



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:00 AM UTC

PDB ID : 8ICJ / pdb_00008icj
Title : DNA POLYMERASE BETA (E.C.2.7.7.7)/DNA COMPLEX + THYMIDIN
E-5'-TRIPHOSPHATE, SOAKED IN THE PRESENCE OF DTTP AND
MGCL2
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-04-19
Resolution : 3.20 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

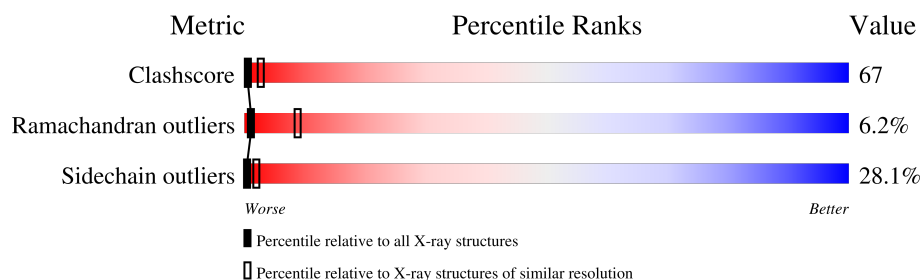
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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	
2	P	7	
3	A	335	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	TTP	A	338	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3058 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

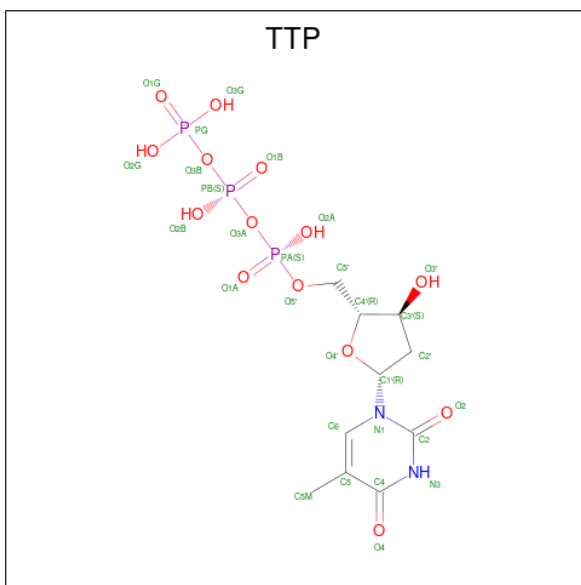
- Molecule 3 is a protein called PROTEIN (DNA POLYMERASE BETA (E.C.2.7.7.7)).

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	T	12	Total O 12 12	0	0
6	P	18	Total O 18 18	0	0
6	A	109	Total O 109 109	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.

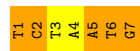
- Molecule 1: DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3')

Chain T: 

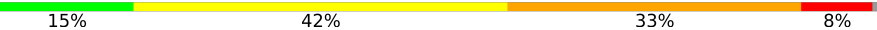


- Molecule 2: DNA (5'-D(*TP*CP*TP*AP*AP*TP*G)-3')

Chain P: 

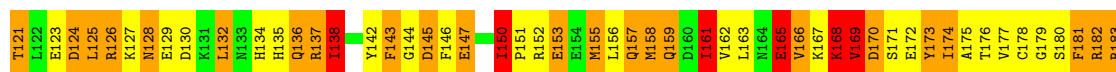


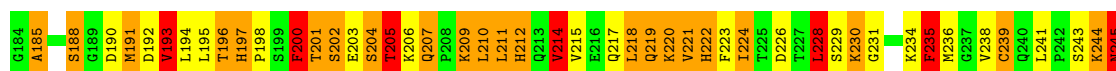
- Molecule 3: PROTEIN (DNA POLYMERASE BETA (E.C.2.7.7.7))

Chain A: 

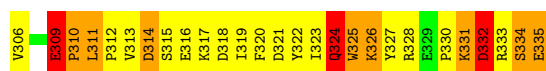












4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.89Å 57.76Å 48.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20	Depositor
% Data completeness (in resolution range)	93.0 (20.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.165 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3058	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

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: TTP, 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	0.93	0/162	3.90	16/249 (6.4%)
2	P	1.35	1/160 (0.6%)	3.22	18/243 (7.4%)
3	A	1.65	22/2672 (0.8%)	2.24	141/3590 (3.9%)
All	All	1.60	23/2994 (0.8%)	2.44	175/4082 (4.3%)

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 (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	138	ILE	N-CA	-7.11	1.37	1.46
2	P	1	DT	OP3-P	6.92	1.62	1.48
3	A	150	ILE	CA-C	6.85	1.58	1.53
3	A	224	ILE	CA-C	-6.48	1.45	1.52
3	A	150	ILE	N-CA	6.29	1.51	1.46
3	A	30	SER	C-N	-6.29	1.26	1.33
3	A	175	ALA	CA-C	-6.08	1.45	1.52
3	A	125	LEU	N-CA	-6.03	1.38	1.46
3	A	15	ILE	CA-C	-5.96	1.45	1.52
3	A	147	GLU	CD-OE2	5.83	1.36	1.25
3	A	106	ILE	CA-C	-5.83	1.46	1.52
3	A	65	VAL	CA-C	-5.60	1.47	1.53
3	A	254	ARG	C-N	-5.58	1.24	1.33
3	A	220	LYS	CA-C	-5.50	1.45	1.52
3	A	224	ILE	CA-CB	-5.41	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	174	ILE	CA-CB	-5.40	1.48	1.54
3	A	158	MET	CA-C	-5.34	1.46	1.52
3	A	77	LEU	C-O	-5.22	1.18	1.24
3	A	67	THR	N-CA	-5.21	1.39	1.46
3	A	193	VAL	CA-CB	-5.13	1.47	1.54
3	A	321	ASP	CG-OD2	5.08	1.34	1.25
3	A	181	PHE	N-CA	-5.05	1.40	1.46
3	A	144	GLY	C-O	-5.02	1.17	1.23

