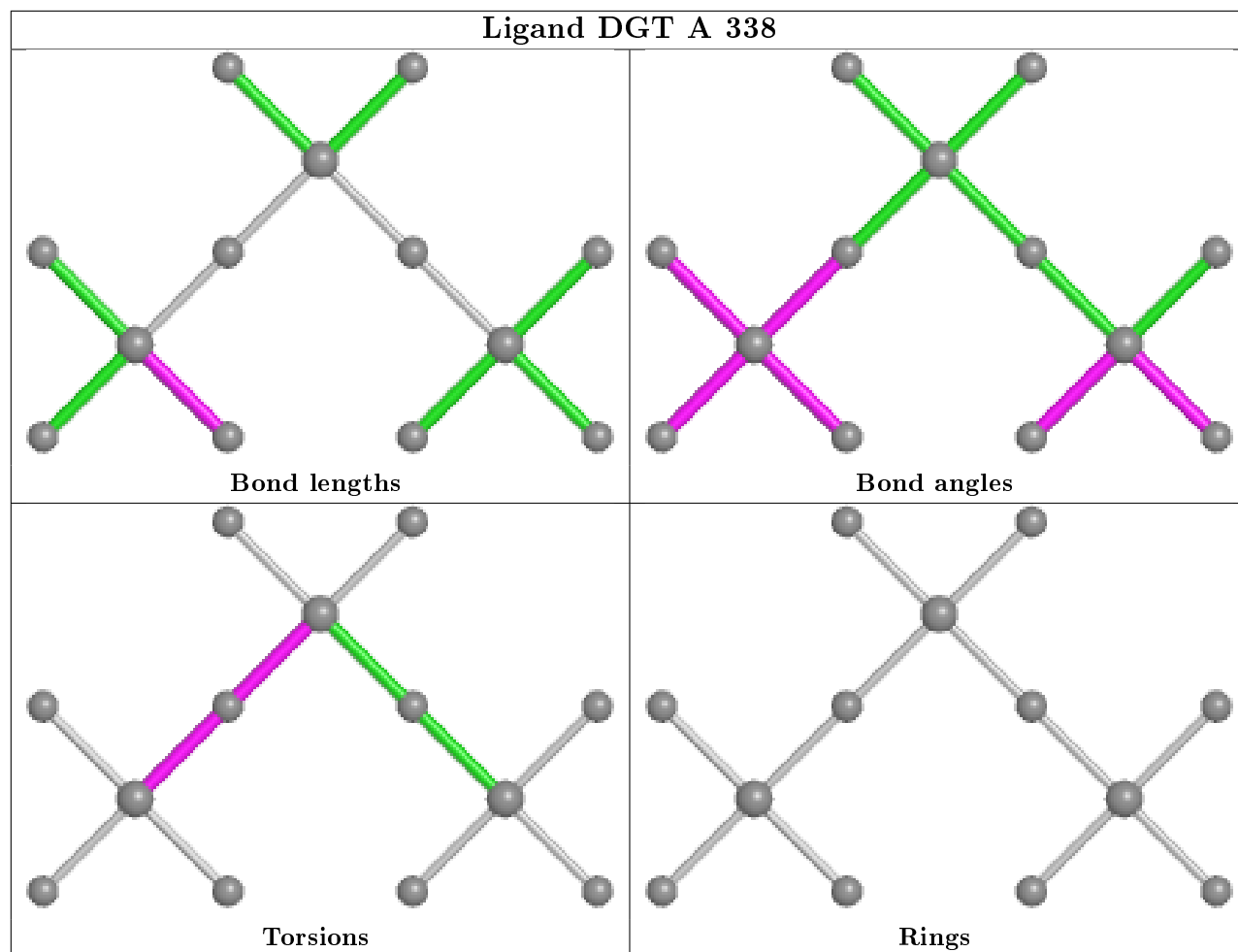
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	338	DGT	PB-O3B-PG-O1G
6	A	338	DGT	PB-O3B-PG-O2G
6	A	338	DGT	PG-O3B-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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	7/7 (100%)	-1.36	0 100 100	14, 29, 68, 97	0
2	P	6/6 (100%)	-1.48	0 100 100	13, 22, 29, 38	0
3	A	324/335 (96%)	-1.24	0 100 100	2, 31, 83, 100	0
All	All	337/348 (96%)	-1.25	0 100 100	2, 31, 84, 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](#)

