



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:15 PM UTC

PDB ID : 2BPF / pdb_00002bpf
Title : STRUCTURES OF TERNARY COMPLEXES OF RAT DNA POLYMERASE BETA, A DNA TEMPLATE-PRIMER, AND DDCTP
Authors : Pelletier, H.; Sawaya, M.R.; Kumar, A.; Wilson, S.H.; Kraut, J.
Deposited on : 1994-05-19
Resolution : 2.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

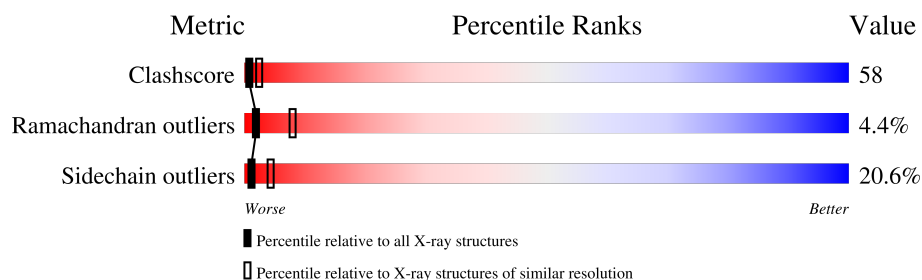
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	T	8	12% 12% 50% 25%
2	P	7	14% 14% 29% 43%
3	A	335	23% 39% 28% 6% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2908 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(*GP*GP*GP*CP*GP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	8	Total	C	N	O	P	0	0	0
			167	77	34	48	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	P	0	0	0
			138	66	27	39	6			

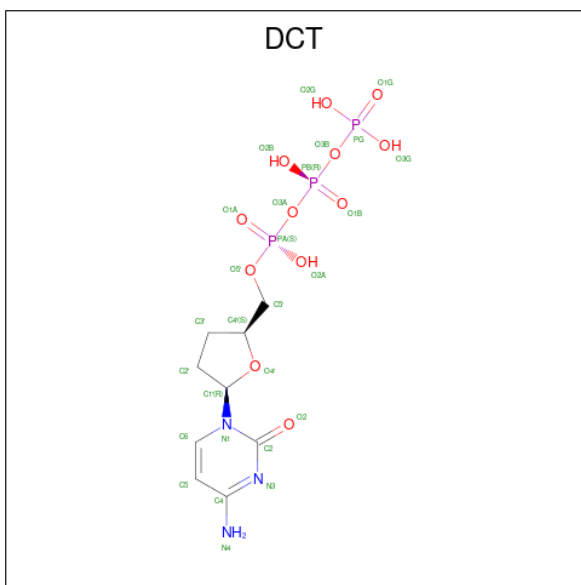
- Molecule 3 is a protein called PROTEIN (DNA POLYMERASE BETA (E.C.2.7.7.7)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	324	Total	C	N	O	S	0	0	0
			2543	1603	449	482	9			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is 2',3'-DIDEOXYCYTIDINE 5'-TRIPHOSPHATE (CCD ID: DCT) (formula: C₉H₁₆N₃O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	9	3	12	3		

- Molecule 6 is water.

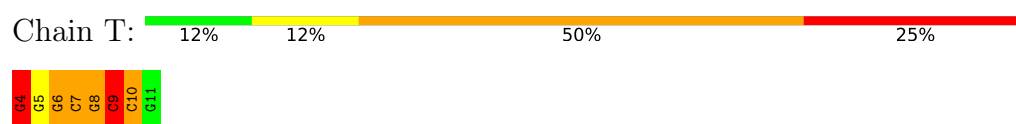
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	T	2	Total O 2 2	0	0
6	P	2	Total O 2 2	0	0
6	A	27	Total O 27 27	0	0

3 Residue-property plots

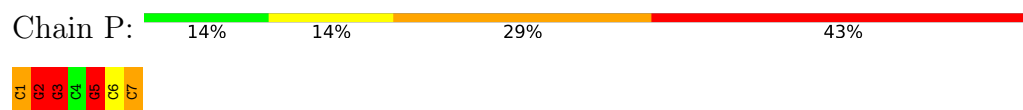
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

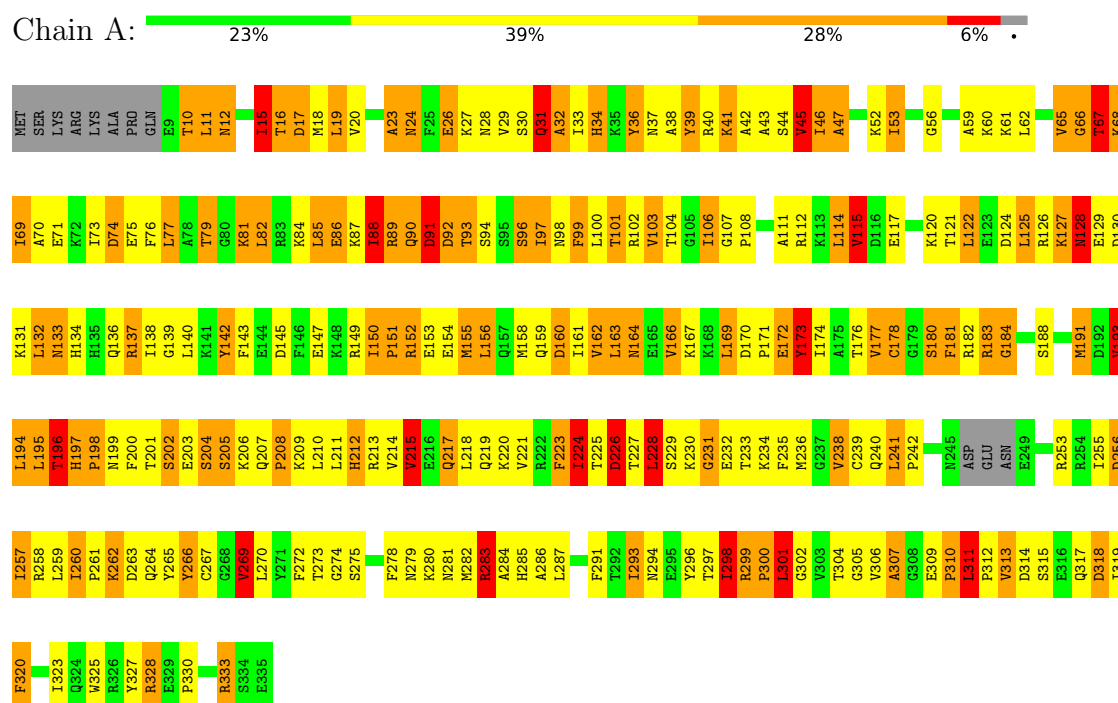
- Molecule 1: DNA (5'-D(*GP*GP*GP*CP*GP*CP*CP*G)-3')



