



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:08 PM UTC

PDB ID : 9ICF / pdb_00009icf
Title : DNA POLYMERASE BETA (E.C.2.7.7.7)/DNA COMPLEX + 2'-DEOXY ADENOSINE-5'-TRIPHOSPHATE, SOAKED IN THE PRESENCE OF DATP AND ZNCL2
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1995-12-15
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

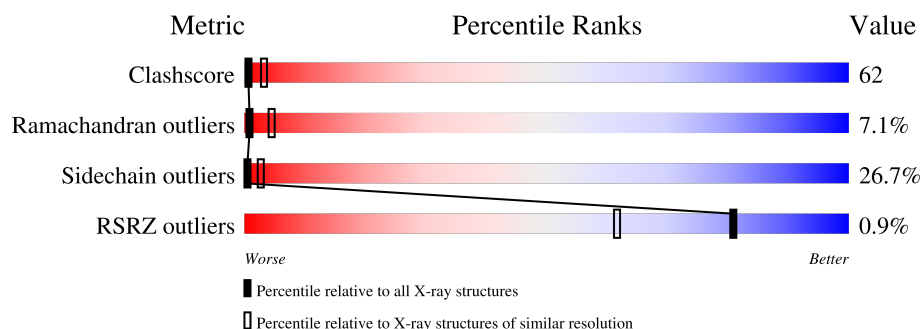
1 Overall quality at a glance

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	8	12% 12% 12% 75%
2	P	8	12% 38% 62%
3	A	335	18% 43% 29% 7% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3072 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*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	8	Total	C	N	O	P	0	0	0
			154	74	24	48	8			

- 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	18	0	0
			2623	1657	458	499	9			

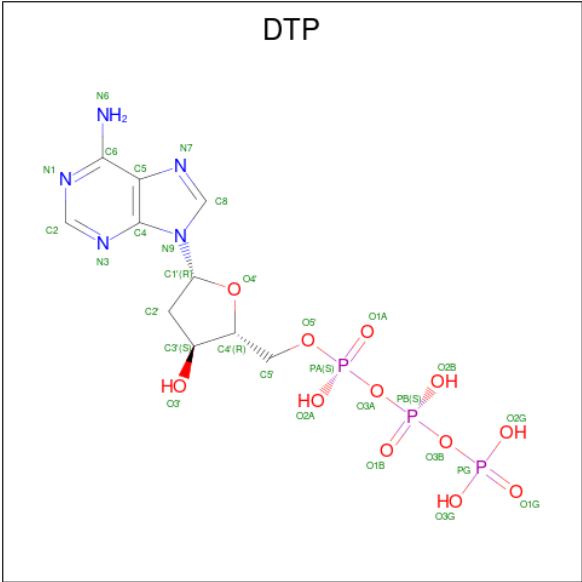
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	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'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			14	11	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	T	16	Total	O	0	0
			16	16		
7	P	15	Total	O	0	0
			15	15		
7	A	101	Total	O	0	0
			101	101		

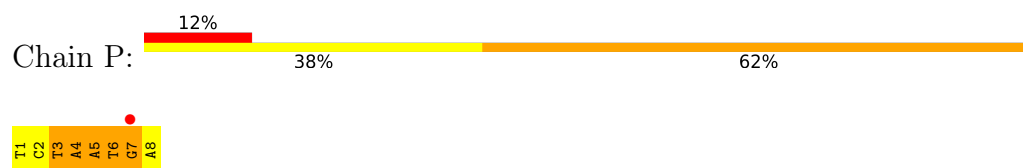
3 Residue-property plots [i](#)

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.

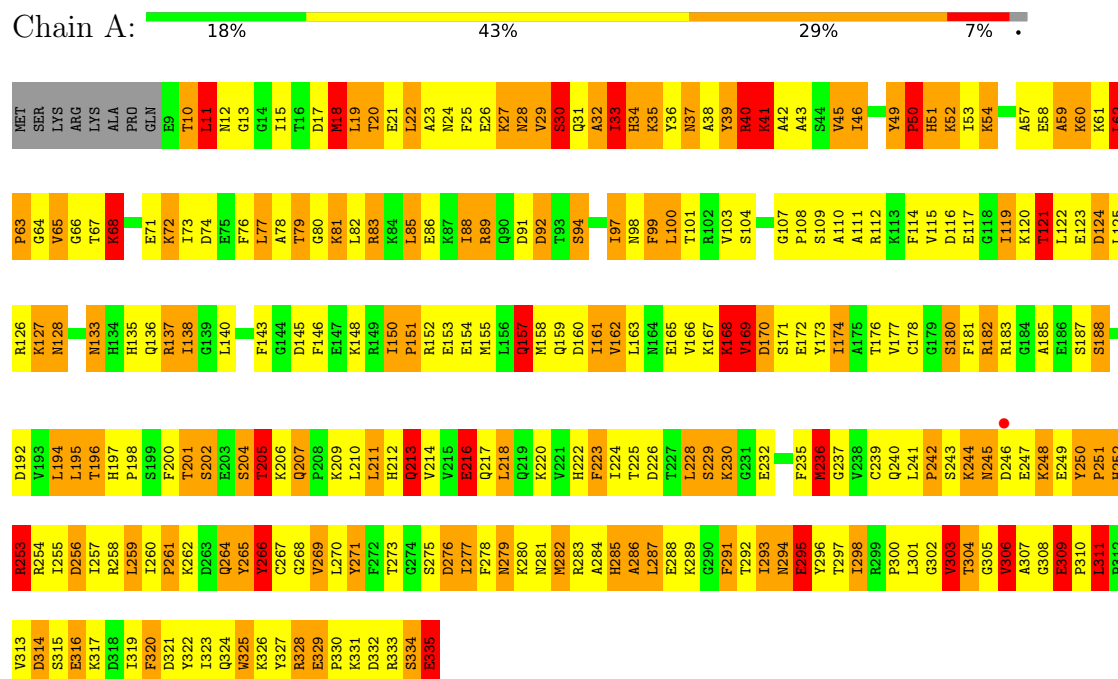
- Molecule 1: DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3')