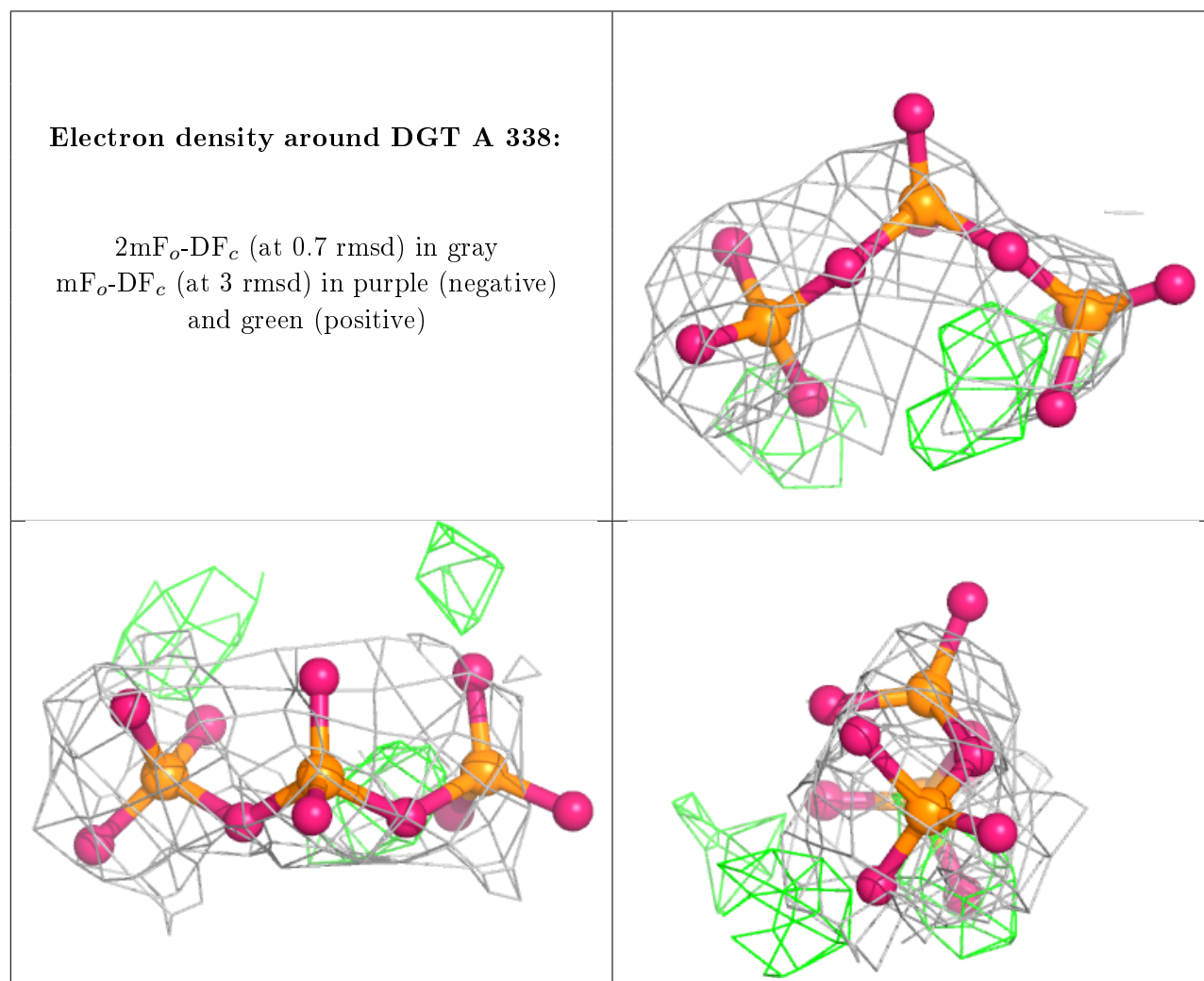
There are no carbohydrates in this entry.

### 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
6	DGT	A	338	13/31	0.88	0.27	67,90,100,100	13
4	MN	A	339	1/1	0.95	0.07	30,30,30,30	1
5	NA	A	341	1/1	0.96	0.11	28,28,28,28	0
4	MN	A	340	1/1	0.97	0.08	30,30,30,30	1
5	NA	A	342	1/1	0.99	0.07	31,31,31,31	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.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.