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	7	DA	C4-N9-C1'	-26.94	86.64	127.05
1	T	7	DA	C8-N9-C1'	26.59	166.93	127.05
2	P	1	DT	C6-N1-C1'	-18.41	91.74	119.35
2	P	1	DT	C2-N1-C1'	17.50	145.61	119.35
1	T	6	DG	C4-N9-C1'	-17.23	101.16	127.00
1	T	6	DG	C8-N9-C1'	17.19	152.78	127.00
1	T	4	DT	C6-N1-C1'	-16.00	95.34	119.35
1	T	4	DT	C2-N1-C1'	15.89	143.18	119.35
2	P	3	DT	C2-N1-C1'	15.19	142.13	119.35
3	A	77	LEU	N-CA-CB	13.82	130.43	110.12
2	P	3	DT	C6-N1-C1'	-13.40	99.25	119.35
1	T	5	DA	C8-N9-C1'	12.66	146.05	127.05
1	T	5	DA	C4-N9-C1'	-12.15	108.83	127.05
2	P	5	DA	C4-N9-C1'	11.68	144.56	127.05
3	A	291	PHE	N-CA-C	11.54	123.46	108.34
3	A	49	TYR	CA-C-N	11.54	132.93	120.12
3	A	49	TYR	C-N-CA	11.54	132.93	120.12
2	P	5	DA	C8-N9-C1'	-11.53	109.75	127.05
3	A	260	ILE	O-C-N	11.43	128.89	121.69
3	A	256	ASP	CA-CB-CG	11.26	123.86	112.60
2	P	2	DC	C2-N1-C1'	10.19	134.98	119.70
3	A	272	PHE	CA-CB-CG	-10.10	103.70	113.80
2	P	4	DA	C4-N9-C1'	-9.00	113.55	127.05
1	T	1	DC	P-O3'-C3'	8.97	133.65	120.20
2	P	6	DT	C2-N1-C1'	8.97	132.81	119.35
2	P	4	DA	C8-N9-C1'	8.70	140.10	127.05
1	T	2	DA	C8-N9-C1'	8.66	140.04	127.05
3	A	72	LYS	CB-CA-C	8.57	124.34	110.88
3	A	150	ILE	N-CA-C	8.51	115.98	107.55
2	P	6	DT	C6-N1-C1'	-8.31	106.88	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	224	ILE	CA-CB-CG1	-8.24	96.39	110.40
1	T	2	DA	C4-N9-C1'	-8.05	114.97	127.05
3	A	65	VAL	N-CA-C	8.02	119.23	106.32
3	A	68	LYS	N-CA-CB	8.01	122.02	110.16
3	A	173	TYR	CB-CA-C	-7.83	97.36	109.89
2	P	2	DC	C6-N1-C1'	-7.70	108.16	119.70
3	A	161	ILE	N-CA-C	7.68	117.79	110.42
3	A	200	PHE	CA-CB-CG	7.64	121.44	113.80
3	A	151	PRO	N-CA-CB	7.55	110.06	103.27
2	P	7	DG	P-O5'-C5'	-7.38	108.94	120.00
3	A	68	LYS	O-C-N	7.22	130.38	122.15
3	A	49	TYR	O-C-N	7.12	129.51	121.32
3	A	296	TYR	N-CA-C	6.98	122.58	114.62
3	A	117	GLU	N-CA-C	-6.96	104.26	112.89
3	A	260	ILE	CA-C-N	6.77	126.73	119.76
3	A	260	ILE	C-N-CA	6.77	126.73	119.76
3	A	219	GLN	CB-CA-C	-6.77	98.32	110.70
3	A	211	LEU	CA-C-N	6.76	129.64	120.38
3	A	211	LEU	C-N-CA	6.76	129.64	120.38
3	A	12	ASN	CB-CA-C	6.71	121.33	109.65
3	A	17	ASP	N-CA-CB	6.68	119.94	110.12
2	P	3	DT	O5'-C5'-C4'	-6.64	100.84	110.80
3	A	271	TYR	CA-CB-CG	-6.58	102.05	113.90
3	A	30	SER	CA-C-N	-6.56	112.06	122.95
3	A	30	SER	C-N-CA	-6.56	112.06	122.95
3	A	170	ASP	N-CA-C	-6.54	99.38	109.52
3	A	211	LEU	N-CA-CB	6.48	119.46	110.07
3	A	321	ASP	CB-CA-C	-6.44	100.50	110.81
3	A	124	ASP	CA-CB-CG	-6.38	106.22	112.60
3	A	70	ALA	N-CA-C	-6.36	104.34	111.28
3	A	53	ILE	N-CA-CB	6.35	117.87	110.82
3	A	181	PHE	CA-CB-CG	-6.34	107.46	113.80
3	A	15	ILE	N-CA-CB	6.34	117.53	110.62
2	P	6	DT	C4-C5-C7	-6.33	112.90	122.40
3	A	246	ASP	N-CA-C	6.30	124.21	110.80
3	A	256	ASP	N-CA-CB	6.29	121.38	110.81
3	A	277	ILE	N-CA-CB	6.29	121.07	110.56
2	P	3	DT	C4'-C3'-O3'	-6.26	100.60	110.00
3	A	271	TYR	N-CA-C	6.26	118.65	111.02
3	A	130	ASP	CA-CB-CG	6.23	118.83	112.60
1	T	7	DA	P-O5'-C5'	-6.21	110.69	120.00
3	A	296	TYR	CB-CA-C	-6.19	101.05	109.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	168	LYS	N-CA-CB	6.14	119.14	110.12
3	A	212	HIS	CA-CB-CG	-6.13	107.67	113.80
3	A	136	GLN	N-CA-C	6.12	118.92	111.82
3	A	270	LEU	O-C-N	6.08	128.58	122.08
3	A	313	VAL	N-CA-C	6.06	116.74	107.77
3	A	299	ARG	N-CA-C	6.06	118.25	109.04
3	A	158	MET	O-C-N	6.05	128.32	122.03
3	A	116	ASP	CA-CB-CG	-6.03	106.57	112.60
3	A	309	GLU	N-CA-C	6.03	123.14	109.81
3	A	134	HIS	CA-CB-CG	6.02	119.82	113.80
3	A	309	GLU	CA-C-N	5.99	127.33	119.84
3	A	309	GLU	C-N-CA	5.99	127.33	119.84
3	A	74	ASP	N-CA-CB	5.96	118.82	109.94
3	A	197	HIS	CA-C-N	5.95	125.65	119.05
3	A	197	HIS	C-N-CA	5.95	125.65	119.05
1	T	3	DT	C2-N1-C1'	5.92	128.23	119.35
3	A	114	PHE	CA-CB-CG	-5.90	107.90	113.80
3	A	94	SER	N-CA-C	-5.88	105.00	111.82
3	A	21	GLU	CA-C-N	5.87	128.94	120.79