- Molecule 2: DNA (5'-D(*CP*GP*GP*CP*GP*CP*C)-3')



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



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	94.90Å 94.90Å 117.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2908	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DCT, MG

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	1.11	0/187	2.89	16/287 (5.6%)
2	P	1.06	0/154	2.50	12/235 (5.1%)
3	A	1.58	25/2589 (1.0%)	2.19	123/3493 (3.5%)
All	All	1.53	25/2930 (0.9%)	2.26	151/4015 (3.8%)

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
1	T	0	4
2	P	0	5
All	All	0	9

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	LEU	N-CA	-10.41	1.33	1.46
3	A	24	ASN	CA-CB	7.53	1.66	1.53
3	A	24	ASN	CA-C	-7.46	1.42	1.52
3	A	299	ARG	CA-C	-7.19	1.46	1.52
3	A	191	MET	CA-C	-6.75	1.44	1.52
3	A	196	THR	CA-C	6.05	1.60	1.52
3	A	226	ASP	CA-C	-6.03	1.45	1.52
3	A	173	TYR	CA-C	-5.91	1.45	1.52
3	A	170	ASP	C-N	-5.86	1.29	1.33
3	A	180	SER	CA-C	-5.86	1.45	1.52
3	A	300	PRO	N-CA	-5.64	1.40	1.47
3	A	217	GLN	N-CA	-5.62	1.39	1.46
3	A	42	ALA	C-O	5.52	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	238	VAL	CA-C	-5.30	1.46	1.52
3	A	211	LEU	N-CA	-5.24	1.40	1.46
3	A	171	PRO	N-CA	-5.24	1.44	1.47
3	A	39	TYR	N-CA	-5.21	1.40	1.46
3	A	298	ILE	CA-C	-5.21	1.46	1.52
3	A	226	ASP	N-CA	-5.17	1.39	1.45
3	A	69	ILE	CA-C	-5.14	1.46	1.52
3	A	269	VAL	CA-CB	-5.12	1.48	1.54
3	A	311	LEU	C-N	-5.05	1.26	1.33
3	A	40	ARG	CA-C	-5.03	1.46	1.52
3	A	161	ILE	CA-CB	-5.03	1.48	1.54
3	A	155	MET	CA-C	-5.02	1.46	1.52