- Molecule 2: DNA (5'-D(*TP*CP*TP*AP*AP*TP*GP*A)-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	179.96Å 57.62Å 48.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	84.0 (20.00-3.00) 83.8 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	5.70	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.70Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.163 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 261.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3072	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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: NA, ZN, DTP

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	1.14	0/162	2.97	15/249 (6.0%)
2	P	1.34	1/171 (0.6%)	4.44	22/259 (8.5%)
3	A	1.61	23/2672 (0.9%)	2.19	123/3590 (3.4%)
All	All	1.57	24/3005 (0.8%)	2.44	160/4098 (3.9%)

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 (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	224	ILE	CA-CB	-7.93	1.44	1.54
3	A	196	THR	CA-C	-7.03	1.44	1.52
3	A	261	PRO	CA-C	-6.96	1.45	1.52
3	A	35	LYS	CA-C	-6.80	1.44	1.52
2	P	1	DT	OP3-P	6.50	1.61	1.48
3	A	251	PRO	N-CA	-6.20	1.39	1.47
3	A	269	VAL	CA-CB	-5.99	1.47	1.54
3	A	109	SER	CA-C	-5.97	1.44	1.52
3	A	137	ARG	C-N	-5.88	1.26	1.33
3	A	63	PRO	N-CA	-5.77	1.40	1.47
3	A	225	THR	CA-C	-5.70	1.44	1.52
3	A	181	PHE	N-CA	-5.67	1.39	1.46
3	A	242	PRO	N-CA	-5.63	1.40	1.47
3	A	192	ASP	CA-CB	5.62	1.60	1.53
3	A	62	LEU	C-N	-5.45	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	140	LEU	C-N	-5.44	1.26	1.34
3	A	29	VAL	CA-CB	-5.42	1.48	1.54
3	A	103	VAL	CA-CB	-5.34	1.47	1.53
3	A	35	LYS	C-N	-5.29	1.27	1.33
3	A	138	ILE	CA-CB	-5.19	1.47	1.54
3	A	65	VAL	C-N	-5.17	1.28	1.33
3	A	151	PRO	N-CA	-5.16	1.41	1.47
3	A	66	GLY	N-CA	-5.08	1.40	1.44
3	A	24	ASN	CA-C	-5.07	1.45	1.52