3	A	21	GLU	C-N-CA	5.87	128.94	120.79
3	A	34	HIS	N-CA-C	5.86	117.54	111.03
3	A	173	TYR	N-CA-C	5.85	118.73	109.96
3	A	209	LYS	O-C-N	5.82	128.29	122.12
3	A	332	ASP	N-CA-C	5.81	119.99	113.02
3	A	157	GLN	N-CA-CB	5.78	119.24	110.28
3	A	143	PHE	CB-CA-C	5.77	120.04	110.81
3	A	311	LEU	CA-C-N	5.76	125.95	119.90
3	A	311	LEU	C-N-CA	5.76	125.95	119.90
3	A	106	ILE	N-CA-C	5.74	116.69	107.73
3	A	94	SER	CA-CB-OG	-5.67	99.75	111.10
3	A	32	ALA	N-CA-C	5.64	118.52	110.68
3	A	136	GLN	CB-CG-CD	-5.63	103.02	112.60
3	A	193	VAL	N-CA-CB	-5.63	104.39	110.53
3	A	137	ARG	N-CA-C	-5.62	104.78	111.69
3	A	30	SER	O-C-N	-5.61	116.69	123.03
3	A	43	ALA	CA-C-N	5.61	129.31	120.89
3	A	43	ALA	C-N-CA	5.61	129.31	120.89
3	A	267	CYS	O-C-N	5.60	127.84	122.07
3	A	17	ASP	CB-CA-C	5.60	120.09	110.79
3	A	38	ALA	CA-C-N	5.59	128.54	120.38
3	A	38	ALA	C-N-CA	5.59	128.54	120.38
3	A	318	ASP	CA-CB-CG	-5.58	107.02	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	192	ASP	CA-CB-CG	5.57	118.17	112.60
3	A	77	LEU	CB-CA-C	5.56	120.01	110.79
3	A	214	VAL	N-CA-C	5.54	116.31	110.72
3	A	270	LEU	CA-C-N	5.52	128.47	120.79
3	A	270	LEU	C-N-CA	5.52	128.47	120.79
3	A	252	HIS	N-CA-CB	5.51	118.50	109.95
3	A	99	PHE	N-CA-C	5.50	118.11	111.40
1	T	3	DT	C6-N1-C1'	-5.49	111.11	119.35
3	A	271	TYR	N-CA-CB	-5.48	101.49	109.82
3	A	245	ASN	N-CA-CB	5.47	116.64	110.35
3	A	41	LYS	CB-CA-C	5.46	120.13	110.85
2	P	3	DT	N1-C1'-C2'	5.43	121.65	113.50
3	A	257	ILE	CA-CB-CG2	-5.42	101.29	110.50
3	A	153	GLU	CA-C-N	5.42	127.98	120.29
3	A	153	GLU	C-N-CA	5.42	127.98	120.29
3	A	239	CYS	N-CA-CB	5.41	119.17	111.05
3	A	202	SER	N-CA-C	5.41	122.32	110.80
3	A	315	SER	N-CA-CB	5.39	119.75	111.56
3	A	282	MET	N-CA-C	-5.39	104.65	111.11
3	A	59	ALA	O-C-N	5.38	127.91	122.09
3	A	48	LYS	O-C-N	5.38	127.90	122.09
3	A	219	GLN	O-C-N	5.38	129.22	122.23
3	A	222	HIS	CA-CB-CG	-5.38	108.42	113.80
3	A	155	MET	CA-C-N	5.37	127.42	120.44
3	A	155	MET	C-N-CA	5.37	127.42	120.44
3	A	196	THR	N-CA-CB	5.36	120.16	111.21
3	A	98	ASN	CB-CA-C	5.35	120.53	110.63
3	A	228	LEU	N-CA-C	-5.34	105.03	112.45
3	A	286	ALA	CA-C-N	5.34	131.74	121.54
3	A	286	ALA	C-N-CA	5.34	131.74	121.54
3	A	324	GLN	N-CA-C	5.33	119.07	111.92
3	A	326	LYS	CD-CE-NZ	5.29	128.82	111.90
3	A	89	ARG	N-CA-CB	-5.27	102.37	110.12
3	A	41	LYS	N-CA-CB	5.27	117.95	110.16
3	A	128	ASN	CA-CB-CG	-5.25	107.35	112.60
3	A	113	LYS	N-CA-CB	5.24	117.75	109.94
3	A	165	GLU	N-CA-CB	5.23	119.32	110.49
3	A	126	ARG	N-CA-C	5.21	116.77	111.14
3	A	205	THR	N-CA-CB	5.21	119.30	110.49
3	A	98	ASN	CA-C-N	5.21	129.41	120.71
3	A	98	ASN	C-N-CA	5.21	129.41	120.71
3	A	229	SER	CA-C-N	-5.20	115.43	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	229	SER	C-N-CA	-5.20	115.43	122.77
3	A	251	PRO	CA-C-O	-5.19	115.43	122.08
3	A	87	LYS	CB-CA-C	5.19	119.50	110.68
3	A	115	VAL	N-CA-C	5.18	115.95	110.72
3	A	291	PHE	CA-C-O	5.15	127.40	121.32
1	T	3	DT	P-O5'-C5'	5.14	127.72	120.00
3	A	314	ASP	N-CA-CB	5.13	118.19	110.65
1	T	5	DA	P-O5'-C5'	-5.12	112.32	120.00
3	A	235	PHE	N-CA-C	-5.07	101.43	109.59
3	A	107	GLY	N-CA-C	-5.04	102.06	112.34
3	A	169	VAL	CB-CA-C	5.03	118.09	111.81
3	A	205	THR	N-CA-C	5.02	121.50	110.80
3	A	12	ASN	N-CA-C	5.02	119.56	113.38
2	P	5	DA	O3'-P-O5'	-5.02	96.47	104.00
3	A	334	SER	CB-CA-C	5.01	120.40	110.42
3	A	116	ASP	CB-CA-C	5.01	120.89	110.32
3	A	150	ILE	N-CA-CB	5.01	117.22	111.31
3	A	312	PRO	N-CA-C	5.01	118.36	110.80
3	A	249	GLU	CB-CG-CD	5.00	121.11	112.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	77	LEU	CA
3	A	246	ASP	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	145	0	80	5	0
2	P	144	0	81	11	0
3	A	2623	0	2641	363	0
4	A	2	0	0	0	0
5	A	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	109	0	0	20	0
6	P	18	0	0	2	0
6	T	12	0	0	0	0
All	All	3058	0	2802	376	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 67.