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	8	DG	C8-N9-C1'	19.13	155.69	127.00
1	T	8	DG	C4-N9-C1'	-18.67	98.99	127.00
2	P	7	DC	C2-N1-C1'	-17.54	93.39	119.70
1	T	10	DC	C2-N1-C1'	-13.96	98.76	119.70
2	P	7	DC	C6-N1-C1'	12.74	138.82	119.70
1	T	9	DC	C2-N1-C1'	-11.84	101.94	119.70
3	A	301	LEU	N-CA-CB	11.37	129.34	110.47
3	A	31	GLN	N-CA-C	-10.73	99.91	113.43
1	T	9	DC	C6-N1-C1'	9.86	134.48	119.70
3	A	196	THR	CA-CB-OG1	-9.49	95.36	109.60
3	A	196	THR	CA-CB-CG2	9.33	126.36	110.50
3	A	23	ALA	CA-C-N	-9.30	105.19	120.72
3	A	23	ALA	C-N-CA	-9.30	105.19	120.72
2	P	2	DG	C8-N9-C1'	-9.01	113.49	127.00
3	A	224	ILE	N-CA-C	-8.94	97.22	109.55
1	T	6	DG	C8-N9-C1'	8.76	140.14	127.00
1	T	7	DC	C2-N1-C1'	-8.76	106.56	119.70
3	A	300	PRO	CA-C-N	-8.73	110.71	123.11
3	A	300	PRO	C-N-CA	-8.73	110.71	123.11
3	A	195	LEU	CA-C-N	-8.73	108.15	122.82
3	A	195	LEU	C-N-CA	-8.73	108.15	122.82
1	T	6	DG	C4-N9-C1'	-8.64	114.04	127.00
3	A	241	LEU	C-N-CD	-8.61	89.69	125.00
1	T	8	DG	P-O5'-C5'	-8.55	107.17	120.00
3	A	40	ARG	O-C-N	8.48	130.80	122.07
3	A	307	ALA	N-CA-C	8.33	121.83	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	212	HIS	CA-CB-CG	-8.30	105.50	113.80
2	P	3	DG	P-O5'-C5'	-8.25	107.63	120.00
3	A	266	TYR	N-CA-C	8.14	120.16	111.28
3	A	223	PHE	CA-CB-CG	-8.09	105.71	113.80
3	A	99	PHE	CA-CB-CG	-8.03	105.77	113.80
3	A	170	ASP	CA-C-N	-8.03	111.79	120.94
3	A	170	ASP	C-N-CA	-8.03	111.79	120.94
1	T	4	DG	C4-N9-C1'	-8.00	115.00	127.00
3	A	293	ILE	N-CA-C	7.92	119.25	108.17
3	A	173	TYR	CB-CA-C	-7.69	97.58	109.89
3	A	215	VAL	N-CA-CB	7.69	121.00	110.54
2	P	6	DC	C2-N1-C1'	-7.69	108.17	119.70
3	A	24	ASN	N-CA-C	7.68	121.91	112.54
3	A	234	LYS	N-CA-CB	7.67	122.08	110.42
1	T	7	DC	C6-N1-C1'	7.62	131.13	119.70
1	T	4	DG	C8-N9-C1'	7.54	138.31	127.00
3	A	160	ASP	CA-CB-CG	-7.53	105.07	112.60
3	A	180	SER	O-C-N	7.20	129.58	122.09
3	A	310	PRO	CB-CA-C	-7.17	104.88	111.40
2	P	6	DC	C6-N1-C1'	7.06	130.29	119.70
2	P	5	DG	C8-N9-C1'	-7.02	116.47	127.00
2	P	5	DG	C4-N9-C1'	7.00	137.50	127.00
3	A	152	ARG	N-CA-CB	6.97	121.15	109.78
3	A	231	GLY	N-CA-C	-6.96	102.64	112.60
3	A	333	ARG	CD-NE-CZ	-6.85	114.81	124.40
3	A	47	ALA	N-CA-C	6.76	118.73	111.36
3	A	193	VAL	N-CA-C	6.75	118.02	108.17
3	A	122	LEU	N-CA-C	-6.74	103.08	112.45
3	A	46	ILE	CB-CA-C	-6.70	101.77	112.16
3	A	269	VAL	CB-CA-C	-6.69	103.28	112.04
3	A	297	THR	N-CA-C	6.65	117.92	108.74
3	A	53	ILE	N-CA-CB	6.63	117.95	110.72
3	A	311	LEU	CB-CA-C	-6.54	99.35	109.62
3	A	197	HIS	CA-CB-CG	-6.50	107.30	113.80
3	A	34	HIS	CA-CB-CG	-6.48	107.32	113.80
3	A	226	ASP	CA-C-N	-6.45	113.67	122.77
3	A	226	ASP	C-N-CA	-6.45	113.67	122.77
3	A	39	TYR	CA-CB-CG	-6.43	102.32	113.90
3	A	90	GLN	CA-C-N	6.38	133.73	121.54
3	A	90	GLN	C-N-CA	6.38	133.73	121.54
3	A	301	LEU	CA-C-O	6.36	127.26	120.46
3	A	318	ASP	N-CA-CB	6.34	119.44	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	52	LYS	CA-C-N	-6.32	114.22	122.37
3	A	52	LYS	C-N-CA	-6.32	114.22	122.37
3	A	313	VAL	N-CA-CB	6.31	121.80	111.58
3	A	193	VAL	O-C-N	6.30	129.88	123.07
3	A	17	ASP	CA-CB-CG	-6.28	106.32	112.60
3	A	256	ASP	CA-CB-CG	-6.25	106.35	112.60
3	A	266	TYR	N-CA-CB	6.25	119.31	110.12
3	A	283	ARG	N-CA-CB	6.22	119.39	110.06
3	A	166	VAL	N-CA-CB	6.21	119.89	110.58
3	A	162	VAL	O-C-N	6.19	128.21	121.83
3	A	40	ARG	N-CA-CB	6.09	118.84	110.01
3	A	267	CYS	CA-CB-SG	-6.08	100.41	114.40
3	A	320	PHE	CA-CB-CG	-6.07	107.73	113.80
3	A	298	ILE	N-CA-CB	6.07	120.23	112.34
3	A	92	ASP	N-CA-C	6.05	123.69	110.80
3	A	196	THR	CA-C-O	6.05	128.59	121.58
3	A	91	ASP	CA-CB-CG	6.04	118.64	112.60
3	A	318	ASP	CA-CB-CG	5.97	118.57	112.60
3	A	293	ILE	CB-CA-C	-5.94	101.98	110.83
2	P	5	DG	P-O5'-C5'	-5.90	111.16	120.00
1	T	10	DC	C6-N1-C1'	5.85	128.47	119.70
3	A	196	THR	N-CA-C	5.83	118.27	109.41
3	A	181	PHE	CA-CB-CG	-5.82	107.98	113.80
3	A	91	ASP	N-CA-C	5.81	123.18	110.80
3	A	66	GLY	O-C-N	5.78	130.16	123.51
3	A	155	MET	O-C-N	5.76	128.23	122.12
3	A	150	ILE	CA-C-N	-5.74	113.28	120.51
3	A	150	ILE	C-N-CA	-5.74	113.28	120.51
3	A	12	ASN	N-CA-C	5.72	119.96	113.15
2	P	7	DC	N1-C1'-C2'	-5.69	104.97	113.50
3	A	273	THR	CA-C-O	5.68	126.49	119.79
3	A	103	VAL	CB-CA-C	-5.66	103.75	111.33
3	A	234	LYS	N-CA-C	5.65	118.78	110.59
3	A	12	ASN	CA-CB-CG	-5.64	106.96	112.60
3	A	96	SER	N-CA-C	5.64	117.43	111.28
2	P	3	DG	C4'-C3'-O3'	-5.61	101.59	110.00
3	A	115	VAL	CB-CA-C	5.61	119.37	112.02
3	A	45	VAL	CA-C-O	-5.58	115.47	121.27
3	A	15	ILE	N-CA-CB	5.56	120.41	111.23
3	A	142	TYR	CB-CA-C	-5.55	101.79	110.94
3	A	269	VAL	N-CA-CB	5.55	117.40	110.47
1	T	10	DC	P-O3'-C3'	-5.49	111.96	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	171	PRO	N-CA-CB	5.49	106.44	101.83
1	T	4	DG	C4'-C3'-O3'	-5.47	101.80	110.00
3	A	297	THR	N-CA-CB	-5.44	102.13	111.21
3	A	128	ASN	CA-CB-CG	-5.39	107.21	112.60
3	A	68	LYS	CA-C-N	-5.36	113.69	120.56
3	A	68	LYS	C-N-CA	-5.36	113.69	120.56
3	A	69	ILE	N-CA-CB	5.34	117.40	110.57
3	A	184	GLY	N-CA-C	5.33	122.98	115.30
1	T	10	DC	P-O5'-C5'	-5.32	112.03	120.00
2	P	5	DG	O4'-C1'-C2'	-5.30	98.44	106.40
3	A	143	PHE	N-CA-C	5.30	120.06	111.37
3	A	208	PRO	N-CA-C	-5.29	105.87	113.75
3	A	257	ILE	CB-CA-C	-5.28	102.68	110.82
3	A	132	LEU	N-CA-C	5.25	118.50	110.20
3	A	134	HIS	N-CA-C	5.24	117.39	111.11
3	A	163	LEU	O-C-N	5.22	127.67	122.08
3	A	333	ARG	N-CA-C	5.21	119.20	113.21
3	A	302	GLY	CA-C-N	5.18	127.29	120.60
3	A	302	GLY	C-N-CA	5.18	127.29	120.60
3	A	228	LEU	N-CA-CB	5.16	118.08	110.33
3	A	93	THR	CA-C-N	5.16	127.45	120.38
3	A	93	THR	C-N-CA	5.16	127.45	120.38
3	A	74	ASP	CB-CA-C	5.16	119.12	110.92
3	A	198	PRO	CA-N-CD	-5.15	104.79	112.00
3	A	106	ILE	N-CA-C	5.14	115.74	107.98
3	A	178	CYS	CA-CB-SG	-5.13	102.59	114.40
3	A	208	PRO	CB-CA-C	-5.12	103.72	112.64
3	A	171	PRO	N-CA-C	-5.11	108.14	114.68
3	A	36	TYR	N-CA-CB	-5.08	102.43	110.06
3	A	283	ARG	O-C-N	5.08	127.51	122.12
3	A	297	THR	CB-CA-C	-5.06	99.90	111.95
3	A	86	GLU	N-CA-CB	5.05	117.63	110.06
3	A	211	LEU	N-CA-C	-5.04	105.70	111.14
3	A	137	ARG	CA-C-N	-5.03	114.12	120.56
3	A	137	ARG	C-N-CA	-5.03	114.12	120.56
3	A	151	PRO	N-CA-CB	5.03	108.06	102.72
3	A	269	VAL	N-CA-C	5.03	116.36	110.62
3	A	266	TYR	CA-C-N	-5.02	113.55	120.28
3	A	266	TYR	C-N-CA	-5.02	113.55	120.28
3	A	299	ARG	O-C-N	5.02	126.64	121.72
3	A	257	ILE	CA-CB-CG1	5.01	118.92	110.40

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	1	DC	Sidechain
2	P	2	DG	Sidechain
2	P	3	DG	Sidechain
2	P	5	DG	Sidechain
2	P	7	DC	Sidechain
1	T	10	DC	Sidechain
1	T	4	DG	Sidechain
1	T	6	DG	Sidechain
1	T	9	DC	Sidechain

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	167	0	89	12	0
2	P	138	0	77	9	0
3	A	2543	0	2491	305	0
4	A	2	0	0	0	0
5	A	27	0	12	7	0
6	A	27	0	0	4	0
6	P	2	0	0	0	0
6	T	2	0	0	0	0
All	All	2908	0	2669	318	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 58.