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	1	DT	C6-N1-C1'	-30.99	72.87	119.35
2	P	1	DT	C2-N1-C1'	29.67	163.86	119.35
2	P	6	DT	C6-N1-C1'	-22.55	85.52	119.35
2	P	6	DT	C2-N1-C1'	22.06	152.44	119.35
1	T	4	DT	C2-N1-C1'	21.51	151.61	119.35
1	T	4	DT	C6-N1-C1'	-21.49	87.11	119.35
2	P	3	DT	C2-N1-C1'	17.51	145.62	119.35
2	P	3	DT	C6-N1-C1'	-16.20	95.05	119.35
2	P	7	DG	C8-N9-C1'	15.94	150.91	127.00
2	P	7	DG	C4-N9-C1'	-15.74	103.39	127.00
1	T	7	DA	C4-N9-C1'	-10.56	111.21	127.05
2	P	7	DG	P-O3'-C3'	10.08	135.31	120.20
3	A	143	PHE	CA-CB-CG	-10.07	103.73	113.80
1	T	7	DA	C8-N9-C1'	10.06	142.14	127.05
3	A	18	MET	CA-C-N	9.45	133.88	120.28
3	A	18	MET	C-N-CA	9.45	133.88	120.28
3	A	116	ASP	CA-CB-CG	-9.08	103.52	112.60
2	P	2	DC	C2-N1-C1'	8.93	133.09	119.70
3	A	309	GLU	CA-C-N	8.72	130.74	119.84
3	A	309	GLU	C-N-CA	8.72	130.74	119.84
1	T	1	DC	P-O3'-C3'	8.48	132.93	120.20
1	T	5	DA	C8-N9-C1'	8.30	139.50	127.05
3	A	222	HIS	CA-CB-CG	-8.09	105.71	113.80
3	A	162	VAL	N-CA-CB	7.89	119.78	110.55
1	T	5	DA	C4-N9-C1'	-7.79	115.37	127.05
3	A	49	TYR	CA-C-N	7.73	129.50	119.84
3	A	49	TYR	C-N-CA	7.73	129.50	119.84
2	P	2	DC	C6-N1-C1'	-7.72	108.13	119.70
3	A	181	PHE	CA-CB-CG	-7.70	106.10	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	VAL	N-CA-C	7.57	120.51	111.05
3	A	30	SER	CA-C-N	-7.56	110.47	123.25
3	A	30	SER	C-N-CA	-7.56	110.47	123.25
3	A	168	LYS	N-CA-CB	7.54	121.32	110.16
3	A	313	VAL	N-CA-C	7.45	118.39	107.37
3	A	34	HIS	CA-CB-CG	-7.39	106.41	113.80
3	A	92	ASP	N-CA-C	7.35	118.93	111.07
3	A	320	PHE	CA-CB-CG	-7.29	106.51	113.80
3	A	146	PHE	N-CA-C	7.28	120.26	111.82
3	A	41	LYS	N-CA-C	-7.21	103.50	111.36
3	A	150	ILE	N-CA-C	7.18	115.81	107.77
3	A	51	HIS	CA-CB-CG	7.15	120.95	113.80
3	A	20	THR	N-CA-CB	7.11	120.66	110.13
3	A	211	LEU	CA-C-N	7.09	130.49	120.28
3	A	211	LEU	C-N-CA	7.09	130.49	120.28
3	A	97	ILE	CB-CA-C	-6.93	102.78	112.14
1	T	2	DA	C4-N9-C1'	-6.87	116.75	127.05
2	P	4	DA	C8-N9-C1'	-6.85	116.78	127.05
3	A	266	TYR	CA-CB-CG	-6.85	101.58	113.90
3	A	177	VAL	N-CA-C	-6.84	97.77	108.23
3	A	40	ARG	N-CA-C	6.80	120.06	111.69
3	A	24	ASN	CA-CB-CG	-6.74	105.86	112.60
3	A	103	VAL	N-CA-CB	-6.62	103.47	110.82
3	A	271	TYR	CA-CB-CG	-6.60	102.01	113.90
3	A	250	TYR	CA-C-O	6.56	125.70	120.19
3	A	92	ASP	CB-CA-C	6.54	121.16	110.88
3	A	59	ALA	O-C-N	6.51	128.77	122.07
3	A	291	PHE	CA-CB-CG	-6.46	107.34	113.80
3	A	18	MET	O-C-N	6.39	128.65	122.07
2	P	5	DA	C4-N9-C1'	6.37	136.61	127.05
3	A	116	ASP	N-CA-CB	6.35	119.45	110.12
3	A	92	ASP	N-CA-CB	6.34	119.21	110.01
3	A	252	HIS	CA-CB-CG	-6.33	107.47	113.80
3	A	29	VAL	N-CA-C	6.33	117.00	110.36
3	A	54	LYS	N-CA-C	6.29	121.24	113.50
2	P	5	DA	C8-N9-C1'	-6.28	117.63	127.05
3	A	253	ARG	N-CA-C	6.26	119.11	108.90
3	A	68	LYS	CB-CA-C	6.26	121.23	110.84
1	T	6	DG	C4-N9-C1'	-6.22	117.68	127.00
3	A	261	PRO	N-CA-C	-6.14	100.85	110.50
3	A	286	ALA	CA-C-N	6.09	128.72	120.44
3	A	286	ALA	C-N-CA	6.09	128.72	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	20	THR	CB-CA-C	6.06	120.97	110.79
3	A	98	ASN	CB-CA-C	6.02	120.91	110.68
2	P	3	DT	O4'-C1'-N1	5.97	117.35	108.40
2	P	4	DA	C4-N9-C1'	5.97	136.00	127.05
3	A	83	ARG	N-CA-CB	5.95	118.70	110.07
3	A	99	PHE	CA-CB-CG	-5.91	107.89	113.80
3	A	222	HIS	N-CA-C	5.91	119.79	112.58
3	A	33	ILE	N-CA-CB	-5.91	103.09	110.47
2	P	6	DT	C4'-C3'-O3'	-5.90	101.14	110.00