All (376) 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:29:VAL:HG21	3:A:94:SER:HB2	1.24	1.17
2:P:1:DT:H2''	2:P:2:DC:H5'	1.29	1.15
3:A:73:ILE:HG22	3:A:77:LEU:HD21	1.33	1.10
3:A:285:HIS:HD2	3:A:323:ILE:HD12	1.25	0.96
3:A:245:ASN:N	3:A:245:ASN:HD22	1.63	0.93
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.49	0.92
3:A:12:ASN:HD21	3:A:53:ILE:H	1.11	0.92
3:A:31:GLN:HE21	3:A:112:ARG:HH22	1.12	0.91
3:A:152:ARG:HA	3:A:155:MET:HB2	1.52	0.91
2:P:5:DA:H2''	2:P:6:DT:H5'	1.54	0.89
3:A:73:ILE:HG23	3:A:77:LEU:HD11	1.52	0.89
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.35	0.88
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.15	0.86
3:A:191:MET:HG2	3:A:255:ILE:HG12	1.57	0.84
3:A:155:MET:HE2	3:A:188:SER:HB2	1.57	0.84
3:A:155:MET:HE2	3:A:188:SER:CB	2.07	0.84
3:A:285:HIS:CD2	3:A:323:ILE:HD12	2.12	0.84
3:A:11:LEU:HD23	3:A:11:LEU:H	1.40	0.83
3:A:129:GLU:HG2	3:A:137:ARG:HD3	1.58	0.83
3:A:19:LEU:HB3	3:A:43:ALA:HB2	1.60	0.83
1:T:6:DG:H2''	1:T:7:DA:C8	2.14	0.83
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.60	0.83
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.11	0.81
3:A:270:LEU:CD2	3:A:319:ILE:HG21	2.11	0.80
3:A:108:PRO:O	3:A:112:ARG:HG3	1.81	0.80
3:A:15:ILE:HD11	3:A:77:LEU:CD1	2.12	0.79
3:A:31:GLN:HE21	3:A:112:ARG:NH2	1.80	0.79
3:A:330:PRO:HA	3:A:333:ARG:HG2	1.63	0.79
3:A:29:VAL:CG2	3:A:94:SER:HB2	2.10	0.78
3:A:299:ARG:HG2	3:A:310:PRO:HD3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.65	0.77
3:A:150:ILE:HD13	3:A:253:ARG:HG2	1.66	0.77
3:A:73:ILE:HG22	3:A:77:LEU:CD2	2.13	0.77
3:A:125:LEU:HD22	3:A:132:LEU:HD21	1.67	0.76
3:A:271:TYR:HB2	6:A:592:HOH:O	1.85	0.76
2:P:5:DA:H2''	2:P:6:DT:C5'	2.16	0.76
3:A:330:PRO:HA	3:A:333:ARG:CG	2.16	0.76
2:P:1:DT:H2''	2:P:2:DC:C5'	2.14	0.75
3:A:121:THR:HG23	3:A:124:ASP:OD1	1.85	0.75
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.84	0.74
3:A:245:ASN:HD22	3:A:245:ASN:H	1.33	0.74
3:A:73:ILE:CG2	3:A:77:LEU:HD11	2.17	0.74
3:A:270:LEU:HD23	3:A:319:ILE:HG21	1.68	0.74
3:A:27:LYS:HB3	3:A:36:TYR:CD1	2.22	0.73
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.70	0.73
3:A:323:ILE:O	3:A:324:GLN:HG2	1.89	0.73
3:A:245:ASN:N	3:A:245:ASN:ND2	2.36	0.72
3:A:62:LEU:HD12	3:A:63:PRO:HD2	1.70	0.72
3:A:243:SER:OG	3:A:249:GLU:HG3	1.90	0.72
3:A:99:PHE:HD2	3:A:100:LEU:HD13	1.55	0.71
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.73	0.71
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.71	0.70
3:A:165:GLU:OE1	3:A:168:LYS:HD3	1.91	0.70
3:A:11:LEU:HA	3:A:52:LYS:NZ	2.06	0.70
3:A:41:LYS:HE2	3:A:64:GLY:HA3	1.74	0.69
3:A:180:SER:HA	3:A:183:ARG:HH21	1.56	0.69
3:A:182:ARG:HG2	3:A:182:ARG:NH1	2.07	0.69
3:A:172:GLU:HG3	3:A:198:PRO:HG2	1.74	0.69
3:A:299:ARG:CD	3:A:310:PRO:HD3	2.23	0.69
3:A:16:THR:HG21	3:A:47:ALA:HB2	1.74	0.68
3:A:56:GLY:O	3:A:59:ALA:HB3	1.93	0.68
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.28	0.68
3:A:270:LEU:HD21	3:A:282:MET:HE2	1.76	0.68
3:A:299:ARG:HG2	3:A:310:PRO:CD	2.24	0.68
3:A:236:MET:HG2	3:A:256:ASP:OD1	1.94	0.67
3:A:165:GLU:O	3:A:168:LYS:N	2.27	0.67
3:A:83:ARG:O	3:A:86:GLU:HG2	1.95	0.67
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.30	0.67
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.28	0.67
3:A:328:ARG:O	3:A:333:ARG:NE	2.26	0.67
3:A:215:VAL:O	3:A:219:GLN:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:38:ALA:O	3:A:41:LYS:HD3	1.95	0.66
3:A:280:LYS:O	3:A:284:ALA:N	2.29	0.66
3:A:295:GLU:HA	6:A:592:HOH:O	1.94	0.66
3:A:155:MET:HA	3:A:158:MET:HE3	1.78	0.66
3:A:253:ARG:HG3	3:A:253:ARG:HH11	1.60	0.66
3:A:12:ASN:ND2	3:A:53:ILE:H	1.91	0.65
3:A:268:GLY:O	3:A:271:TYR:HB3	1.97	0.65
3:A:59:ALA:O	3:A:62:LEU:HB2	1.96	0.65
3:A:299:ARG:CG	3:A:310:PRO:HD3	2.26	0.65
3:A:115:VAL:O	3:A:118:GLY:N	2.29	0.65
3:A:41:LYS:O	3:A:44:SER:HB3	1.97	0.65
3:A:60:LYS:HA	3:A:65:VAL:HG12	1.79	0.65
3:A:121:THR:HG23	3:A:124:ASP:CG	2.22	0.65
3:A:125:LEU:HD22	3:A:132:LEU:CD2	2.27	0.65
3:A:214:VAL:HG23	3:A:218:LEU:HD22	1.79	0.64
3:A:270:LEU:HA	3:A:316:GLU:OE2	1.97	0.64
3:A:319:ILE:O	3:A:322:TYR:HB2	1.98	0.64
3:A:207:GLN:O	3:A:210:LEU:HB2	1.98	0.64
3:A:180:SER:HB3	3:A:183:ARG:NH2	2.11	0.64
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.27	0.64