All (318) 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:16:THR:HG23	3:A:46:ILE:HD11	1.23	1.12
3:A:270:LEU:HD21	3:A:282:MET:HE1	1.42	1.01
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.37	1.00
3:A:180:SER:HA	3:A:183:ARG:HH12	1.24	0.99
1:T:9:DC:N4	2:P:3:DG:H1	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:158:MET:HG2	3:A:241:LEU:HD11	1.54	0.89
3:A:270:LEU:CD2	3:A:282:MET:HE1	2.04	0.88
3:A:180:SER:HA	3:A:183:ARG:NH1	1.88	0.88
1:T:4:DG:N3	3:A:283:ARG:HD2	1.91	0.85
3:A:233:THR:HG21	3:A:258:ARG:HH11	1.41	0.85
1:T:9:DC:H42	2:P:3:DG:H1	0.89	0.85
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.05	0.84
3:A:16:THR:HG23	3:A:46:ILE:CD1	2.07	0.84
3:A:233:THR:HG22	3:A:258:ARG:HD2	1.59	0.83
3:A:233:THR:HG21	3:A:258:ARG:NH1	1.96	0.81
3:A:16:THR:CG2	3:A:46:ILE:HD11	2.10	0.81
5:A:338:DCT:C5'	5:A:338:DCT:H6	2.12	0.80
3:A:15:ILE:HG12	3:A:16:THR:N	1.97	0.80
1:T:4:DG:H21	3:A:283:ARG:CZ	1.93	0.79
1:T:8:DG:H5''	3:A:231:GLY:HA3	1.65	0.79
3:A:11:LEU:H	3:A:11:LEU:HD22	1.49	0.77
3:A:299:ARG:HG2	3:A:299:ARG:HH11	1.48	0.77
3:A:264:GLN:HE22	3:A:296:TYR:HB3	1.50	0.77
3:A:214:VAL:O	3:A:218:LEU:HD12	1.86	0.76
3:A:67:THR:HG23	3:A:68:LYS:H	1.50	0.75
3:A:264:GLN:NE2	3:A:296:TYR:HB3	2.02	0.75
3:A:174:ILE:O	3:A:195:LEU:HD12	1.87	0.75
3:A:198:PRO:HB3	3:A:262:LYS:HD3	1.69	0.75
3:A:154:GLU:O	3:A:158:MET:HG3	1.87	0.74
3:A:12:ASN:ND2	3:A:53:ILE:H	1.86	0.73
3:A:82:LEU:CB	3:A:85:LEU:HB3	2.18	0.73
3:A:12:ASN:HD21	3:A:53:ILE:H	1.35	0.73
3:A:16:THR:HG21	3:A:47:ALA:HB2	1.70	0.73
3:A:169:LEU:HB3	3:A:213:ARG:NH2	2.04	0.73
3:A:266:TYR:HA	3:A:269:VAL:CG2	2.19	0.72
3:A:197:HIS:ND1	3:A:198:PRO:HD2	2.05	0.72
3:A:204:SER:CB	3:A:206:LYS:HE2	2.20	0.71
3:A:108:PRO:HB2	3:A:112:ARG:NH2	2.05	0.71
3:A:41:LYS:O	3:A:44:SER:HB3	1.91	0.70
3:A:140:LEU:HD12	3:A:140:LEU:O	1.91	0.70
3:A:133:ASN:H	3:A:136:GLN:NE2	1.89	0.70
3:A:228:LEU:N	3:A:228:LEU:HD23	2.06	0.70
3:A:266:TYR:HA	3:A:269:VAL:HG23	1.74	0.70
3:A:41:LYS:NZ	3:A:41:LYS:HB3	2.05	0.70
1:T:8:DG:OP1	3:A:231:GLY:HA3	1.92	0.69
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:195:LEU:O	3:A:259:LEU:HD12	1.92	0.69
3:A:169:LEU:N	3:A:169:LEU:HD23	2.06	0.69
3:A:103:VAL:CB	3:A:106:ILE:HD12	2.23	0.68
3:A:183:ARG:HH11	3:A:183:ARG:HB2	1.58	0.68
2:P:5:DG:OP2	3:A:108:PRO:HD2	1.93	0.68
3:A:11:LEU:H	3:A:11:LEU:HD13	1.58	0.67
3:A:233:THR:CG2	3:A:258:ARG:HH11	2.08	0.67
3:A:38:ALA:CA	3:A:41:LYS:HZ2	2.07	0.67
3:A:158:MET:HG2	3:A:241:LEU:CD1	2.24	0.67
3:A:11:LEU:HD13	3:A:11:LEU:N	2.10	0.67
3:A:180:SER:HB2	3:A:188:SER:OG	1.94	0.67
3:A:133:ASN:C	3:A:133:ASN:HD22	2.03	0.67
3:A:88:ILE:O	3:A:90:GLN:N	2.28	0.66
3:A:23:ALA:HB1	3:A:36:TYR:CD1	2.30	0.66
3:A:31:GLN:O	3:A:33:ILE:N	2.28	0.66
3:A:212:HIS:HD2	3:A:230:LYS:HE2	1.60	0.66
3:A:160:ASP:O	3:A:164:ASN:ND2	2.30	0.65
3:A:11:LEU:HD22	3:A:11:LEU:N	2.11	0.65
3:A:328:ARG:CG	3:A:328:ARG:HH11	2.10	0.65
3:A:97:ILE:HG22	3:A:98:ASN:N	2.12	0.65
3:A:115:VAL:CG2	3:A:120:LYS:HB3	2.27	0.64
3:A:149:ARG:O	3:A:151:PRO:HD3	1.97	0.64
3:A:125:LEU:O	3:A:128:ASN:N	2.30	0.64
3:A:299:ARG:HG2	3:A:299:ARG:NH1	2.12	0.64
3:A:36:TYR:O	3:A:39:TYR:HB2	1.97	0.64
3:A:279:ASN:O	3:A:283:ARG:HG3	1.97	0.64
3:A:196:THR:HG21	3:A:262:LYS:HA	1.78	0.64
3:A:17:ASP:O	3:A:20:VAL:HG12	1.98	0.64
3:A:183:ARG:HH11	3:A:183:ARG:CG	2.11	0.64
3:A:208:PRO:CD	3:A:209:LYS:H	2.10	0.64
3:A:330:PRO:HA	3:A:333:ARG:HE	1.63	0.63
3:A:104:THR:HG22	3:A:139:GLY:CA	2.28	0.63
3:A:115:VAL:HG22	3:A:120:LYS:HB3	1.80	0.63
3:A:133:ASN:ND2	3:A:136:GLN:H	1.96	0.63
2:P:5:DG:P	3:A:107:GLY:HA3	2.39	0.63
3:A:82:LEU:O	3:A:86:GLU:N	2.29	0.62
3:A:197:HIS:CE1	3:A:198:PRO:HD2	2.33	0.62
3:A:233:THR:CG2	3:A:258:ARG:HD2	2.28	0.62
3:A:27:LYS:HB2	3:A:36:TYR:CD1	2.35	0.61
3:A:38:ALA:HA	3:A:41:LYS:HZ2	1.64	0.61
3:A:86:GLU:HA	3:A:86:GLU:OE1	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:154:GLU:OE1	3:A:253:ARG:NH2	2.30	0.61
3:A:301:LEU:HD23	3:A:301:LEU:O	2.00	0.61
3:A:333:ARG:HD2	6:A:405:HOH:O	2.02	0.60
3:A:38:ALA:C	3:A:41:LYS:HZ2	2.10	0.60
3:A:317:GLN:HG3	3:A:327:TYR:CD2	2.36	0.60
3:A:238:VAL:HG12	3:A:239:CYS:N	2.16	0.59
3:A:328:ARG:HH11	3:A:328:ARG:HB3	1.66	0.59
3:A:328:ARG:HH11	3:A:328:ARG:CB	2.15	0.59
3:A:159:GLN:O	3:A:163:LEU:HG	2.01	0.59
3:A:121:THR:HG1	3:A:124:ASP:H	1.48	0.59
3:A:100:LEU:HD11	3:A:125:LEU:CD2	2.33	0.59
2:P:2:DG:H2''	2:P:3:DG:H5'	1.85	0.58
3:A:38:ALA:O	3:A:41:LYS:NZ	2.35	0.58
3:A:104:THR:HG22	3:A:139:GLY:HA3	1.84	0.58
3:A:299:ARG:HB2	3:A:300:PRO:HD2	1.85	0.58
3:A:166:VAL:CG1	3:A:173:TYR:HB3	2.34	0.58
3:A:88:ILE:C	3:A:90:GLN:H	2.11	0.58
3:A:125:LEU:HB3	3:A:140:LEU:HD22	1.85	0.58