3	A	250	TYR	N-CA-C	5.90	117.51	110.07
3	A	271	TYR	N-CA-C	5.90	118.21	111.02
3	A	68	LYS	N-CA-C	5.88	121.02	111.37
3	A	74	ASP	N-CA-CB	5.88	118.53	110.01
2	P	6	DT	O3'-P-O5'	-5.85	95.22	104.00
1	T	1	DC	C6-N1-C1'	-5.85	110.93	119.70
3	A	157	GLN	N-CA-CB	5.84	118.53	110.07
3	A	11	LEU	N-CA-C	-5.83	105.66	112.89
3	A	99	PHE	N-CA-C	5.81	118.48	111.40
3	A	176	THR	CA-C-N	-5.80	115.11	122.37
3	A	176	THR	C-N-CA	-5.80	115.11	122.37
2	P	5	DA	P-O5'-C5'	-5.78	111.34	120.00
3	A	32	ALA	N-CA-C	5.75	118.25	109.62
3	A	192	ASP	CB-CA-C	5.75	120.30	110.81
3	A	314	ASP	N-CA-CB	5.73	119.38	110.44
3	A	320	PHE	O-C-N	5.73	127.99	122.03
3	A	116	ASP	CB-CA-C	5.71	120.27	110.79
3	A	285	HIS	N-CA-C	5.71	117.17	111.07
1	T	2	DA	C8-N9-C1'	5.70	135.60	127.05
1	T	3	DT	P-O5'-C5'	5.64	128.46	120.00
3	A	151	PRO	N-CA-CB	5.64	108.32	103.36
3	A	276	ASP	CA-CB-CG	-5.61	106.99	112.60
3	A	121	THR	CA-C-N	5.61	127.79	120.28
3	A	121	THR	C-N-CA	5.61	127.79	120.28
3	A	223	PHE	CA-C-N	-5.60	115.88	122.93
3	A	223	PHE	C-N-CA	-5.60	115.88	122.93
3	A	196	THR	CB-CA-C	-5.60	98.39	111.09
3	A	256	ASP	N-CA-CB	5.57	120.16	110.81
3	A	57	ALA	CA-C-N	5.54	128.16	120.29
3	A	57	ALA	C-N-CA	5.54	128.16	120.29
3	A	259	LEU	N-CA-C	5.52	117.73	108.73
2	P	3	DT	N1-C1'-C2'	5.51	121.77	113.50
3	A	28	ASN	CA-CB-CG	-5.49	107.11	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	320	PHE	CA-C-N	5.46	129.01	120.82
3	A	320	PHE	C-N-CA	5.46	129.01	120.82
3	A	216	GLU	CB-CG-CD	-5.43	103.37	112.60
3	A	29	VAL	N-CA-CB	5.42	116.53	110.51
3	A	124	ASP	N-CA-C	-5.42	105.37	111.28
3	A	50	PRO	CB-CA-C	-5.42	102.62	111.56
3	A	170	ASP	N-CA-C	-5.40	99.89	109.06
3	A	224	ILE	CA-CB-CG1	-5.40	101.23	110.40
3	A	236	MET	CA-C-O	-5.39	114.39	120.32
2	P	7	DG	O5'-C5'-C4'	5.38	118.87	110.80
3	A	223	PHE	N-CA-C	-5.37	105.87	112.90
1	T	2	DA	N9-C1'-C2'	-5.37	105.45	113.50
3	A	213	GLN	CB-CG-CD	-5.36	103.49	112.60
3	A	169	VAL	N-CA-CB	5.35	116.45	110.62
3	A	104	SER	N-CA-C	-5.35	102.13	110.10
3	A	232	GLU	N-CA-C	5.34	119.42	113.01
1	T	1	DC	C2-N1-C1'	5.30	127.64	119.70
3	A	229	SER	CA-C-N	-5.29	113.50	121.86
3	A	229	SER	C-N-CA	-5.29	113.50	121.86
3	A	218	LEU	CB-CA-C	5.28	119.56	110.79
1	T	6	DG	C8-N9-C1'	5.26	134.88	127.00
3	A	109	SER	CA-CB-OG	-5.25	100.59	111.10
3	A	311	LEU	CA-C-N	5.25	126.40	119.84
3	A	311	LEU	C-N-CA	5.25	126.40	119.84
3	A	332	ASP	N-CA-CB	5.24	117.59	110.42
3	A	295	GLU	CB-CG-CD	5.23	121.48	112.60
3	A	335	GLU	N-CA-CB	5.21	119.35	110.50
3	A	334	SER	N-CA-C	5.17	118.69	112.38
3	A	117	GLU	CA-C-N	-5.14	115.54	122.63
3	A	117	GLU	C-N-CA	-5.14	115.54	122.63
3	A	281	ASN	CA-C-N	-5.12	111.98	120.68
3	A	281	ASN	C-N-CA	-5.12	111.98	120.68
3	A	306	VAL	CB-CA-C	-5.11	104.19	111.34
3	A	39	TYR	CA-CB-CG	-5.11	104.71	113.90
3	A	282	MET	CA-CB-CG	-5.10	103.89	114.10
3	A	303	VAL	CB-CA-C	5.10	120.07	112.16
3	A	309	GLU	O-C-N	5.10	127.18	121.32
3	A	68	LYS	CA-C-N	5.09	129.04	120.29
3	A	68	LYS	C-N-CA	5.09	129.04	120.29
2	P	6	DT	C5'-C4'-C3'	-5.07	107.30	114.90
3	A	216	GLU	CB-CA-C	-5.07	102.28	110.79
3	A	195	LEU	N-CA-C	5.06	117.59	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	269	VAL	CB-CA-C	-5.04	105.34	112.14
3	A	146	PHE	N-CA-CB	5.04	118.09	110.28
3	A	17	ASP	CB-CA-C	5.03	119.94	110.63
3	A	177	VAL	CB-CA-C	5.02	117.04	110.96
3	A	281	ASN	N-CA-CB	5.01	117.48	110.12