3:A:137:ARG:NH1	6:A:515:HOH:O	2.30	0.63
3:A:79:THR:O	3:A:81:LYS:N	2.32	0.63
3:A:119:ILE:HG23	3:A:124:ASP:CB	2.29	0.63
3:A:125:LEU:CD2	3:A:132:LEU:HD21	2.29	0.63
3:A:180:SER:HB2	3:A:185:ALA:CB	2.28	0.63
3:A:11:LEU:H	3:A:11:LEU:CD2	2.08	0.63
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.29	0.63
3:A:152:ARG:NH2	3:A:181:PHE:O	2.30	0.62
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.81	0.62
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.29	0.62
3:A:41:LYS:NZ	3:A:64:GLY:O	2.29	0.62
3:A:18:MET:O	3:A:21:GLU:HB2	2.00	0.62
3:A:207:GLN:HB3	3:A:210:LEU:HG	1.81	0.62
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.29	0.62
3:A:245:ASN:H	3:A:245:ASN:ND2	1.97	0.61
3:A:165:GLU:OE2	3:A:221:VAL:HG11	2.00	0.61
3:A:255:ILE:HD13	3:A:256:ASP:N	2.16	0.61
3:A:103:VAL:HG22	3:A:143:PHE:CD2	2.35	0.61
3:A:58:GLU:O	3:A:61:LYS:HG3	2.00	0.61
3:A:212:HIS:HB3	6:A:541:HOH:O	2.01	0.61
6:P:612:HOH:O	3:A:109:SER:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:288:GLU:C	3:A:290:GLY:H	2.09	0.60
3:A:188:SER:HB3	6:A:522:HOH:O	2.02	0.60
3:A:200:PHE:O	3:A:262:LYS:N	2.29	0.60
3:A:294:ASN:O	3:A:296:TYR:N	2.34	0.60
3:A:310:PRO:HB3	6:A:626:HOH:O	2.00	0.60
3:A:129:GLU:CG	3:A:137:ARG:HD3	2.29	0.60
3:A:15:ILE:CG2	3:A:46:ILE:HD13	2.31	0.60
3:A:275:SER:OG	3:A:277:ILE:HD13	2.00	0.60
3:A:278:PHE:HE1	3:A:325:TRP:CZ3	2.19	0.60
3:A:103:VAL:HG22	3:A:143:PHE:CE2	2.36	0.60
3:A:201:THR:HA	3:A:261:PRO:HB3	1.83	0.60
3:A:163:LEU:HD23	3:A:163:LEU:N	2.11	0.60
3:A:270:LEU:HD21	3:A:282:MET:CE	2.32	0.59
3:A:298:ILE:HA	6:A:593:HOH:O	2.01	0.59
3:A:284:ALA:O	3:A:287:LEU:HB2	2.01	0.59
3:A:200:PHE:HB2	6:A:625:HOH:O	2.03	0.59
3:A:180:SER:HA	3:A:183:ARG:NH2	2.18	0.59
3:A:239:CYS:SG	3:A:255:ILE:HB	2.44	0.58
3:A:323:ILE:C	3:A:324:GLN:HG2	2.28	0.58
3:A:92:ASP:HA	3:A:95:SER:HB2	1.86	0.58
3:A:83:ARG:O	3:A:87:LYS:N	2.28	0.58
3:A:218:LEU:CB	3:A:224:ILE:HD12	2.34	0.58
3:A:77:LEU:HD13	3:A:77:LEU:N	2.19	0.58
3:A:291:PHE:CD1	3:A:300:PRO:HA	2.39	0.58
3:A:180:SER:CB	3:A:183:ARG:HH21	2.17	0.58
3:A:115:VAL:C	3:A:118:GLY:H	2.12	0.57
3:A:200:PHE:CE1	3:A:261:PRO:HD3	2.39	0.57
3:A:68:LYS:HB2	3:A:68:LYS:NZ	2.19	0.57
3:A:177:VAL:CG1	3:A:191:MET:HE2	2.34	0.57
3:A:14:GLY:O	3:A:18:MET:N	2.30	0.57
3:A:180:SER:HB2	3:A:185:ALA:HB2	1.86	0.57
3:A:165:GLU:O	3:A:168:LYS:HG2	2.04	0.57
3:A:217:GLN:NE2	3:A:217:GLN:HA	2.19	0.57
1:T:5:DA:H2''	1:T:6:DG:O5'	2.05	0.57
3:A:253:ARG:NH1	6:A:503:HOH:O	2.37	0.57
3:A:285:HIS:CE1	3:A:289:LYS:HG2	2.40	0.57
3:A:127:LYS:HB2	3:A:128:ASN:ND2	2.19	0.57
3:A:274:GLY:O	3:A:278:PHE:HD2	1.88	0.57
3:A:243:SER:HB3	3:A:249:GLU:HA	1.87	0.56
3:A:330:PRO:CA	3:A:333:ARG:HG2	2.34	0.56
3:A:11:LEU:HA	3:A:52:LYS:HZ1	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:292:THR:O	3:A:293:ILE:HD13	2.06	0.56
3:A:291:PHE:HD1	3:A:300:PRO:HA	1.70	0.56
3:A:182:ARG:HG2	3:A:273:THR:HG23	1.87	0.56
3:A:217:GLN:O	3:A:221:VAL:HG13	2.05	0.56
3:A:327:TYR:HD1	3:A:328:ARG:N	2.03	0.56
3:A:33:ILE:O	3:A:36:TYR:HD2	1.87	0.56
3:A:44:SER:OG	3:A:45:VAL:N	2.36	0.56
3:A:183:ARG:HD3	3:A:273:THR:O	2.05	0.56
2:P:5:DA:H2'	6:P:648:HOH:O	2.06	0.56
3:A:44:SER:O	3:A:47:ALA:HB3	2.06	0.56
3:A:124:ASP:O	3:A:128:ASN:ND2	2.27	0.55
3:A:108:PRO:HA	3:A:111:ALA:HB3	1.88	0.55
3:A:294:ASN:HB2	3:A:295:GLU:OE1	2.05	0.55
3:A:104:SER:N	6:A:600:HOH:O	2.27	0.55
3:A:179:GLY:O	3:A:182:ARG:HB3	2.07	0.55
3:A:292:THR:C	3:A:293:ILE:HD13	2.32	0.55
3:A:62:LEU:HD12	3:A:63:PRO:CD	2.37	0.55
3:A:12:ASN:HD21	3:A:53:ILE:N	1.94	0.54
3:A:177:VAL:HG11	3:A:191:MET:HE2	1.90	0.54
3:A:331:LYS:HG2	3:A:332:ASP:N	2.06	0.54
2:P:1:DT:H2'	2:P:2:DC:C6	2.43	0.54
3:A:270:LEU:CD2	3:A:282:MET:HE2	2.38	0.54
3:A:200:PHE:HE1	3:A:261:PRO:HD3	1.73	0.54
3:A:204:SER:O	3:A:206:LYS:N	2.40	0.54
3:A:11:LEU:HA	3:A:52:LYS:HZ2	1.72	0.53
3:A:180:SER:HB3	3:A:183:ARG:HH21	1.71	0.53
3:A:11:LEU:HD23	3:A:11:LEU:N	2.14	0.53
3:A:73:ILE:O	3:A:77:LEU:HD22	2.08	0.53
3:A:207:GLN:HB2	6:A:625:HOH:O	2.08	0.53
3:A:277:ILE:HG12	3:A:335:GLU:HA	1.91	0.53
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.90	0.53
3:A:172:GLU:HB3	3:A:197:HIS:NE2	2.23	0.53
3:A:178:CYS:SG	3:A:269:VAL:HG22	2.48	0.53
3:A:183:ARG:HG3	3:A:273:THR:HG22	1.91	0.53