3:A:133:ASN:HD21	3:A:136:GLN:HG3	1.69	0.58
3:A:183:ARG:HH11	3:A:183:ARG:CB	2.17	0.57
3:A:227:THR:C	3:A:228:LEU:HD23	2.29	0.57
3:A:278:PHE:HB2	3:A:333:ARG:O	2.02	0.57
3:A:281:ASN:O	3:A:284:ALA:HB3	2.04	0.57
3:A:153:GLU:O	3:A:156:LEU:HB2	2.04	0.57
3:A:301:LEU:HD23	3:A:301:LEU:C	2.30	0.57
3:A:60:LYS:HA	3:A:65:VAL:HG22	1.86	0.57
3:A:77:LEU:HD13	3:A:77:LEU:N	2.19	0.57
3:A:129:GLU:HA	3:A:132:LEU:HD12	1.86	0.57
2:P:2:DG:C2'	2:P:3:DG:H5'	2.35	0.56
3:A:75:GLU:O	3:A:79:THR:HG23	2.05	0.56
3:A:265:TYR:O	3:A:269:VAL:HG22	2.05	0.56
3:A:62:LEU:O	3:A:65:VAL:HG13	2.05	0.56
3:A:98:ASN:O	3:A:101:THR:HB	2.04	0.56
3:A:224:ILE:HD13	3:A:235:PHE:CZ	2.40	0.56
3:A:31:GLN:HG3	3:A:32:ALA:N	2.19	0.56
3:A:100:LEU:O	3:A:103:VAL:HG23	2.06	0.56
3:A:210:LEU:O	3:A:214:VAL:HG12	2.07	0.55
3:A:102:ARG:HH21	3:A:147:GLU:CD	2.13	0.55
1:T:8:DG:H5''	3:A:231:GLY:CA	2.34	0.55
3:A:204:SER:HB2	3:A:206:LYS:HG2	1.87	0.55
3:A:293:ILE:HG12	3:A:298:ILE:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:328:ARG:HH11	3:A:328:ARG:HG2	1.72	0.55
3:A:330:PRO:HD3	3:A:333:ARG:NH2	2.21	0.55
3:A:133:ASN:H	3:A:136:GLN:HE21	1.53	0.55
3:A:300:PRO:HD3	3:A:309:GLU:O	2.07	0.55
3:A:122:LEU:HD13	3:A:122:LEU:C	2.32	0.54
3:A:198:PRO:HD2	3:A:199:ASN:H	1.71	0.54
3:A:279:ASN:HA	6:A:426:HOH:O	2.08	0.54
3:A:282:MET:HE2	6:A:426:HOH:O	2.06	0.54
3:A:194:LEU:HD13	3:A:195:LEU:N	2.22	0.54
3:A:59:ALA:O	3:A:62:LEU:HB2	2.07	0.54
3:A:164:ASN:O	3:A:167:LYS:N	2.41	0.54
3:A:102:ARG:NH2	3:A:147:GLU:OE2	2.41	0.54
3:A:100:LEU:HD11	3:A:125:LEU:HD21	1.88	0.54
3:A:223:PHE:O	3:A:239:CYS:HA	2.08	0.54
3:A:16:THR:HG22	3:A:43:ALA:HB1	1.90	0.53
3:A:274:GLY:CA	5:A:338:DCT:H2'	2.39	0.53
3:A:283:ARG:O	3:A:287:LEU:HD13	2.08	0.53
3:A:108:PRO:HB2	3:A:112:ARG:HH22	1.73	0.53
3:A:240:GLN:O	3:A:242:PRO:HD3	2.09	0.53
3:A:104:THR:HG22	3:A:139:GLY:HA2	1.90	0.53
3:A:202:SER:N	3:A:263:ASP:OD1	2.37	0.53
3:A:41:LYS:HB3	3:A:41:LYS:HZ2	1.74	0.52
3:A:140:LEU:HD12	3:A:140:LEU:C	2.31	0.52
3:A:71:GLU:O	3:A:74:ASP:N	2.42	0.52
3:A:149:ARG:NH2	5:A:338:DCT:O2G	2.42	0.52
3:A:287:LEU:HD12	3:A:291:PHE:O	2.08	0.52
5:A:338:DCT:H6	5:A:338:DCT:H5'	1.89	0.52
3:A:285:HIS:CD2	3:A:325:TRP:NE1	2.78	0.52
3:A:46:ILE:HD12	3:A:47:ALA:HA	1.91	0.52
3:A:84:LYS:O	3:A:87:LYS:HB3	2.10	0.52
3:A:128:ASN:N	3:A:128:ASN:ND2	2.57	0.52
3:A:56:GLY:O	3:A:59:ALA:HB3	2.10	0.52
3:A:70:ALA:O	3:A:73:ILE:HB	2.09	0.51
3:A:82:LEU:O	3:A:85:LEU:N	2.44	0.51
2:P:1:DC:O3'	2:P:2:DG:O4'	2.28	0.51
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.91	0.51
3:A:33:ILE:HG23	3:A:34:HIS:N	2.26	0.51
3:A:85:LEU:O	3:A:88:ILE:HG22	2.10	0.51
3:A:215:VAL:HG11	3:A:235:PHE:CD2	2.45	0.51
3:A:177:VAL:HG22	3:A:181:PHE:CD2	2.46	0.51
3:A:15:ILE:O	3:A:18:MET:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:221:VAL:HG12	3:A:221:VAL:O	2.11	0.50
3:A:182:ARG:C	3:A:184:GLY:H	2.19	0.50
3:A:106:ILE:CG2	3:A:111:ALA:HB2	2.41	0.50
3:A:238:VAL:CG1	3:A:239:CYS:N	2.74	0.50
3:A:133:ASN:ND2	3:A:136:GLN:HG3	2.27	0.50
3:A:198:PRO:CB	3:A:262:LYS:HD3	2.39	0.50
3:A:274:GLY:HA3	5:A:338:DCT:H2''	1.94	0.50
5:A:338:DCT:O2B	5:A:338:DCT:O1A	2.30	0.50
3:A:12:ASN:HD21	3:A:53:ILE:N	2.06	0.50
3:A:159:GLN:N	3:A:191:MET:HE1	2.27	0.50
3:A:96:SER:O	3:A:99:PHE:HB3	2.12	0.50
3:A:117:GLU:OE1	3:A:131:LYS:NZ	2.42	0.49
3:A:311:LEU:HB3	3:A:312:PRO:HD2	1.92	0.49
3:A:46:ILE:HD12	3:A:46:ILE:C	2.37	0.49
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.46	0.49
1:T:9:DC:H5'	3:A:229:SER:HB3	1.93	0.49
3:A:152:ARG:O	3:A:156:LEU:HD22	2.13	0.49
3:A:193:VAL:O	3:A:193:VAL:HG22	2.12	0.49
3:A:204:SER:O	3:A:206:LYS:HD3	2.13	0.49
3:A:152:ARG:NH2	3:A:181:PHE:O	2.45	0.48
3:A:197:HIS:O	3:A:200:PHE:HB3	2.13	0.48
3:A:278:PHE:CE2	3:A:333:ARG:CD	2.96	0.48
3:A:209:LYS:HA	3:A:212:HIS:HB2	1.94	0.48
3:A:212:HIS:CD2	3:A:230:LYS:HE2	2.44	0.48
3:A:299:ARG:CD	3:A:307:ALA:HB1	2.44	0.48
3:A:183:ARG:HE	3:A:275:SER:HB3	1.78	0.48
3:A:204:SER:HB3	3:A:206:LYS:HE2	1.93	0.48
3:A:60:LYS:HA	3:A:65:VAL:CG2	2.44	0.48
3:A:162:VAL:HG12	3:A:163:LEU:HD23	1.95	0.48
3:A:62:LEU:HB3	3:A:65:VAL:HG11	1.96	0.48
3:A:180:SER:CA	3:A:183:ARG:HH12	2.11	0.48
3:A:194:LEU:HA	3:A:194:LEU:HD22	1.48	0.47
1:T:4:DG:H2''	1:T:5:DG:O5'	2.14	0.47
3:A:133:ASN:O	3:A:137:ARG:HG3	2.15	0.47
3:A:138:ILE:CG2	3:A:142:TYR:HD2	2.27	0.47
3:A:197:HIS:CG	3:A:198:PRO:CD	2.97	0.47
3:A:158:MET:HB2	3:A:191:MET:HE1	1.97	0.47
3:A:217:GLN:O	3:A:221:VAL:HG23	2.14	0.47
3:A:330:PRO:HD3	3:A:333:ARG:HH21	1.80	0.47
3:A:299:ARG:HB2	3:A:300:PRO:CD	2.43	0.47
3:A:46:ILE:HG13	3:A:47:ALA:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:270:LEU:HD21	3:A:282:MET:CE	2.30	0.47
3:A:158:MET:HB2	3:A:191:MET:CE	2.45	0.46