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	68	LYS	CA
3	A	92	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	6	0
2	P	154	0	85	11	0
3	A	2623	0	2641	335	0
4	A	2	0	0	0	0
5	A	2	0	0	0	0
6	A	14	0	0	2	0
7	A	101	0	0	20	0
7	P	15	0	0	2	0
7	T	16	0	0	1	0
All	All	3072	0	2806	349	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 62.

All (349) 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:293:ILE:HD13	3:A:298:ILE:HG13	1.33	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:270:LEU:HD21	3:A:282:MET:HE1	1.31	1.07
2:P:5:DA:H2''	2:P:6:DT:H5'	1.39	1.03
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.38	1.03
3:A:245:ASN:HD22	3:A:245:ASN:N	1.53	0.98
3:A:18:MET:HE3	3:A:76:PHE:HB2	1.45	0.96
3:A:245:ASN:H	3:A:245:ASN:ND2	1.57	0.96
3:A:29:VAL:HG22	3:A:97:ILE:HD12	1.48	0.94
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.52	0.90
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.53	0.89
3:A:41:LYS:HD3	3:A:42:ALA:H	1.38	0.88
3:A:41:LYS:HE2	3:A:64:GLY:HA3	1.56	0.87
3:A:155:MET:HA	3:A:158:MET:HE3	1.57	0.87
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.05	0.86
3:A:270:LEU:HD21	3:A:282:MET:CE	2.07	0.84
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.60	0.83
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.60	0.83
3:A:172:GLU:HG3	3:A:198:PRO:HG2	1.58	0.83
3:A:277:ILE:HG12	3:A:335:GLU:HA	1.60	0.81
3:A:253:ARG:HG3	3:A:253:ARG:HH11	1.46	0.81
3:A:41:LYS:HD3	3:A:42:ALA:N	1.96	0.79
2:P:5:DA:H2''	2:P:6:DT:C5'	2.12	0.78
2:P:5:DA:H1'	7:P:565:HOH:O	1.82	0.78
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.48	0.78
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.15	0.77
3:A:259:LEU:C	3:A:260:ILE:HD13	2.10	0.77
3:A:302:GLY:HA3	3:A:307:ALA:HB2	1.66	0.77
3:A:12:ASN:HD21	3:A:53:ILE:H	1.32	0.76
3:A:68:LYS:O	3:A:72:LYS:HE3	1.83	0.76
3:A:195:LEU:O	3:A:259:LEU:HD12	1.86	0.76
3:A:330:PRO:HA	3:A:333:ARG:CG	2.15	0.76
3:A:243:SER:HB3	3:A:249:GLU:HA	1.66	0.76
3:A:236:MET:HG3	3:A:256:ASP:OD1	1.85	0.76
3:A:293:ILE:HD13	3:A:298:ILE:CG1	2.15	0.75
3:A:172:GLU:CG	3:A:198:PRO:HG2	2.16	0.75
1:T:6:DG:H2''	1:T:7:DA:C8	2.21	0.75
3:A:30:SER:HA	7:A:558:HOH:O	1.87	0.75
3:A:68:LYS:HB2	3:A:68:LYS:NZ	2.02	0.75
3:A:172:GLU:HB3	3:A:197:HIS:NE2	2.02	0.75
3:A:33:ILE:O	3:A:37:ASN:HB2	1.87	0.74
3:A:207:GLN:O	3:A:210:LEU:HB2	1.87	0.74
3:A:182:ARG:HG2	3:A:182:ARG:NH1	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:264:GLN:NE2	3:A:296:TYR:HB3	2.03	0.72
3:A:279:ASN:O	3:A:283:ARG:HG3	1.88	0.72
3:A:271:TYR:HB2	7:A:592:HOH:O	1.90	0.72
3:A:19:LEU:HB3	3:A:43:ALA:HB2	1.72	0.72
3:A:18:MET:HE3	3:A:76:PHE:CB	2.20	0.71
3:A:18:MET:O	3:A:21:GLU:HB2	1.90	0.71
3:A:266:TYR:HA	3:A:269:VAL:HB	1.72	0.71
3:A:18:MET:CE	3:A:76:PHE:HB2	2.20	0.71
3:A:291:PHE:CD1	3:A:300:PRO:HA	2.26	0.71
3:A:291:PHE:HD1	3:A:300:PRO:HA	1.56	0.70
3:A:268:GLY:O	3:A:271:TYR:HB3	1.93	0.69
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.75	0.68
3:A:108:PRO:O	3:A:112:ARG:HG3	1.93	0.68
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.24	0.68
3:A:68:LYS:HB2	3:A:68:LYS:HZ3	1.59	0.67
1:T:6:DG:N7	7:T:652:HOH:O	2.27	0.67
3:A:323:ILE:O	3:A:324:GLN:HG2	1.93	0.67
2:P:6:DT:H1'	2:P:7:DG:H5''	1.77	0.67
3:A:12:ASN:HB3	3:A:46:ILE:CD1	2.25	0.67
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.29	0.67
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.77	0.66
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.29	0.66
3:A:302:GLY:N	3:A:307:ALA:HB3	2.11	0.66
3:A:245:ASN:HD22	3:A:245:ASN:H	0.77	0.66
