



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:49 PM UTC

PDB ID : 9ICT / pdb_00009ict
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

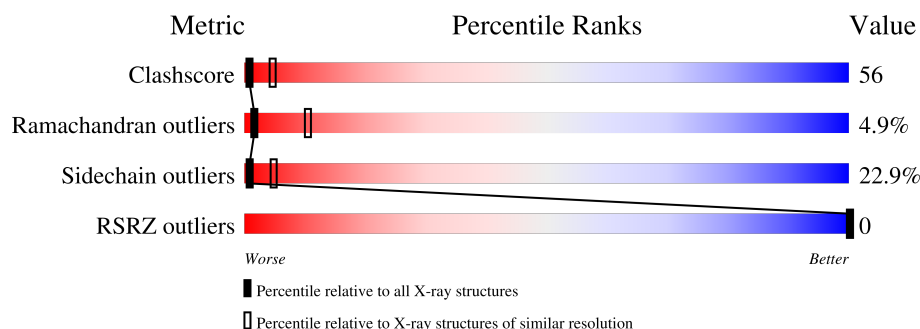
1 Overall quality at a glance

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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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			

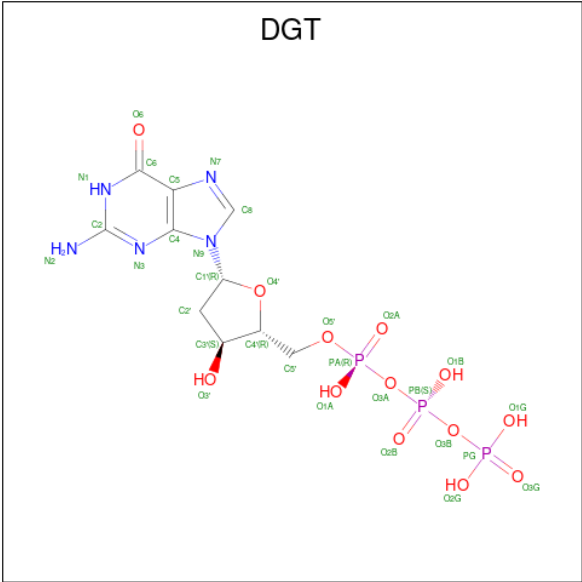
- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 5 is SODIUM ION (CCD ID: 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 (CCD ID: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

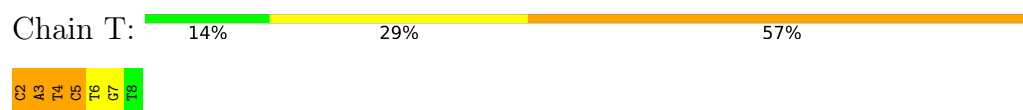
- Molecule 7 is water.

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

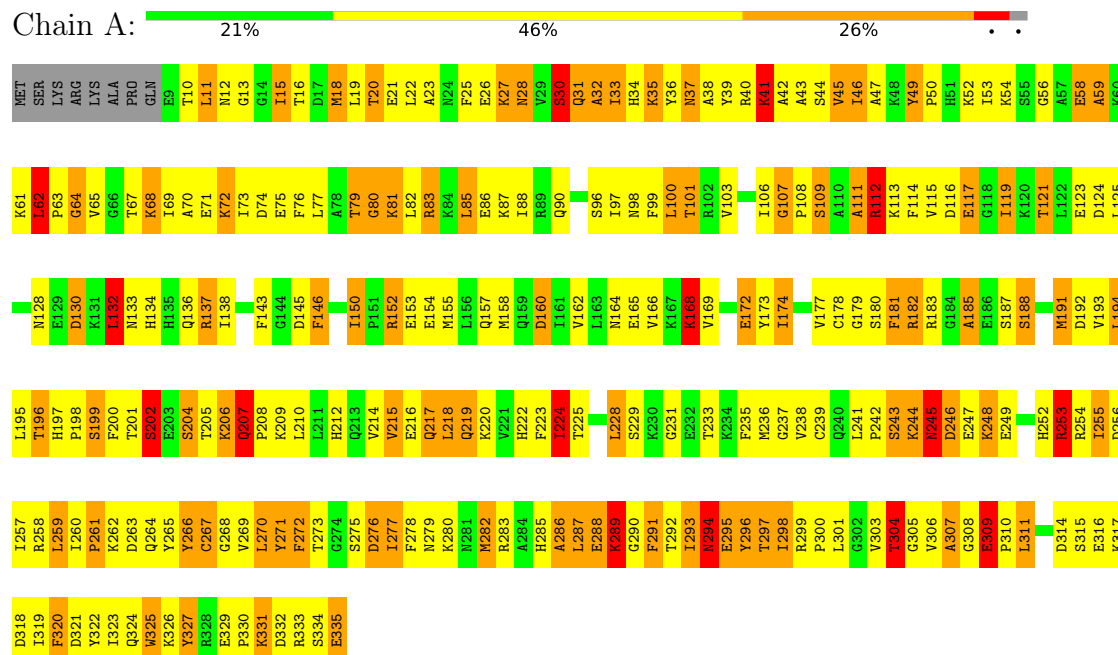
- Molecule 1: DNA (5'-D(*CP*AP*TP*CP*TP*GP*T)-3')