3:A:299:ARG:HG2	3:A:310:PRO:N	2.24	0.53
3:A:120:LYS:N	3:A:124:ASP:OD2	2.31	0.53
3:A:180:SER:CA	3:A:183:ARG:HH21	2.20	0.53
3:A:243:SER:O	3:A:244:LYS:O	2.27	0.53
2:P:5:DA:O5'	3:A:107:GLY:HA3	2.08	0.52
3:A:92:ASP:O	3:A:96:SER:N	2.30	0.52
3:A:15:ILE:CD1	3:A:77:LEU:HD11	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:299:ARG:HD2	3:A:310:PRO:HD3	1.90	0.52
3:A:218:LEU:HB2	3:A:224:ILE:HD12	1.89	0.52
3:A:218:LEU:HB3	3:A:224:ILE:CD1	2.40	0.52
3:A:212:HIS:N	3:A:212:HIS:CD2	2.78	0.52
3:A:176:THR:HG22	3:A:178:CYS:SG	2.49	0.52
3:A:230:LYS:HG3	3:A:235:PHE:HD2	1.73	0.52
3:A:326:LYS:HG3	3:A:326:LYS:O	2.10	0.52
3:A:263:ASP:C	3:A:264:GLN:HG2	2.34	0.51
3:A:212:HIS:CD2	3:A:212:HIS:H	2.27	0.51
3:A:303:VAL:O	3:A:305:GLY:N	2.44	0.51
3:A:303:VAL:C	3:A:305:GLY:H	2.19	0.51
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.91	0.51
3:A:172:GLU:HB2	6:A:551:HOH:O	2.09	0.51
3:A:217:GLN:O	3:A:220:LYS:HB3	2.09	0.51
3:A:191:MET:HG2	3:A:255:ILE:CG1	2.33	0.51
3:A:165:GLU:CD	3:A:168:LYS:HD3	2.36	0.51
3:A:228:LEU:HB2	3:A:236:MET:O	2.10	0.51
3:A:293:ILE:HA	6:A:593:HOH:O	2.10	0.51
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.55	0.51
3:A:25:PHE:CE2	3:A:88:ILE:HG12	2.46	0.51
3:A:287:LEU:HA	3:A:291:PHE:O	2.10	0.51
3:A:288:GLU:O	3:A:290:GLY:N	2.39	0.51
3:A:298:ILE:HG22	6:A:578:HOH:O	2.10	0.51
3:A:278:PHE:HE1	3:A:325:TRP:HZ3	1.59	0.51
3:A:15:ILE:HG22	3:A:46:ILE:HD13	1.92	0.50
3:A:277:ILE:HG13	3:A:335:GLU:HB2	1.94	0.50
3:A:316:GLU:O	3:A:320:PHE:HD2	1.95	0.50
3:A:35:LYS:O	3:A:38:ALA:HB3	2.12	0.50
3:A:83:ARG:HA	3:A:86:GLU:HG2	1.93	0.50
3:A:204:SER:O	3:A:204:SER:OG	2.29	0.50
3:A:60:LYS:HE3	3:A:66:GLY:C	2.37	0.50
3:A:278:PHE:CE1	3:A:325:TRP:HZ3	2.30	0.50
3:A:19:LEU:HD23	3:A:43:ALA:HA	1.93	0.50
3:A:123:GLU:O	3:A:126:ARG:N	2.45	0.50
3:A:282:MET:HE1	3:A:319:ILE:HG22	1.92	0.50
3:A:270:LEU:CD2	3:A:319:ILE:HD13	2.42	0.49
3:A:298:ILE:HG23	3:A:298:ILE:O	2.12	0.49
3:A:201:THR:HA	3:A:261:PRO:CB	2.41	0.49
3:A:165:GLU:HG3	3:A:217:GLN:HG3	1.94	0.49
3:A:183:ARG:HG2	3:A:330:PRO:O	2.12	0.49
2:P:6:DT:H2"	2:P:7:DG:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:167:LYS:O	3:A:170:ASP:O	2.31	0.49
3:A:155:MET:HE2	3:A:188:SER:OG	2.12	0.49
3:A:170:ASP:OD1	3:A:171:SER:N	2.46	0.48
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.49	0.48
3:A:326:LYS:O	3:A:328:ARG:HG2	2.13	0.48
3:A:200:PHE:CE1	3:A:261:PRO:N	2.82	0.48
3:A:276:ASP:O	3:A:280:LYS:HG3	2.14	0.48
3:A:165:GLU:HB3	3:A:217:GLN:CG	2.43	0.48
3:A:91:ASP:O	3:A:95:SER:HB2	2.13	0.48
3:A:15:ILE:HD11	3:A:77:LEU:HD12	1.94	0.48
3:A:218:LEU:HB3	3:A:224:ILE:HD12	1.96	0.48
3:A:283:ARG:O	3:A:287:LEU:HD23	2.14	0.48
3:A:128:ASN:ND2	3:A:128:ASN:N	2.61	0.48
3:A:145:ASP:OD1	3:A:145:ASP:N	2.46	0.48
3:A:282:MET:HA	3:A:325:TRP:CH2	2.49	0.48
3:A:29:VAL:HA	3:A:97:ILE:HD12	1.95	0.47
3:A:57:ALA:O	3:A:60:LYS:HB3	2.14	0.47
3:A:259:LEU:O	3:A:260:ILE:HD13	2.13	0.47
3:A:183:ARG:HH11	3:A:275:SER:HA	1.79	0.47
3:A:317:LYS:O	3:A:320:PHE:HB2	2.14	0.47
3:A:15:ILE:HG22	3:A:46:ILE:CD1	2.45	0.47
3:A:162:VAL:HG12	3:A:162:VAL:O	2.14	0.47
1:T:4:DT:H2"	1:T:5:DA:C8	2.49	0.47
3:A:182:ARG:NH1	3:A:273:THR:CG2	2.77	0.47
3:A:182:ARG:NE	6:A:576:HOH:O	2.45	0.47
3:A:195:LEU:O	3:A:260:ILE:N	2.48	0.47
3:A:200:PHE:CD1	3:A:261:PRO:HA	2.49	0.47
3:A:234:LYS:HD3	6:A:617:HOH:O	2.14	0.47
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.63	0.47
3:A:59:ALA:O	3:A:62:LEU:N	2.43	0.47
3:A:243:SER:CB	3:A:249:GLU:HA	2.45	0.47
3:A:298:ILE:N	6:A:578:HOH:O	2.39	0.47
3:A:79:THR:C	3:A:81:LYS:H	2.23	0.47
3:A:182:ARG:NH1	3:A:182:ARG:CG	2.76	0.47
3:A:165:GLU:CG	3:A:217:GLN:HG3	2.46	0.46
3:A:170:ASP:HB3	3:A:173:TYR:CD2	2.51	0.46
3:A:12:ASN:HA	6:A:553:HOH:O	2.15	0.46
3:A:200:PHE:HE1	3:A:261:PRO:CD	2.28	0.46
3:A:152:ARG:CA	3:A:155:MET:HB2	2.36	0.46
3:A:16:THR:CG2	3:A:47:ALA:HB2	2.45	0.46
3:A:211:LEU:HD12	3:A:211:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:230:LYS:CB	3:A:230:LYS:NZ	2.77	0.46
2:P:6:DT:H2''	2:P:7:DG:H5''	1.98	0.46
1:T:7:DA:O5'	1:T:8:DA:OP2	2.34	0.46
3:A:332:ASP:C	3:A:334:SER:H	2.24	0.46
3:A:62:LEU:CD1	3:A:63:PRO:HD2	2.42	0.46
3:A:125:LEU:HD23	3:A:125:LEU:HA	1.71	0.46
3:A:289:LYS:HA	3:A:289:LYS:HD3	1.52	0.46