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.31	0.65
3:A:286:ALA:HB2	3:A:323:ILE:HG21	1.79	0.65
3:A:280:LYS:O	3:A:284:ALA:N	2.28	0.65
3:A:79:THR:O	3:A:81:LYS:N	2.29	0.65
3:A:285:HIS:NE2	7:A:583:HOH:O	2.29	0.65
3:A:27:LYS:HB2	3:A:36:TYR:CD1	2.32	0.65
3:A:145:ASP:OD2	3:A:252:HIS:HB2	1.97	0.65
3:A:286:ALA:HA	3:A:323:ILE:CG2	2.26	0.64
2:P:3:DT:H4'	7:P:569:HOH:O	1.97	0.64
3:A:150:ILE:HG12	3:A:253:ARG:HG2	1.80	0.63
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.13	0.63
3:A:329:GLU:O	3:A:333:ARG:HG2	1.98	0.63
3:A:323:ILE:C	3:A:324:GLN:HG2	2.21	0.63
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.79	0.63
3:A:306:VAL:HG22	7:A:650:HOH:O	1.98	0.62
3:A:119:ILE:HG23	3:A:124:ASP:CB	2.29	0.62
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:165:GLU:OE1	3:A:168:LYS:NZ	2.31	0.62
3:A:303:VAL:C	3:A:305:GLY:H	2.07	0.62
3:A:122:LEU:C	3:A:122:LEU:HD23	2.25	0.62
3:A:286:ALA:HA	3:A:323:ILE:HG21	1.81	0.61
3:A:243:SER:CB	3:A:249:GLU:HA	2.29	0.61
3:A:128:ASN:N	3:A:128:ASN:ND2	2.49	0.61
3:A:52:LYS:HD3	3:A:54:LYS:HE3	1.83	0.60
3:A:41:LYS:NZ	3:A:64:GLY:O	2.31	0.60
3:A:123:GLU:O	3:A:127:LYS:HG2	2.00	0.60
3:A:174:ILE:O	3:A:195:LEU:HD12	2.01	0.60
3:A:15:ILE:HD13	3:A:73:ILE:HG23	1.84	0.60
3:A:286:ALA:O	3:A:291:PHE:N	2.31	0.60
3:A:11:LEU:HD23	3:A:11:LEU:H	1.67	0.60
3:A:200:PHE:O	3:A:262:LYS:N	2.32	0.60
3:A:155:MET:HE2	3:A:188:SER:HB2	1.83	0.60
3:A:240:GLN:NE2	3:A:250:TYR:O	2.33	0.60
3:A:306:VAL:HG23	3:A:307:ALA:N	2.15	0.60
3:A:165:GLU:O	3:A:169:VAL:HG12	2.01	0.60
3:A:150:ILE:O	3:A:187:SER:HA	2.03	0.59
3:A:124:ASP:O	3:A:128:ASN:ND2	2.36	0.59
3:A:62:LEU:HD12	3:A:63:PRO:HD2	1.83	0.59
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.84	0.59
3:A:11:LEU:H	3:A:11:LEU:CD2	2.15	0.59
3:A:270:LEU:HD12	7:A:584:HOH:O	2.03	0.59
3:A:122:LEU:HB3	7:A:623:HOH:O	2.03	0.58
3:A:237:GLY:O	3:A:254:ARG:NH1	2.36	0.58
3:A:157:GLN:O	3:A:160:ASP:HB3	2.04	0.58
3:A:282:MET:HB3	7:A:555:HOH:O	2.03	0.58
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.67	0.58
3:A:195:LEU:O	3:A:260:ILE:N	2.28	0.58
3:A:320:PHE:O	3:A:324:GLN:N	2.37	0.58
3:A:83:ARG:HA	3:A:86:GLU:HG2	1.86	0.57
3:A:128:ASN:N	3:A:128:ASN:HD22	2.02	0.57
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.86	0.57
3:A:73:ILE:HG22	3:A:77:LEU:HD22	1.85	0.57
3:A:150:ILE:HG22	3:A:155:MET:HG2	1.85	0.57
3:A:27:LYS:HG3	3:A:28:ASN:N	2.17	0.57
3:A:277:ILE:HD11	3:A:334:SER:O	2.05	0.57
3:A:172:GLU:HB3	3:A:197:HIS:CD2	2.40	0.57
3:A:209:LYS:HA	3:A:212:HIS:HB2	1.85	0.57
3:A:286:ALA:HB2	3:A:293:ILE:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:286:ALA:CA	3:A:323:ILE:HG21	2.34	0.57
3:A:178:CYS:HA	3:A:182:ARG:HD3	1.86	0.57
3:A:163:LEU:HD23	3:A:163:LEU:N	2.19	0.56
3:A:253:ARG:HH11	3:A:253:ARG:CG	2.17	0.56
3:A:259:LEU:O	3:A:260:ILE:HD13	2.03	0.56
3:A:223:PHE:O	3:A:239:CYS:HA	2.05	0.56
3:A:278:PHE:HB2	3:A:333:ARG:O	2.06	0.56
3:A:26:GLU:HG3	3:A:35:LYS:HB3	1.87	0.56
3:A:265:TYR:O	3:A:268:GLY:N	2.39	0.56
3:A:294:ASN:O	3:A:296:TYR:N	2.38	0.56
3:A:266:TYR:O	3:A:270:LEU:N	2.30	0.56
3:A:58:GLU:O	3:A:61:LYS:HG3	2.05	0.56
3:A:155:MET:HE2	3:A:188:SER:CB	2.35	0.56
3:A:253:ARG:NH2	7:A:620:HOH:O	2.27	0.56
3:A:152:ARG:HA	3:A:155:MET:HB2	1.88	0.55
3:A:201:THR:HA	3:A:261:PRO:CB	2.37	0.55
3:A:182:ARG:NH2	3:A:316:GLU:OE2	2.37	0.55
3:A:201:THR:HA	3:A:261:PRO:HB3	1.88	0.55
3:A:277:ILE:HG13	3:A:335:GLU:HB2	1.88	0.55
3:A:250:TYR:HB3	7:A:577:HOH:O	2.07	0.55
3:A:121:THR:HG23	3:A:124:ASP:OD2	2.07	0.54
3:A:133:ASN:HD22	3:A:135:HIS:H	1.54	0.54