- 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 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.54Å 57.72Å 48.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-3.00) 94.1 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	4.30	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	38.2	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 327.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3032	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MN, DGT, NA

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	0.99	0/135	2.47	13/207 (6.3%)
2	P	1.28	2/141 (1.4%)	2.49	10/214 (4.7%)
3	A	1.64	25/2672 (0.9%)	2.14	98/3590 (2.7%)
All	All	1.60	27/2948 (0.9%)	2.18	121/4011 (3.0%)

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 (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	90	GLN	CA-C	-7.93	1.44	1.53
2	P	1	DC	OP3-P	7.03	1.62	1.48
3	A	65	VAL	CA-CB	-6.31	1.46	1.53
3	A	138	ILE	CA-CB	-6.28	1.47	1.54
3	A	138	ILE	N-CA	-6.19	1.39	1.46
3	A	146	PHE	CA-C	-6.11	1.44	1.52
3	A	119	ILE	CA-C	-5.95	1.46	1.52
3	A	160	ASP	CG-OD2	5.92	1.36	1.25
3	A	224	ILE	CA-CB	-5.90	1.47	1.54
3	A	270	LEU	C-N	-5.70	1.27	1.33
3	A	30	SER	C-N	-5.55	1.24	1.33
3	A	271	TYR	N-CA	-5.53	1.39	1.46
3	A	196	THR	CA-C	-5.50	1.46	1.52
3	A	239	CYS	CA-C	-5.47	1.45	1.52
2	P	5	DT	N1-C2	5.43	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	65	VAL	CA-C	-5.42	1.47	1.52
3	A	58	GLU	CA-C	-5.30	1.45	1.52
3	A	217	GLN	N-CA	-5.24	1.40	1.46
3	A	119	ILE	CA-CB	-5.22	1.47	1.53
3	A	87	LYS	CA-C	5.21	1.59	1.52
3	A	224	ILE	CA-C	-5.21	1.46	1.52
3	A	192	ASP	CA-C	-5.20	1.46	1.52
3	A	35	LYS	CA-C	-5.09	1.46	1.52
3	A	116	ASP	CA-C	-5.08	1.45	1.52
3	A	125	LEU	CA-C	-5.03	1.46	1.52
3	A	132	LEU	CA-C	-5.02	1.46	1.52
3	A	137	ARG	C-N	-5.02	1.27	1.33