3:A:224:ILE:HD13	3:A:235:PHE:CE1	2.50	0.46
3:A:172:GLU:HG2	3:A:198:PRO:HG3	1.97	0.46
3:A:41:LYS:O	3:A:45:VAL:HG12	2.14	0.46
3:A:304:THR:HG23	3:A:305:GLY:N	2.31	0.46
3:A:76:PHE:HD1	3:A:77:LEU:CD1	2.28	0.46
3:A:77:LEU:HA	3:A:77:LEU:HD12	1.22	0.46
3:A:208:PRO:CG	3:A:209:LYS:H	2.28	0.46
3:A:115:VAL:HG23	3:A:120:LYS:HB3	1.98	0.46
3:A:183:ARG:HH11	3:A:183:ARG:HG3	1.77	0.46
3:A:88:ILE:HG23	3:A:89:ARG:N	2.31	0.46
1:T:4:DG:H21	3:A:283:ARG:NE	2.11	0.46
3:A:294:ASN:OD1	3:A:296:TYR:HB2	2.16	0.46
3:A:255:ILE:CG1	3:A:256:ASP:N	2.79	0.45
3:A:19:LEU:HD12	3:A:19:LEU:HA	1.52	0.45
3:A:127:LYS:HB3	3:A:127:LYS:HE2	1.76	0.45
3:A:23:ALA:O	3:A:36:TYR:HD1	1.99	0.45
3:A:76:PHE:HD1	3:A:77:LEU:HD13	1.81	0.45
3:A:196:THR:CG2	3:A:262:LYS:HA	2.46	0.45
3:A:46:ILE:CG1	3:A:47:ALA:N	2.78	0.45
3:A:202:SER:HB3	3:A:264:GLN:OE1	2.17	0.45
3:A:75:GLU:OE2	3:A:82:LEU:HA	2.15	0.45
2:P:1:DC:H2''	2:P:2:DG:C8	2.51	0.45
3:A:88:ILE:HG23	3:A:89:ARG:H	1.82	0.45
3:A:208:PRO:CG	3:A:209:LYS:N	2.80	0.45
3:A:317:GLN:O	3:A:320:PHE:HB2	2.17	0.45
3:A:330:PRO:CD	3:A:333:ARG:HH21	2.30	0.45
3:A:198:PRO:CD	3:A:199:ASN:H	2.30	0.44
3:A:133:ASN:C	3:A:133:ASN:ND2	2.73	0.44
3:A:219:GLN:C	3:A:221:VAL:H	2.25	0.44
3:A:225:THR:OG1	3:A:226:ASP:OD1	2.29	0.44
3:A:126:ARG:NH1	3:A:126:ARG:HG3	2.33	0.44
3:A:150:ILE:HG22	3:A:155:MET:HG2	2.00	0.44
1:T:7:DC:H2''	1:T:8:DG:O5'	2.17	0.44
3:A:93:THR:HG23	3:A:94:SER:N	2.32	0.44
3:A:323:ILE:HG13	3:A:325:TRP:HB2	2.00	0.44
3:A:204:SER:C	3:A:206:LYS:HG2	2.43	0.44
3:A:255:ILE:HG13	3:A:256:ASP:N	2.32	0.44
3:A:299:ARG:HB3	3:A:310:PRO:HA	2.00	0.44
3:A:66:GLY:O	3:A:69:ILE:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:103:VAL:CG2	3:A:106:ILE:HD12	2.49	0.43
3:A:164:ASN:O	3:A:167:LYS:HB2	2.19	0.43
3:A:126:ARG:NE	3:A:140:LEU:HD11	2.32	0.43
3:A:208:PRO:CD	3:A:209:LYS:N	2.80	0.43
3:A:278:PHE:CE2	3:A:333:ARG:HD3	2.52	0.43
3:A:317:GLN:HA	3:A:327:TYR:HD2	1.83	0.43
3:A:266:TYR:O	3:A:269:VAL:HG23	2.19	0.43
3:A:255:ILE:HG13	3:A:256:ASP:H	1.83	0.43
3:A:214:VAL:CG2	3:A:218:LEU:HD11	2.48	0.43
3:A:260:ILE:HD13	3:A:260:ILE:HA	1.68	0.43
3:A:11:LEU:H	3:A:11:LEU:CD1	2.22	0.43
3:A:163:LEU:HD23	3:A:163:LEU:N	2.25	0.43
3:A:204:SER:HB2	3:A:206:LYS:CG	2.48	0.43
3:A:228:LEU:N	3:A:228:LEU:CD2	2.79	0.43
3:A:36:TYR:C	3:A:39:TYR:HB2	2.44	0.43
3:A:328:ARG:CB	3:A:328:ARG:NH1	2.82	0.43
5:A:338:DCT:H6	5:A:338:DCT:C4'	2.28	0.43
3:A:114:LEU:HD23	3:A:114:LEU:HA	1.50	0.42
3:A:156:LEU:HD13	3:A:156:LEU:HA	1.44	0.42
3:A:201:THR:C	3:A:203:GLU:H	2.27	0.42
3:A:23:ALA:HB1	3:A:36:TYR:HD1	1.81	0.42
3:A:91:ASP:CG	3:A:92:ASP:N	2.77	0.42
3:A:178:CYS:HA	3:A:182:ARG:HB3	2.01	0.42
3:A:195:LEU:HD12	3:A:195:LEU:HA	1.79	0.42
3:A:333:ARG:HD3	3:A:333:ARG:HH11	1.46	0.42
3:A:204:SER:HB2	3:A:206:LYS:HE2	1.99	0.42
3:A:177:VAL:HG22	3:A:181:PHE:HD2	1.85	0.42
3:A:215:VAL:HG21	3:A:230:LYS:HE3	2.01	0.42
3:A:270:LEU:HD12	6:A:405:HOH:O	2.19	0.42
3:A:330:PRO:HG3	3:A:333:ARG:HH21	1.85	0.42
3:A:299:ARG:NE	3:A:307:ALA:HB1	2.34	0.42
3:A:112:ARG:O	3:A:115:VAL:N	2.53	0.42
3:A:169:LEU:HD23	3:A:169:LEU:H	1.81	0.42
3:A:314:ASP:O	3:A:315:SER:HB3	2.20	0.42
3:A:319:ILE:H	3:A:319:ILE:HG13	1.68	0.42
3:A:76:PHE:CD1	3:A:76:PHE:C	2.98	0.41
2:P:2:DG:C2'	2:P:3:DG:C5'	2.98	0.41
3:A:104:THR:O	3:A:104:THR:HG23	2.20	0.41
3:A:198:PRO:CD	3:A:199:ASN:N	2.83	0.41
3:A:126:ARG:HG3	3:A:126:ARG:HH11	1.86	0.41
3:A:182:ARG:C	3:A:184:GLY:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:196:THR:OG1	3:A:260:ILE:O	2.28	0.41
3:A:201:THR:O	3:A:203:GLU:N	2.54	0.41
3:A:286:ALA:HA	3:A:323:ILE:HG22	2.03	0.41
3:A:79:THR:C	3:A:81:LYS:N	2.77	0.41
3:A:169:LEU:N	3:A:169:LEU:CD2	2.79	0.41
3:A:206:LYS:HG3	3:A:207:GLN:HG2	2.02	0.41
3:A:206:LYS:HB2	3:A:207:GLN:H	1.39	0.41
3:A:328:ARG:HB3	3:A:328:ARG:NH1	2.31	0.41
3:A:15:ILE:C	3:A:17:ASP:N	2.78	0.41
3:A:24:ASN:HA	3:A:27:LYS:HB3	2.03	0.41
3:A:138:ILE:HG23	3:A:142:TYR:CD2	2.56	0.41
3:A:200:PHE:C	3:A:201:THR:HG23	2.46	0.41
3:A:208:PRO:HB3	3:A:232:GLU:HB3	2.01	0.41
3:A:219:GLN:O	3:A:221:VAL:N	2.53	0.41
3:A:327:TYR:O	3:A:328:ARG:HG3	2.21	0.41
3:A:235:PHE:CD1	3:A:235:PHE:C	2.97	0.41
3:A:26:GLU:O	3:A:30:SER:HB2	2.22	0.40
3:A:75:GLU:O	3:A:75:GLU:HG2	2.21	0.40
3:A:127:LYS:C	3:A:128:ASN:ND2	2.79	0.40
3:A:28:ASN:C	3:A:30:SER:H	2.29	0.40
3:A:26:GLU:HG3	3:A:32:ALA:CB	2.52	0.40
3:A:142:TYR:O	3:A:145:ASP:HB2	2.22	0.40
3:A:201:THR:HB	3:A:263:ASP:OD1	2.22	0.40
1:T:4:DG:C2	3:A:283:ARG:HD2	2.54	0.40
3:A:11:LEU:H	3:A:11:LEU:CD2	2.16	0.40
3:A:280:LYS:O	3:A:284:ALA:HB2	2.21	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	320/335 (96%)	258 (81%)	48 (15%)	14 (4%)	2 8