3:A:207:GLN:HB2	7:A:625:HOH:O	2.07	0.54
3:A:41:LYS:O	3:A:45:VAL:HG13	2.08	0.54
3:A:89:ARG:HD3	3:A:89:ARG:C	2.33	0.54
3:A:49:TYR:CE2	3:A:51:HIS:HB2	2.42	0.54
3:A:260:ILE:HG22	3:A:261:PRO:N	2.22	0.54
3:A:316:GLU:O	3:A:320:PHE:HD1	1.91	0.54
3:A:302:GLY:HA3	3:A:307:ALA:CB	2.36	0.54
3:A:277:ILE:CG1	3:A:335:GLU:HA	2.35	0.53
3:A:298:ILE:O	3:A:311:LEU:HB2	2.09	0.53
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.38	0.53
3:A:195:LEU:O	3:A:259:LEU:HA	2.08	0.53
3:A:150:ILE:CG1	3:A:253:ARG:HG2	2.38	0.53
3:A:26:GLU:HB2	3:A:36:TYR:HB2	1.90	0.53
3:A:295:GLU:HA	7:A:592:HOH:O	2.09	0.53
3:A:110:ALA:HB2	7:A:568:HOH:O	2.08	0.52
3:A:62:LEU:C	3:A:65:VAL:HG22	2.35	0.52
3:A:111:ALA:O	3:A:115:VAL:HG23	2.09	0.52
3:A:114:PHE:HB3	3:A:119:ILE:HB	1.92	0.52
3:A:54:LYS:N	3:A:58:GLU:OE1	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:211:LEU:HD12	3:A:211:LEU:O	2.10	0.52
3:A:328:ARG:HB3	3:A:328:ARG:CZ	2.38	0.52
3:A:25:PHE:CE2	3:A:88:ILE:HG12	2.45	0.51
3:A:267:CYS:O	3:A:271:TYR:HB2	2.11	0.51
3:A:35:LYS:O	3:A:38:ALA:HB3	2.11	0.51
3:A:77:LEU:HD13	3:A:77:LEU:N	2.25	0.51
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.57	0.51
3:A:212:HIS:N	3:A:212:HIS:CD2	2.76	0.51
3:A:60:LYS:O	3:A:60:LYS:HG2	2.10	0.51
3:A:278:PHE:O	3:A:282:MET:N	2.42	0.51
3:A:303:VAL:O	3:A:305:GLY:N	2.44	0.51
3:A:285:HIS:CE1	3:A:289:LYS:HG2	2.46	0.51
3:A:183:ARG:HD3	3:A:273:THR:O	2.11	0.51
3:A:68:LYS:O	3:A:71:GLU:HB3	2.11	0.51
3:A:133:ASN:ND2	3:A:135:HIS:H	2.08	0.51
3:A:155:MET:HE2	3:A:188:SER:OG	2.11	0.51
3:A:32:ALA:O	3:A:36:TYR:HB3	2.10	0.50
3:A:279:ASN:O	3:A:282:MET:N	2.43	0.50
3:A:154:GLU:OE2	3:A:250:TYR:HE1	1.93	0.50
3:A:171:SER:O	3:A:171:SER:OG	2.30	0.50
3:A:260:ILE:HG22	3:A:261:PRO:O	2.11	0.50
3:A:29:VAL:HG21	3:A:94:SER:HB2	1.93	0.50
3:A:34:HIS:O	3:A:38:ALA:N	2.45	0.50
3:A:197:HIS:O	3:A:262:LYS:HB2	2.11	0.50
3:A:326:LYS:HG3	3:A:326:LYS:O	2.10	0.50
3:A:31:GLN:NE2	3:A:112:ARG:HH12	2.10	0.50
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.42	0.50
2:P:8:DA:OP1	6:A:338:DTP:O2A	2.30	0.50
3:A:133:ASN:O	3:A:137:ARG:HG3	2.12	0.49
3:A:194:LEU:O	3:A:265:TYR:OH	2.31	0.49
3:A:320:PHE:HD2	3:A:325:TRP:HB3	1.76	0.49
3:A:62:LEU:HB2	3:A:65:VAL:HG21	1.95	0.49
3:A:326:LYS:O	3:A:328:ARG:HG2	2.12	0.49
3:A:209:LYS:O	3:A:213:GLN:N	2.42	0.49
3:A:82:LEU:HD23	3:A:85:LEU:HD22	1.95	0.49
3:A:11:LEU:HD23	3:A:11:LEU:N	2.28	0.49
3:A:333:ARG:NH1	7:A:584:HOH:O	2.45	0.49
3:A:120:LYS:N	3:A:124:ASP:OD2	2.45	0.48
3:A:180:SER:OG	6:A:338:DTP:O1G	2.30	0.48
3:A:166:VAL:CG1	3:A:173:TYR:HB3	2.42	0.48
3:A:242:PRO:HB2	7:A:589:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:196:THR:OG1	3:A:197:HIS:N	2.43	0.48
3:A:23:ALA:O	3:A:36:TYR:HD1	1.97	0.48
3:A:248:LYS:O	3:A:248:LYS:HG2	2.13	0.48
3:A:315:SER:OG	3:A:316:GLU:N	2.45	0.48
1:T:2:DA:N6	2:P:5:DA:N6	2.62	0.48
3:A:30:SER:HB3	7:A:561:HOH:O	2.13	0.48
3:A:216:GLU:O	3:A:220:LYS:N	2.44	0.48
3:A:41:LYS:NZ	3:A:42:ALA:HB2	2.29	0.48
3:A:276:ASP:O	3:A:280:LYS:HG3	2.14	0.48
3:A:22:LEU:HD13	3:A:22:LEU:HA	1.32	0.47
3:A:178:CYS:SG	3:A:194:LEU:HD23	2.53	0.47
3:A:212:HIS:CD2	3:A:212:HIS:H	2.32	0.47
3:A:245:ASN:N	3:A:245:ASN:ND2	2.29	0.47
3:A:277:ILE:HG13	3:A:335:GLU:CB	2.44	0.47
3:A:19:LEU:HD23	3:A:43:ALA:HA	1.97	0.47
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.55	0.47
3:A:79:THR:O	3:A:79:THR:OG1	2.29	0.47
3:A:121:THR:HG23	3:A:124:ASP:CG	2.39	0.47
3:A:278:PHE:CE2	3:A:333:ARG:CD	2.98	0.47
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.50	0.47
3:A:278:PHE:HZ	3:A:320:PHE:CZ	2.32	0.47