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	5	DT	C2-N1-C1'	13.29	139.29	119.35
3	A	49	TYR	CA-C-N	13.15	132.70	119.82
3	A	49	TYR	C-N-CA	13.15	132.70	119.82
2	P	5	DT	C6-N1-C1'	-12.46	100.66	119.35
3	A	99	PHE	CA-CB-CG	-12.03	101.77	113.80
1	T	6	DT	C6-N1-C1'	-11.86	101.57	119.35
3	A	272	PHE	CA-CB-CG	-11.60	102.20	113.80
2	P	6	DG	C4-N9-C1'	-10.56	111.16	127.00
3	A	34	HIS	CA-CB-CG	-10.49	103.31	113.80
1	T	4	DT	C6-N1-C1'	-10.44	103.68	119.35
1	T	4	DT	C2-N1-C1'	10.39	134.94	119.35
2	P	6	DG	C8-N9-C1'	10.39	142.59	127.00
1	T	6	DT	C2-N1-C1'	10.02	134.37	119.35
3	A	49	TYR	O-C-N	9.37	128.78	121.47
1	T	5	DC	C2-N1-C1'	9.31	133.67	119.70
3	A	40	ARG	N-CA-C	9.16	121.34	111.36
1	T	5	DC	C6-N1-C1'	-8.83	106.46	119.70
3	A	271	TYR	CA-CB-CG	-8.54	98.53	113.90
3	A	152	ARG	N-CA-CB	8.48	124.82	110.49
3	A	30	SER	N-CA-C	-8.21	97.13	109.86
3	A	318	ASP	CA-CB-CG	-8.21	104.39	112.60
3	A	30	SER	CA-C-N	-8.19	109.38	122.23
3	A	30	SER	C-N-CA	-8.19	109.38	122.23
3	A	291	PHE	N-CA-C	8.00	121.06	109.14
2	P	3	DG	C8-N9-C1'	7.70	138.56	127.00
1	T	7	DG	C4-N9-C1'	-7.56	115.67	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	20	THR	CB-CA-C	7.52	122.61	110.95
3	A	65	VAL	N-CA-C	7.17	117.77	106.88
3	A	168	LYS	N-CA-CB	7.09	120.55	110.12
3	A	146	PHE	N-CA-C	6.95	118.86	111.28
3	A	261	PRO	CB-CA-C	-6.94	102.90	111.64
3	A	245	ASN	CA-CB-CG	6.82	119.42	112.60
3	A	20	THR	N-CA-CB	6.73	119.74	109.98
3	A	138	ILE	CB-CA-C	-6.73	103.36	111.97
3	A	64	GLY	N-CA-C	-6.69	106.51	115.21
3	A	329	GLU	N-CA-C	-6.64	100.92	110.08
3	A	28	ASN	N-CA-C	6.63	118.59	111.36
2	P	3	DG	C4-N9-C1'	-6.57	117.14	127.00
3	A	266	TYR	N-CA-C	6.55	120.13	111.75
3	A	90	GLN	O-C-N	6.54	129.90	122.19
3	A	87	LYS	CB-CA-C	6.42	120.96	110.88
3	A	74	ASP	N-CA-CB	6.41	119.49	109.94
3	A	96	SER	N-CA-C	6.39	118.25	111.28
1	T	7	DG	C8-N9-C1'	6.37	136.55	127.00
3	A	296	TYR	N-CA-C	6.36	122.11	113.97
2	P	4	DA	P-O3'-C3'	6.30	129.66	120.20
3	A	83	ARG	N-CA-CB	6.30	119.11	109.91
3	A	253	ARG	N-CA-C	6.27	119.62	109.40
3	A	41	LYS	N-CA-C	-6.22	104.58	111.36
3	A	86	GLU	N-CA-CB	6.11	119.20	110.16
3	A	327	TYR	N-CA-CB	6.10	119.15	109.51
3	A	49	TYR	CA-C-O	6.08	124.88	119.59
3	A	222	HIS	CB-CA-C	-6.03	100.03	111.06
3	A	181	PHE	CA-CB-CG	-6.00	107.80	113.80
3	A	150	ILE	N-CA-C	5.98	113.47	107.55
3	A	320	PHE	O-C-N	5.96	128.96	122.11
3	A	70	ALA	N-CA-C	-5.93	104.81	111.28
3	A	34	HIS	O-C-N	5.89	128.14	122.07
3	A	146	PHE	N-CA-CB	5.83	118.68	110.12
3	A	270	LEU	CA-C-O	5.82	127.11	121.00
3	A	192	ASP	CB-CA-C	-5.81	100.78	110.19
3	A	238	VAL	CA-C-N	-5.80	112.69	123.01
3	A	238	VAL	C-N-CA	-5.80	112.69	123.01
3	A	243	SER	CB-CA-C	5.77	119.75	110.29
3	A	329	GLU	CB-CA-C	5.67	118.40	109.27
3	A	31	GLN	N-CA-C	-5.65	106.27	114.12
3	A	304	THR	N-CA-CB	-5.63	100.98	110.49
3	A	246	ASP	N-CA-C	5.61	122.75	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	286	ALA	CA-C-N	5.60	128.24	120.29
3	A	286	ALA	C-N-CA	5.60	128.24	120.29
3	A	296	TYR	CB-CA-C	-5.55	99.75	109.07
3	A	138	ILE	O-C-N	5.54	127.34	121.91
2	P	4	DA	C4-N9-C1'	-5.54	118.74	127.05
3	A	59	ALA	O-C-N	5.48	127.95	122.03
3	A	107	GLY	N-CA-C	-5.46	101.20	112.34
1	T	4	DT	N1-C1'-C2'	5.44	121.66	113.50
3	A	168	LYS	N-CA-C	5.43	117.19	111.28
3	A	117	GLU	N-CA-C	-5.41	105.49	113.61
3	A	98	ASN	CA-CB-CG	-5.41	107.19	112.60
3	A	257	ILE	CB-CA-C	-5.39	102.47	110.33
3	A	286	ALA	O-C-N	5.38	127.83	122.12
3	A	87	LYS	CA-C-N	5.38	127.83	120.46
3	A	87	LYS	C-N-CA	5.38	127.83	120.46
3	A	241	LEU	O-C-N	5.38	125.99	121.31
1	T	3	DA	C8-N9-C1'	5.35	135.08	127.05
3	A	225	THR	N-CA-C	5.35	120.46	113.88
3	A	150	ILE	N-CA-CB	5.34	117.62	111.31
3	A	62	LEU	CA-C-N	5.32	125.73	119.99
3	A	62	LEU	C-N-CA	5.32	125.73	119.99
3	A	146	PHE	CA-CB-CG	-5.30	108.50	113.80
3	A	34	HIS	CA-C-N	5.30	127.33	120.44
3	A	34	HIS	C-N-CA	5.30	127.33	120.44
3	A	112	ARG	N-CA-C	5.29	116.73	111.07
1	T	2	DC	C6-N1-C1'	-5.28	111.78	119.70
3	A	334	SER	CB-CA-C	5.28	119.31	110.92
3	A	267	CYS	N-CA-C	-5.26	105.62	111.36
3	A	138	ILE	CA-CB-CG2	-5.26	101.55	110.50
3	A	223	PHE	CA-CB-CG	-5.26	108.54	113.80
3	A	109	SER	O-C-N	5.26	127.70	122.08
3	A	123	GLU	CB-CA-C	5.24	119.10	110.88
1	T	2	DC	C2-N1-C1'	5.22	127.54	119.70
3	A	329	GLU	N-CA-CB	5.22	117.74	110.11
3	A	297	THR	CB-CA-C	-5.21	100.95	111.17
3	A	215	VAL	N-CA-CB	5.21	116.98	110.47
3	A	241	LEU	CA-C-N	5.21	126.35	119.84
3	A	241	LEU	C-N-CA	5.21	126.35	119.84
3	A	294	ASN	N-CA-CB	5.21	119.90	111.21
2	P	4	DA	C8-N9-C1'	5.20	134.84	127.05
3	A	266	TYR	CA-CB-CG	-5.20	104.55	113.90
3	A	41	LYS	N-CA-CB	5.18	117.82	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	199	SER	N-CA-CB	-5.17	99.92	110.67
1	T	5	DC	P-O3'-C3'	5.16	127.94	120.20
3	A	335	GLU	N-CA-CB	5.12	119.21	110.50
3	A	223	PHE	N-CA-C	-5.08	105.39	112.45
2	P	2	DA	C5'-C4'-O4'	-5.07	101.79	109.40
3	A	229	SER	CB-CA-C	5.06	119.69	109.68
3	A	96	SER	O-C-N	5.05	127.47	122.12
3	A	291	PHE	CA-CB-CG	-5.04	108.76	113.80
3	A	21	GLU	CB-CA-C	-5.03	102.39	110.74
3	A	86	GLU	CB-CA-C	5.00	119.35	110.85
3	A	111	ALA	N-CA-C	-5.00	105.83	111.28