3:A:99:PHE:HD2	3:A:100:LEU:CD1	2.27	0.45
3:A:254:ARG:CZ	3:A:254:ARG:HB3	2.47	0.45
3:A:278:PHE:O	3:A:282:MET:HB3	2.16	0.45
3:A:193:VAL:H	3:A:193:VAL:HG23	1.35	0.45
3:A:115:VAL:HG13	3:A:120:LYS:HE2	1.98	0.45
3:A:135:HIS:C	3:A:135:HIS:CD2	2.94	0.45
3:A:18:MET:HE3	3:A:76:PHE:HB2	1.99	0.45
3:A:200:PHE:HE1	3:A:260:ILE:C	2.25	0.45
3:A:209:LYS:HD3	3:A:209:LYS:HA	1.64	0.45
3:A:295:GLU:H	3:A:295:GLU:CD	2.24	0.45
3:A:62:LEU:HD12	3:A:62:LEU:HA	1.53	0.45
2:P:5:DA:P	3:A:107:GLY:HA3	2.57	0.45
3:A:166:VAL:O	3:A:169:VAL:HG13	2.17	0.44
3:A:241:LEU:HB2	3:A:250:TYR:CD2	2.52	0.44
3:A:301:LEU:HD12	3:A:301:LEU:HA	1.53	0.44
3:A:200:PHE:CE1	3:A:261:PRO:CD	3.00	0.44
3:A:102:ARG:HH21	3:A:147:GLU:CD	2.25	0.44
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.32	0.44
3:A:279:ASN:O	3:A:283:ARG:N	2.42	0.44
3:A:146:PHE:HZ	3:A:238:VAL:HG22	1.83	0.44
3:A:166:VAL:HG13	3:A:173:TYR:CB	2.48	0.44
3:A:235:PHE:CD1	3:A:235:PHE:C	2.95	0.44
3:A:287:LEU:HB3	3:A:288:GLU:OE2	2.17	0.44
3:A:278:PHE:CD2	3:A:333:ARG:HB3	2.53	0.44
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.32	0.44
3:A:180:SER:OG	5:A:338:TTP:O2G	2.32	0.44
3:A:250:TYR:HB3	6:A:577:HOH:O	2.18	0.44
1:T:4:DT:O5'	3:A:231:GLY:HA3	2.17	0.43
3:A:138:ILE:HG21	3:A:228:LEU:HD11	2.00	0.43
3:A:214:VAL:HG22	3:A:215:VAL:N	2.33	0.43
3:A:85:LEU:HA	3:A:85:LEU:HD12	1.21	0.43
3:A:142:TYR:CE2	3:A:238:VAL:HG11	2.52	0.43
3:A:45:VAL:HG21	3:A:63:PRO:O	2.18	0.43
3:A:177:VAL:HG11	3:A:191:MET:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:68:LYS:O	3:A:72:LYS:HE2	2.19	0.43
3:A:103:VAL:CG2	3:A:143:PHE:CE2	3.02	0.43
3:A:200:PHE:CE1	3:A:260:ILE:C	2.96	0.43
3:A:27:LYS:CB	3:A:36:TYR:CD1	2.98	0.43
3:A:292:THR:O	3:A:298:ILE:HA	2.19	0.43
3:A:183:ARG:HE	3:A:183:ARG:HB2	1.07	0.43
3:A:194:LEU:HD21	3:A:272:PHE:CD2	2.53	0.43
3:A:42:ALA:C	3:A:44:SER:N	2.76	0.43
3:A:82:LEU:HB3	3:A:85:LEU:CB	2.43	0.43
3:A:155:MET:HE3	3:A:181:PHE:HB2	1.99	0.43
3:A:200:PHE:HE1	3:A:261:PRO:N	2.16	0.43
3:A:260:ILE:HG22	3:A:261:PRO:O	2.19	0.43
3:A:15:ILE:HG21	3:A:46:ILE:HD13	1.99	0.43
3:A:260:ILE:CG2	3:A:261:PRO:CD	2.96	0.43
3:A:306:VAL:HG22	6:A:650:HOH:O	2.18	0.43
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.49	0.43
3:A:46:ILE:HG13	3:A:47:ALA:N	2.31	0.43
3:A:85:LEU:O	3:A:89:ARG:HB2	2.19	0.43
3:A:270:LEU:HD23	3:A:319:ILE:HD13	2.01	0.43
3:A:27:LYS:HB3	3:A:36:TYR:CG	2.53	0.42
3:A:157:GLN:O	3:A:161:ILE:HG13	2.18	0.42
3:A:26:GLU:O	3:A:30:SER:O	2.36	0.42
3:A:303:VAL:C	3:A:305:GLY:N	2.78	0.42
3:A:83:ARG:O	3:A:86:GLU:N	2.52	0.42
3:A:267:CYS:HA	3:A:319:ILE:HD11	2.01	0.42
3:A:282:MET:HE1	3:A:319:ILE:CG2	2.49	0.42
3:A:214:VAL:CG2	3:A:215:VAL:N	2.76	0.42
3:A:277:ILE:CG1	3:A:335:GLU:CB	2.98	0.42
3:A:93:THR:HG22	3:A:94:SER:N	2.35	0.42
3:A:196:THR:OG1	3:A:197:HIS:N	2.43	0.42
3:A:223:PHE:O	3:A:239:CYS:HA	2.19	0.42
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.54	0.42
3:A:100:LEU:HA	3:A:100:LEU:HD12	1.43	0.42
3:A:248:LYS:O	3:A:248:LYS:HG2	2.20	0.42
3:A:190:ASP:N	3:A:190:ASP:OD1	2.48	0.41
3:A:99:PHE:CD2	3:A:99:PHE:C	2.98	0.41
3:A:261:PRO:HG2	3:A:264:GLN:HG3	2.02	0.41
3:A:274:GLY:HA3	3:A:275:SER:HA	1.88	0.41
3:A:205:THR:O	3:A:206:LYS:HB2	2.20	0.41
3:A:15:ILE:CG2	3:A:46:ILE:CD1	2.97	0.41
3:A:166:VAL:CG1	3:A:173:TYR:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:197:HIS:HA	3:A:198:PRO:HD3	1.81	0.41
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.86	0.41
2:P:1:DT:C2'	2:P:2:DC:H5'	2.22	0.41
3:A:22:LEU:HD12	3:A:22:LEU:HA	1.56	0.41
3:A:330:PRO:O	3:A:333:ARG:HG2	2.20	0.41
3:A:54:LYS:HA	3:A:54:LYS:HD2	1.29	0.41
3:A:119:ILE:HG23	3:A:124:ASP:HB2	2.00	0.41
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.86	0.41
3:A:68:LYS:O	3:A:71:GLU:HB3	2.22	0.40
3:A:34:HIS:O	3:A:38:ALA:N	2.54	0.40
3:A:270:LEU:HD22	3:A:319:ILE:HD13	2.03	0.40
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.99	0.40
3:A:163:LEU:HD23	3:A:163:LEU:HA	1.44	0.40
3:A:288:GLU:C	3:A:290:GLY:N	2.78	0.40
3:A:159:GLN:O	3:A:159:GLN:HG3	2.21	0.40
3:A:193:VAL:C	3:A:194:LEU:HD12	2.46	0.40
3:A:19:LEU:HD12	3:A:19:LEU:HA	1.78	0.40
3:A:23:ALA:HB2	3:A:39:TYR:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	325/335 (97%)	267 (82%)	38 (12%)	20 (6%)	1 9