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	32	ALA
3	A	89	ARG
3	A	91	ASP
3	A	10	THR
3	A	67	THR
3	A	82	LEU
3	A	88	ILE
3	A	204	SER
3	A	205	SER
3	A	220	LYS
3	A	262	LYS
3	A	164	ASN
3	A	202	SER
3	A	81	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	267/296 (90%)	212 (79%)	55 (21%)	1 4

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	THR
3	A	11	LEU
3	A	15	ILE
3	A	16	THR
3	A	19	LEU
3	A	26	GLU
3	A	29	VAL

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Mol	Chain	Res	Type
3	A	31	GLN
3	A	37	ASN
3	A	41	LYS
3	A	45	VAL
3	A	61	LYS
3	A	65	VAL
3	A	67	THR
3	A	77	LEU
3	A	79	THR
3	A	85	LEU
3	A	88	ILE
3	A	97	ILE
3	A	101	THR
3	A	114	LEU
3	A	115	VAL
3	A	125	LEU
3	A	127	LYS
3	A	128	ASN
3	A	130	ASP
3	A	133	ASN
3	A	156	LEU
3	A	169	LEU
3	A	172	GLU
3	A	173	TYR
3	A	176	THR
3	A	177	VAL
3	A	183	ARG
3	A	193	VAL
3	A	194	LEU
3	A	196	THR
3	A	205	SER
3	A	215	VAL
3	A	224	ILE
3	A	226	ASP
3	A	228	LEU
3	A	236	MET
3	A	257	ILE
3	A	260	ILE
3	A	269	VAL
3	A	272	PHE
3	A	283	ARG
3	A	298	ILE