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	303	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	314	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 56.

All (314) 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:18:MET:HE1	3:A:76:PHE:HB2	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:150:ILE:HG21	3:A:158:MET:HE1	1.55	0.87
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
2:P:1:DC:C2'	2:P:2:DA:H5''	2.12	0.79
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.48	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
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:212:HIS:HB3	7:A:541:HOH:O	1.85	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:150:ILE:HG21	3:A:158:MET:CE	2.15	0.76
3:A:32:ALA:HB1	3:A:35:LYS:HB2	1.66	0.75
3:A:155:MET:CE	3:A:188:SER:HB2	2.16	0.75
3:A:12:ASN:HB3	3:A:46:ILE:CD1	2.17	0.74
3:A:155:MET:HE3	3:A:188:SER:HB2	1.68	0.74
3:A:300:PRO:HD3	3:A:311:LEU:HD13	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:18:MET:CE	3:A:76:PHE:HB2	2.21	0.71
3:A:330:PRO:CA	3:A:333:ARG:HG3	2.21	0.71
3:A:59:ALA:O	3:A:62:LEU:HB2	1.91	0.70
3:A:111:ALA:O	3:A:115:VAL:HG23	1.92	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:12:ASN:HB3	3:A:46:ILE:HD11	1.74	0.69
3:A:31:GLN:N	7:A:641:HOH:O	2.25	0.69
3:A:18:MET:HE1	3:A:76:PHE:CB	2.23	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
2:P:3:DG:H1'	7:P:511:HOH:O	1.96	0.66
3:A:319:ILE:O	3:A:322:TYR:HB2	1.95	0.66
3:A:41:LYS:HD3	3:A:42:ALA:H	1.60	0.66
3:A:215:VAL:O	3:A:219:GLN:HG3	1.95	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
2:P:2:DA:N7	7:P:598:HOH:O	2.30	0.65
3:A:293:ILE:HD13	3:A:298:ILE:CG1	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	3:A:11:LEU:CD2	2.09	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:79:THR:O	3:A:81:LYS:N	2.31	0.62
3:A:166:VAL:O	3:A:169:VAL:HG12	2.00	0.62
3:A:155:MET:HE3	3:A:188:SER:CB	2.30	0.61
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:HG3	3:A:326:LYS:O	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
1:T:4:DT:H2''	1:T:5:DC:O5'	2.03	0.59
3:A:182:ARG:HG2	3:A:182:ARG:NH1	2.15	0.59
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.85	0.59
3:A:79:THR:C	3:A:81:LYS:H	2.10	0.58
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: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:69:ILE:O	3:A:73:ILE:HG13	2.03	0.57
3:A:248:LYS:O	3:A:248:LYS:HG2	2.04	0.57
3:A:155:MET:HA	3:A:158:MET:HE3	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:330:PRO:C	3:A:333:ARG:HG3	2.30	0.56
3:A:75:GLU:O	3:A:79:THR:HG23	2.06	0.55
3:A:288:GLU:C	3:A:290:GLY:H	2.15	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:15:ILE:HG21	3:A:46:ILE:CD1	2.38	0.54
3:A:288:GLU:OE1	3:A:288:GLU:HA	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:295:GLU:CD	3:A:295:GLU:H	2.16	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:HH11	3:A:253:ARG:HG3	1.72	0.53
3:A:243:SER:OG	3:A:249:GLU:HA	2.08	0.53
3:A:145:ASP:CG	3:A:252:HIS:H	2.17	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
3:A:177:VAL:HG11	3:A:191:MET:HE2	1.90	0.52
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:316:GLU:O	3:A:320:PHE:HD2	1.93	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:303:VAL:C	3:A:305:GLY:H	2.18	0.51
3:A:254:ARG:HH11	3:A:255:ILE:N	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:195:LEU:O	3:A:260:ILE:N	2.44	0.50
3:A:259:LEU:HD12	3:A:260:ILE:H	1.76	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
2:P:5:DT:H1'	7:P:565:HOH:O	2.11	0.49
3:A:56:GLY:O	3:A:59:ALA:HB3	2.12	0.49
3:A:201:THR:HA	3:A:261:PRO:HB2	1.93	0.49
3:A:292:THR:HG21	3:A:299:ARG:HH21	1.78	0.49
3:A:43:ALA:O	3:A:47:ALA:HB2	2.13	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: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: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: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:205:THR:HG23	3:A:205:THR:O	2.13	0.48