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	202	SER
3	A	205	THR
3	A	244	LYS

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Mol	Chain	Res	Type
3	A	246	ASP
3	A	289	LYS
3	A	295	GLU
3	A	13	GLY
3	A	80	GLY
3	A	185	ALA
3	A	222	HIS
3	A	247	GLU
3	A	265	TYR
3	A	304	THR
3	A	91	ASP
3	A	207	GLN
3	A	310	PRO
3	A	33	ILE
3	A	309	GLU
3	A	204	SER
3	A	166	VAL

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	288/295 (98%)	207 (72%)	81 (28%)	0 2

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	THR
3	A	11	LEU
3	A	18	MET
3	A	19	LEU
3	A	21	GLU
3	A	22	LEU
3	A	27	LYS
3	A	30	SER
3	A	33	ILE

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Mol	Chain	Res	Type
3	A	37	ASN
3	A	41	LYS
3	A	44	SER
3	A	46	ILE
3	A	54	LYS
3	A	60	LYS
3	A	61	LYS
3	A	62	LEU
3	A	67	THR
3	A	68	LYS
3	A	77	LEU
3	A	85	LEU
3	A	87	LYS
3	A	89	ARG
3	A	92	ASP
3	A	93	THR
3	A	95	SER
3	A	100	LEU
3	A	119	ILE
3	A	121	THR
3	A	132	LEU
3	A	136	GLN
3	A	138	ILE
3	A	145	ASP
3	A	150	ILE
3	A	153	GLU
3	A	156	LEU
3	A	159	GLN
3	A	161	ILE
3	A	165	GLU
3	A	168	LYS
3	A	169	VAL
3	A	174	ILE
3	A	182	ARG
3	A	183	ARG
3	A	188	SER
3	A	191	MET
3	A	193	VAL
3	A	200	PHE
3	A	201	THR
3	A	203	GLU
3	A	210	LEU

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Mol	Chain	Res	Type
3	A	214	VAL
3	A	218	LEU
3	A	221	VAL
3	A	226	ASP
3	A	228	LEU
3	A	230	LYS
3	A	235	PHE
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE
3	A	264	GLN
3	A	270	LEU
3	A	277	ILE
3	A	282	MET
3	A	287	LEU
3	A	293	ILE
3	A	294	ASN
3	A	295	GLU
3	A	298	ILE
3	A	301	LEU
3	A	304	THR
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	324	GLN
3	A	325	TRP
3	A	331	LYS
3	A	332	ASP
3	A	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	28	ASN
3	A	31	GLN
3	A	51	HIS
3	A	133	ASN
3	A	212	HIS
3	A	217	GLN
3	A	219	GLN

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Mol	Chain	Res	Type
3	A	245	ASN
3	A	279	ASN
3	A	294	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	TTP	A	338	-	4,4,30	1.77	2 (50%)	6,6,47	1.45	2 (33%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	338	TTP	PG-O2G	-2.21	1.48	1.54
5	A	338	TTP	PG-O3B	2.15	1.60	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	338	TTP	O3G-PG-O3B	-2.42	100.37	107.91
5	A	338	TTP	O2G-PG-O1G	2.16	118.57	110.95

There are no chirality outliers.

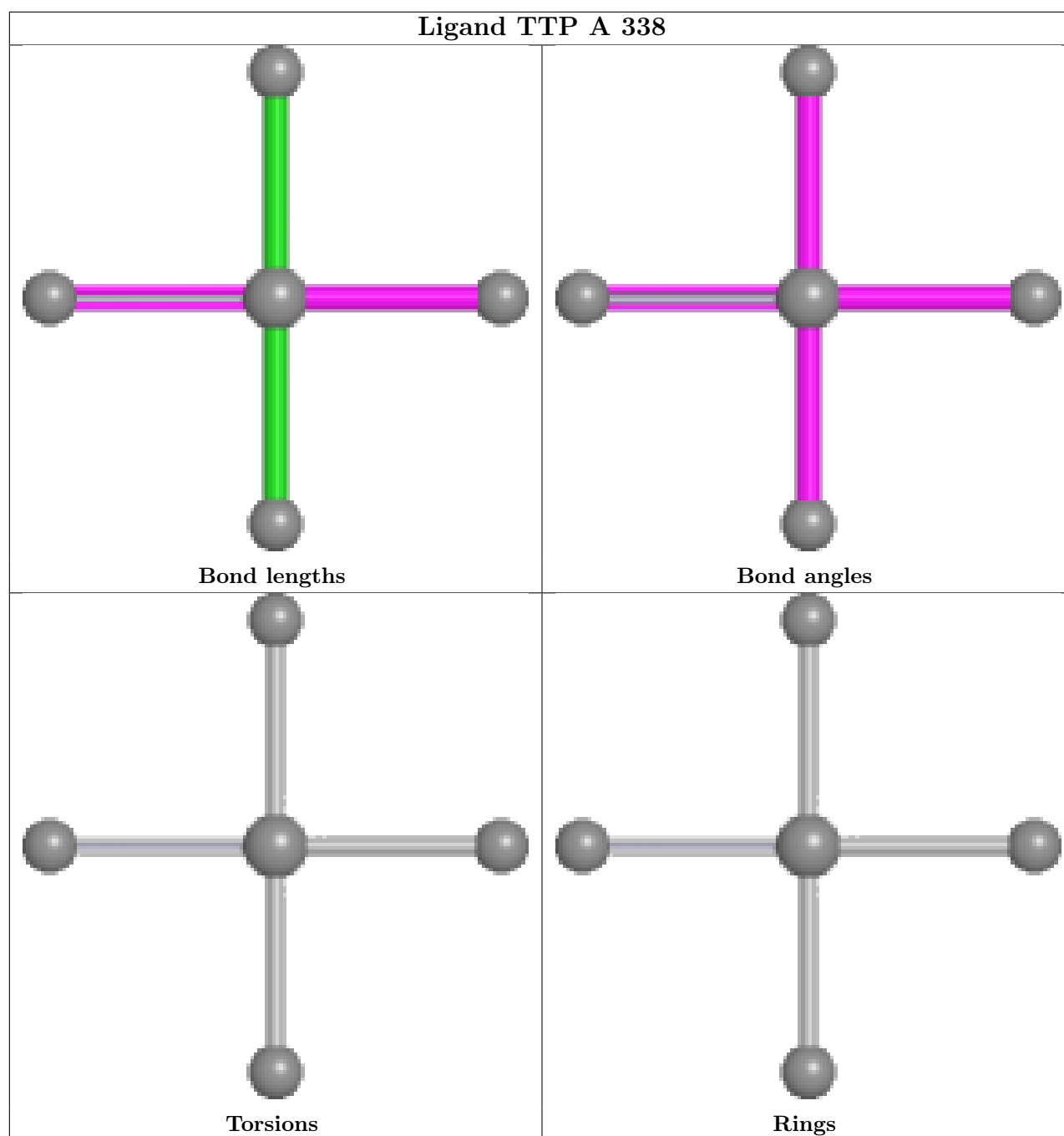
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	338	TTP	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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.