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Mol	Chain	Res	Type
3	A	301	LEU
3	A	306	VAL
3	A	311	LEU
3	A	313	VAL
3	A	318	ASP
3	A	328	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	31	GLN
3	A	37	ASN
3	A	51	HIS
3	A	98	ASN
3	A	128	ASN
3	A	133	ASN
3	A	136	GLN
3	A	164	ASN
3	A	199	ASN
3	A	252	HIS
3	A	279	ASN
3	A	281	ASN
3	A	285	HIS
3	A	324	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 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
5	DCT	A	338	4	27,28,28	2.71	4 (14%)	37,43,43	4.78	8 (21%)

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
5	DCT	A	338	4	-	7/22/31/31	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	338	DCT	PB-O3A	-9.66	1.49	1.59
5	A	338	DCT	PB-O3B	-8.24	1.50	1.59
5	A	338	DCT	PG-O2G	-2.84	1.44	1.54
5	A	338	DCT	O5'-C5'	-2.58	1.34	1.44

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	338	DCT	C1'-N1-C2	20.98	153.83	117.83
5	A	338	DCT	C1'-N1-C6	-18.26	85.62	121.53
5	A	338	DCT	C3'-C2'-C1'	-4.37	97.84	102.87
5	A	338	DCT	C2'-C1'-N1	3.03	118.15	112.40
5	A	338	DCT	O2A-PA-O1A	2.91	125.98	112.44
5	A	338	DCT	O4'-C4'-C5'	-2.85	104.19	109.34
5	A	338	DCT	C4'-O4'-C1'	-2.13	107.80	109.81
5	A	338	DCT	O5'-PA-O1A	-2.09	100.65	108.94

There are no chirality outliers.

All (7) torsion outliers are listed below:

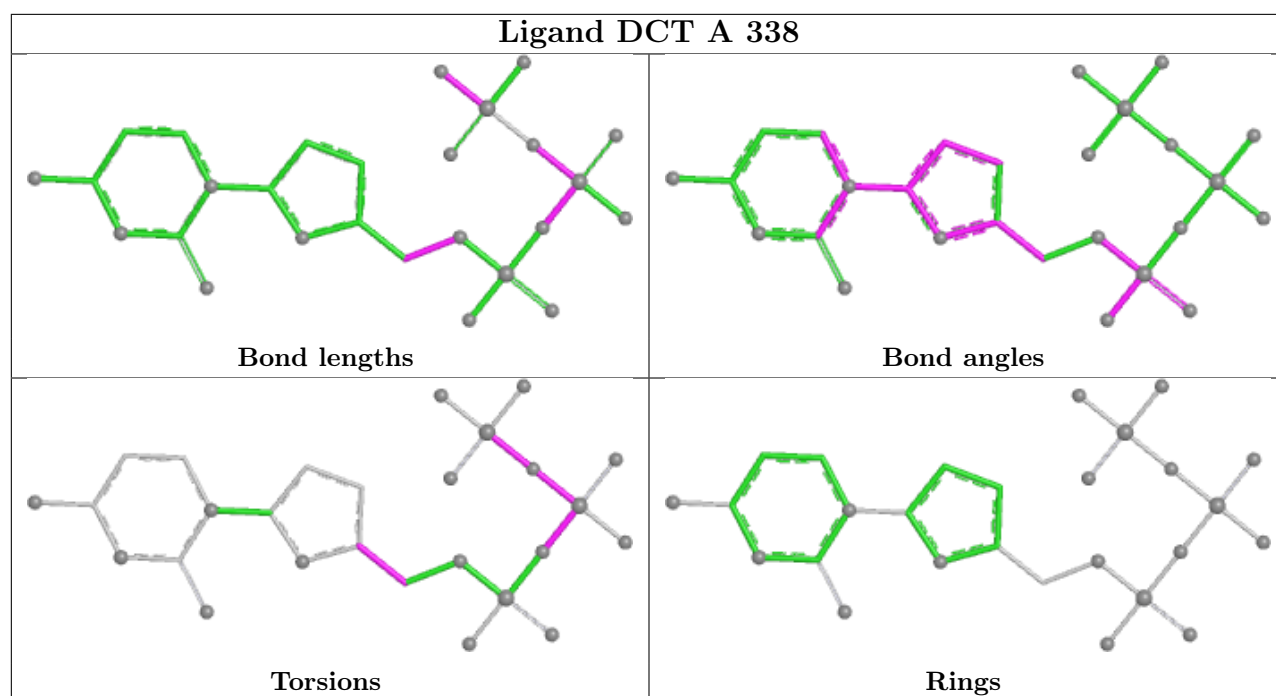
Mol	Chain	Res	Type	Atoms
5	A	338	DCT	C3'-C4'-C5'-O5'
5	A	338	DCT	PB-O3B-PG-O3G
5	A	338	DCT	O4'-C4'-C5'-O5'
5	A	338	DCT	PA-O3A-PB-O1B
5	A	338	DCT	PG-O3B-PB-O2B
5	A	338	DCT	PA-O3A-PB-O2B
5	A	338	DCT	PG-O3B-PB-O1B

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	338	DCT	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.