3:A:16:THR:O	3:A:20:THR:HG23	2.14	0.48
3:A:32:ALA:O	3:A:36:TYR:HB3	2.14	0.48
3:A:103:VAL:HG22	3:A:143:PHE:HD2	1.78	0.48
3:A:207:GLN:O	3:A:210:LEU:HB2	2.13	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: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: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:294:ASN:C	3:A:294:ASN:HD22	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:P:2:DA:H5'	2:P:2:DA:H2'	1.57	0.46
3:A:216:GLU:O	3:A:220:LYS:N	2.43	0.46
3:A:72:LYS:HG2	3:A:82:LEU:HD11	1.97	0.46
3:A:103:VAL:HG22	3:A:143:PHE:CE2	2.51	0.46
3:A:262:LYS:O	3:A:262:LYS:HG3	2.10	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:CD2	3:A:11:LEU:N	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:49:TYR:CE2	3:A:53:ILE:HG12	2.51	0.45
3:A:209:LYS:HA	3:A:209:LYS:HD3	1.47	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:235:PHE:CD1	3:A:235:PHE:C	2.95	0.45
3:A:157:GLN:NE2	3:A:244:LYS:NZ	2.65	0.45
3:A:218:LEU:HB2	3:A:224:ILE:HD12	1.98	0.45
3:A:217:GLN:NE2	3:A:217:GLN:HA	2.31	0.45
3:A:298:ILE:HG21	3:A:322:TYR:HD2	1.82	0.45
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:HD12	3:A:85:LEU:HA	1.82	0.45
3:A:37:ASN:HD22	3:A:37:ASN:HA	1.63	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:36:TYR:CD1	3:A:37:ASN:N	2.85	0.44
3:A:200:PHE:O	3:A:262:LYS:N	2.46	0.44
1:T:4:DT:H5''	3:A:231:GLY:HA3	1.98	0.44
3:A:18:MET:HE3	3:A:76:PHE:CD1	2.52	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
3:A:23:ALA:HA	3:A:39:TYR:CD2	2.52	0.44
3:A:18:MET:HE2	3:A:82:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:300:PRO:HG3	3:A:311:LEU:HD11	2.00	0.44
3:A:80:GLY:C	3:A:81:LYS:HG2	2.41	0.44
2:P:5:DT:P	3:A:107:GLY:HA3	2.57	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
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:44:SER:O	3:A:47:ALA:HB3	2.18	0.43
3:A:183:ARG:HG3	3:A:273:THR:HG22	2.01	0.43
1:T:4:DT:H5'	7:T:617:HOH:O	2.18	0.43
3:A:36:TYR:CD1	3:A:36:TYR:C	2.95	0.43
3:A:194:LEU:HD13	3:A:194:LEU:HA	1.61	0.43
3:A:299:ARG:HA	3:A:300:PRO:HD3	1.88	0.43
3:A:197:HIS:CE1	3:A:198:PRO:HD2	2.53	0.43
3:A:273:THR:HG22	3:A:273:THR:O	2.18	0.43
3:A:322:TYR:C	3:A:324:GLN:H	2.25	0.43
3:A:146:PHE:HD1	3:A:146:PHE:HA	1.58	0.43
3:A:301:LEU:HD12	3:A:301:LEU:HA	1.71	0.43
3:A:25:PHE:CD1	3:A:25:PHE:C	2.96	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:88:ILE:HD13	3:A:88:ILE:HG21	1.71	0.43
3:A:182:ARG:NH1	3:A:273:THR:CG2	2.82	0.43
3:A:205:THR:O	3:A:206:LYS:O	2.36	0.43
3:A:267:CYS:SG	3:A:297:THR:HA	2.59	0.43
3:A:272:PHE:HD1	7:A:587:HOH:O	2.02	0.43
1:T:2:DC:H6	1:T:2:DC:H2'	1.50	0.42
3:A:26:GLU:HA	3:A:30:SER:OG	2.18	0.42
3:A:100:LEU:HA	3:A:100:LEU:HD12	1.70	0.42
3:A:79:THR:C	3:A:81:LYS:N	2.77	0.42
3:A:299:ARG:HB3	3:A:300:PRO:HD2	2.02	0.42
1:T:4:DT:P	3:A:231:GLY:HA3	2.59	0.42
3:A:155:MET:SD	3:A:158:MET:HE3	2.60	0.42
3:A:295:GLU:HG2	3:A:296:TYR:CE1	2.55	0.42
3:A:254:ARG:HD2	3:A:254:ARG:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:172:GLU:CG	3:A:198:PRO:CG	2.97	0.42
3:A:180:SER:HB2	3:A:185:ALA:CB	2.49	0.42
3:A:288:GLU:C	3:A:290:GLY:N	2.77	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
1:T:4:DT:C5'	3:A:231:GLY:HA3	2.51	0.41
3:A:68:LYS:NZ	3:A:68:LYS:CB	2.79	0.41
3:A:264:GLN:HB3	3:A:296:TYR:O	2.21	0.41
3:A:280:LYS:O	3:A:283:ARG:N	2.53	0.41
3:A:264:GLN:HA	7:A:508:HOH:O	2.21	0.41
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.33	0.41
3:A:300:PRO:HG3	3:A:311:LEU:CD1	2.51	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:282:MET:HE3	3:A:323:ILE:HD11	2.01	0.41
3:A:311:LEU:HD12	3:A:311:LEU:HA	1.80	0.41
3:A:15:ILE:CG2	3:A:46:ILE:CD1	2.98	0.41
3:A:197:HIS:CG	3:A:198:PRO:CD	3.00	0.41
3:A:298:ILE:HG21	3:A:322:TYR:CD2	2.55	0.40
3:A:115:VAL:C	3:A:117:GLU:N	2.79	0.40
3:A:128:ASN:C	3:A:130:ASP:N	2.77	0.40
3:A:150:ILE:HB	3:A:155:MET:HE2	2.04	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 [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%)	275 (85%)	34 (10%)	16 (5%)	1	10

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 [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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	288/295 (98%)	222 (77%)	66 (23%)	1 5

All (66) 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	27	LYS
3	A	30	SER
3	A	33	ILE
3	A	37	ASN
3	A	41	LYS
3	A	45	VAL
3	A	46	ILE
3	A	52	LYS
3	A	54	LYS
3	A	62	LEU
3	A	67	THR
3	A	68	LYS
3	A	72	LYS
3	A	79	THR
3	A	81	LYS
3	A	85	LEU
3	A	100	LEU
3	A	101	THR
3	A	112	ARG
3	A	121	THR
3	A	130	ASP
3	A	132	LEU
3	A	153	GLU
3	A	168	LYS
3	A	172	GLU
3	A	174	ILE
3	A	182	ARG
3	A	188	SER
3	A	191	MET
3	A	194	LEU

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Mol	Chain	Res	Type
3	A	202	SER
3	A	204	SER
3	A	207	GLN
3	A	214	VAL
3	A	218	LEU
3	A	219	GLN
3	A	224	ILE
3	A	228	LEU
3	A	233	THR
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE
3	A	258	ARG
3	A	259	LEU
3	A	276	ASP
3	A	277	ILE
3	A	282	MET
3	A	287	LEU
3	A	288	GLU
3	A	289	LYS
3	A	293	ILE
3	A	294	ASN
3	A	295	GLU
3	A	298	ILE
3	A	304	THR
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	325	TRP
3	A	331	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) 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

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Mol	Chain	Res	Type
3	A	136	GLN
3	A	157	GLN
3	A	159	GLN
3	A	164	ASN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	219	GLN
3	A	245	ASN
3	A	279	ASN
3	A	281	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 oligosaccharides 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	10,12,33	1.65	2 (20%)	17,20,52	1.31	3 (17%)

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	-	5/12/12/34	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	338	DGT	PG-O3G	2.78	1.59	1.50
6	A	338	DGT	PB-O3A	2.22	1.61	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	338	DGT	O2G-PG-O1G	2.93	118.78	107.80
6	A	338	DGT	O3B-PG-O3G	-2.45	98.15	111.04
6	A	338	DGT	O1A-PA-O2A	2.06	118.85	110.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

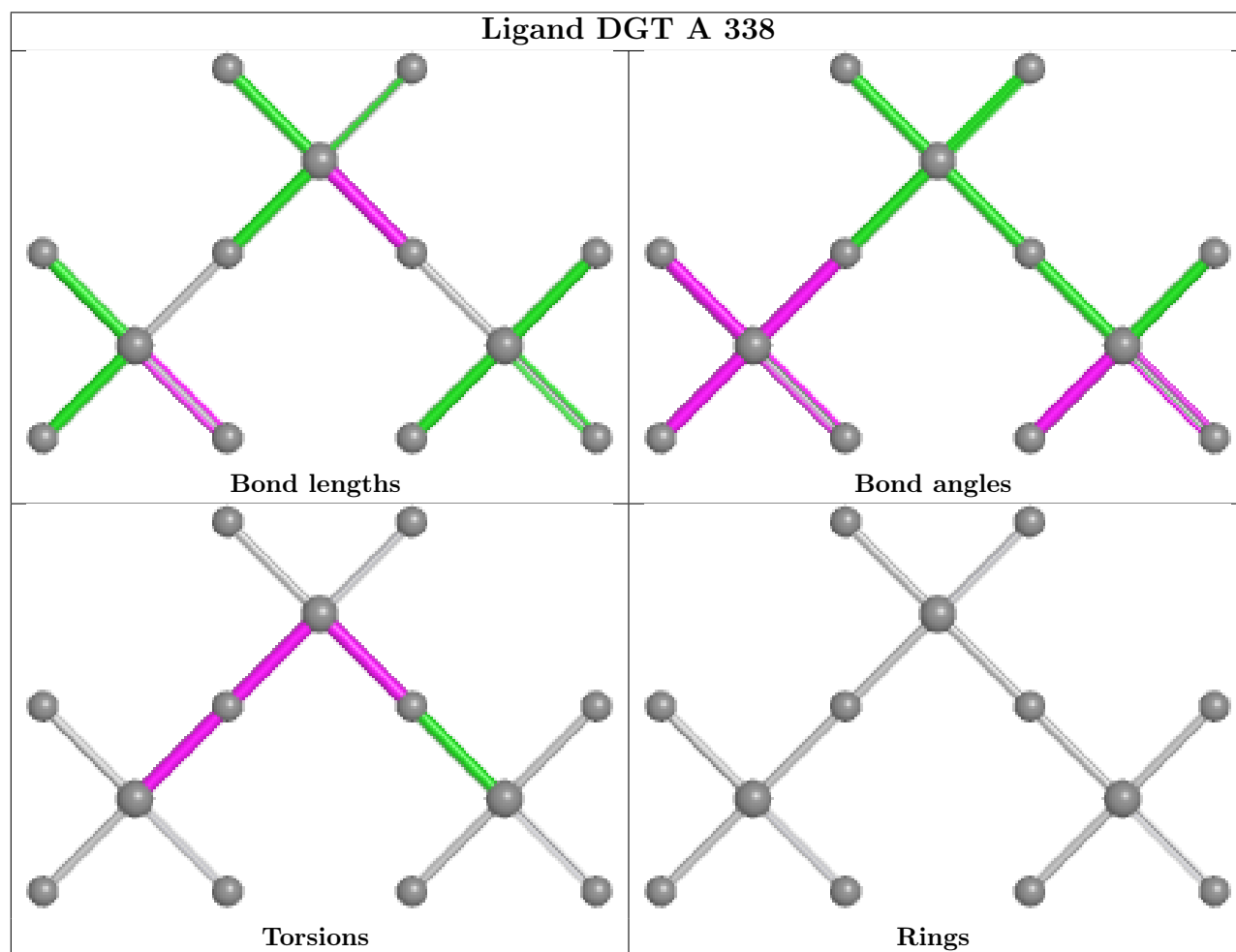
Mol	Chain	Res	Type	Atoms
6	A	338	DGT	PB-O3B-PG-O1G
6	A	338	DGT	PB-O3B-PG-O2G
6	A	338	DGT	PG-O3B-PB-O2B
6	A	338	DGT	PG-O3B-PB-O1B
6	A	338	DGT	PA-O3A-PB-O1B

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	T	7/7 (100%)	-1.02	0 100 100	14, 28, 68, 97	0
2	P	6/6 (100%)	-1.20	0 100 100	13, 22, 29, 38	0
3	A	324/335 (96%)	-0.96	0 100 100	2, 31, 83, 100	0
All	All	337/348 (96%)	-0.97	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](#)

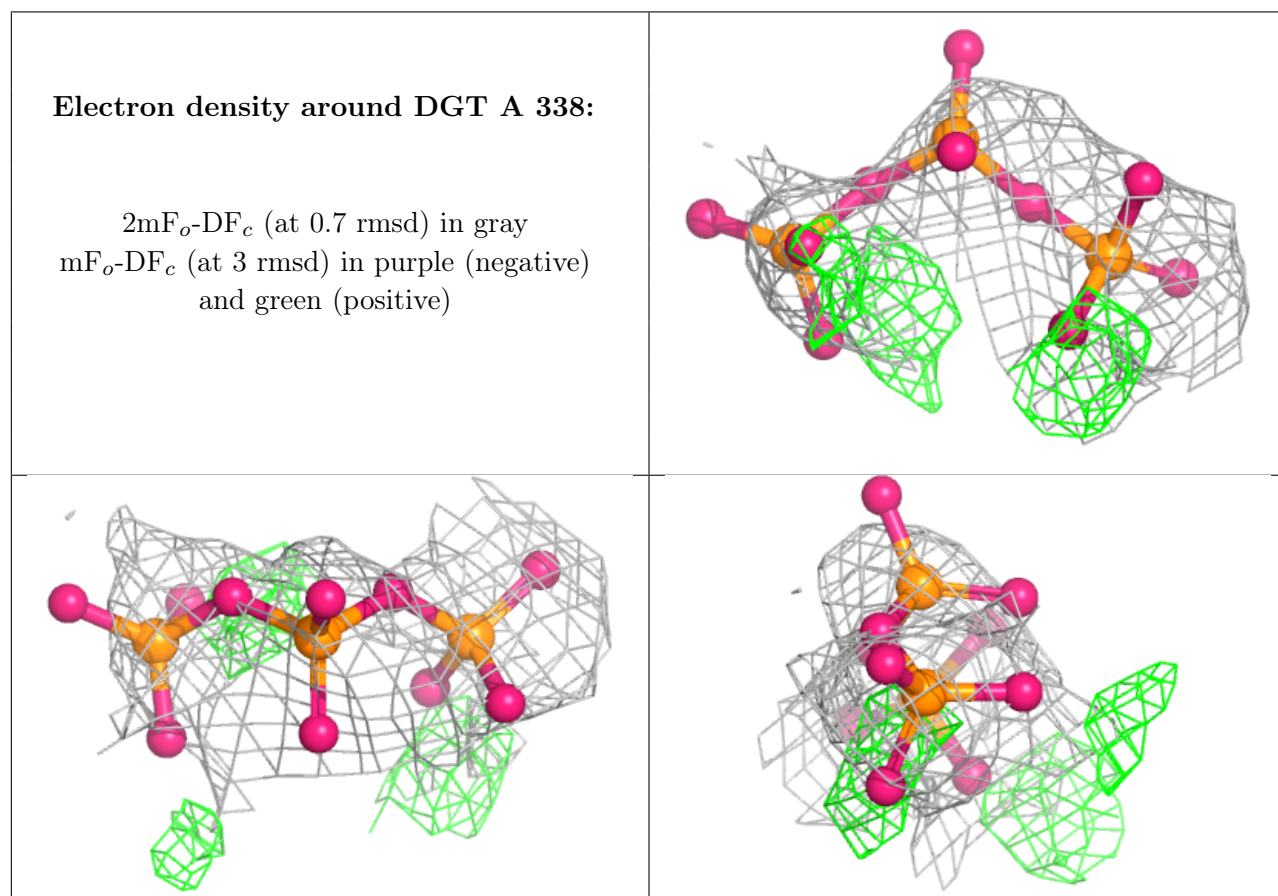
There are no oligosaccharides in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	DGT	A	338	13/31	0.86	0.20	67,90,100,100	13
4	MN	A	340	1/1	0.92	0.06	30,30,30,30	1
5	NA	A	341	1/1	0.96	0.05	28,28,28,28	0
4	MN	A	339	1/1	0.96	0.05	30,30,30,30	1
5	NA	A	342	1/1	0.98	0.05	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 [i](#)

There are no such residues in this entry.