3:A:18:MET:HE2	3:A:82:LEU:HD13	1.96	0.47
3:A:296:TYR:C	3:A:297:THR:HG23	2.40	0.47
3:A:19:LEU:HD23	3:A:43:ALA:HB2	1.97	0.47
3:A:41:LYS:HZ3	3:A:42:ALA:HB2	1.78	0.47
3:A:121:THR:O	3:A:124:ASP:HB2	2.14	0.47
3:A:228:LEU:HB2	3:A:236:MET:HB3	1.97	0.47
3:A:315:SER:C	3:A:317:LYS:H	2.23	0.47
3:A:99:PHE:CD1	3:A:99:PHE:C	2.93	0.47
3:A:180:SER:HB3	3:A:183:ARG:HH21	1.80	0.47
3:A:195:LEU:HD12	3:A:195:LEU:HA	1.62	0.47
3:A:228:LEU:HD12	3:A:228:LEU:HA	1.52	0.47
3:A:239:CYS:O	3:A:240:GLN:HB2	2.14	0.47
3:A:159:GLN:HG2	3:A:160:ASP:N	2.21	0.47
3:A:182:ARG:HH11	3:A:182:ARG:CG	2.22	0.47
3:A:319:ILE:O	3:A:322:TYR:HB2	2.14	0.47
3:A:150:ILE:HD11	3:A:253:ARG:HG2	1.95	0.47
3:A:262:LYS:O	3:A:262:LYS:HG3	2.10	0.47
3:A:264:GLN:NE2	3:A:296:TYR:CB	2.77	0.47
3:A:260:ILE:HD13	3:A:260:ILE:N	2.17	0.46
3:A:286:ALA:O	3:A:291:PHE:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:59:ALA:O	3:A:62:LEU:HB2	2.15	0.46
3:A:249:GLU:HG3	3:A:250:TYR:N	2.29	0.46
3:A:12:ASN:HA	7:A:553:HOH:O	2.16	0.46
1:T:2:DA:H2''	1:T:3:DT:OP2	2.15	0.46
3:A:15:ILE:HD13	3:A:73:ILE:CG2	2.44	0.46
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.51	0.46
3:A:292:THR:O	3:A:298:ILE:HA	2.15	0.46
2:P:5:DA:H5''	3:A:107:GLY:N	2.31	0.46
3:A:151:PRO:HB3	3:A:153:GLU:HG2	1.98	0.46
3:A:194:LEU:HA	3:A:194:LEU:HD12	1.04	0.46
3:A:285:HIS:NE2	3:A:289:LYS:CG	2.79	0.46
3:A:309:GLU:N	3:A:310:PRO:CD	2.79	0.46
3:A:25:PHE:CD2	3:A:88:ILE:CD1	2.99	0.45
3:A:327:TYR:HD1	3:A:328:ARG:N	2.13	0.45
3:A:250:TYR:HA	3:A:251:PRO:HD3	1.79	0.45
3:A:286:ALA:HB1	3:A:291:PHE:HB2	1.98	0.45
3:A:308:GLY:O	3:A:309:GLU:HB2	2.16	0.45
3:A:79:THR:H	3:A:79:THR:HG23	1.26	0.45
3:A:88:ILE:HD13	3:A:88:ILE:HG21	1.76	0.45
3:A:183:ARG:HH11	3:A:275:SER:HA	1.81	0.45
3:A:278:PHE:CD2	3:A:333:ARG:HD2	2.52	0.45
1:T:5:DA:H2''	1:T:6:DG:O5'	2.16	0.45
2:P:6:DT:H6	2:P:6:DT:H2'	0.85	0.45
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.52	0.45
3:A:317:LYS:HE3	3:A:321:ASP:OD1	2.17	0.45
3:A:125:LEU:HA	3:A:125:LEU:HD23	1.31	0.44
3:A:279:ASN:HD22	3:A:279:ASN:HA	1.45	0.44
3:A:122:LEU:HD21	3:A:126:ARG:CZ	2.47	0.44
3:A:49:TYR:HA	3:A:50:PRO:HD2	1.48	0.44
3:A:79:THR:C	3:A:81:LYS:H	2.22	0.44
3:A:260:ILE:CG2	3:A:261:PRO:N	2.79	0.44
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.96	0.44
3:A:82:LEU:HD23	3:A:85:LEU:HB2	2.00	0.44
3:A:288:GLU:OE1	3:A:288:GLU:HA	2.17	0.44
3:A:294:ASN:HB2	3:A:295:GLU:OE1	2.17	0.44
3:A:298:ILE:O	3:A:298:ILE:HG23	2.17	0.44
3:A:148:LYS:HB3	7:A:620:HOH:O	2.18	0.44
3:A:315:SER:C	3:A:317:LYS:N	2.76	0.44
3:A:73:ILE:HG22	3:A:77:LEU:CD2	2.48	0.44
3:A:278:PHE:HZ	3:A:320:PHE:HZ	1.66	0.44
3:A:286:ALA:HA	3:A:323:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:320:PHE:CE2	3:A:328:ARG:HG3	2.53	0.44
3:A:162:VAL:HG13	3:A:218:LEU:HD21	1.98	0.44
3:A:289:LYS:N	3:A:289:LYS:HD3	2.32	0.44
3:A:170:ASP:HB3	3:A:173:TYR:CD2	2.53	0.43
3:A:327:TYR:C	3:A:327:TYR:CD1	2.95	0.43
3:A:133:ASN:HD22	3:A:135:HIS:N	2.15	0.43
3:A:257:ILE:HG22	3:A:258:ARG:N	2.34	0.43
3:A:38:ALA:O	3:A:41:LYS:HD3	2.19	0.43
3:A:42:ALA:O	3:A:46:ILE:HG23	2.18	0.43
3:A:282:MET:HE3	7:A:555:HOH:O	2.18	0.43
3:A:322:TYR:C	3:A:324:GLN:H	2.25	0.43
3:A:29:VAL:HG21	3:A:94:SER:CB	2.48	0.43
3:A:77:LEU:N	3:A:77:LEU:CD1	2.79	0.43
3:A:172:GLU:HG2	3:A:198:PRO:HG2	1.97	0.43
2:P:5:DA:C2'	2:P:6:DT:H5'	2.29	0.43
3:A:210:LEU:HD23	3:A:210:LEU:HA	1.78	0.43
3:A:228:LEU:O	3:A:229:SER:HB3	2.19	0.43
3:A:65:VAL:HG23	3:A:65:VAL:O	2.18	0.43
3:A:77:LEU:HD12	3:A:77:LEU:HA	1.69	0.43
3:A:151:PRO:CB	3:A:153:GLU:HG2	2.49	0.43
3:A:21:GLU:OE1	3:A:85:LEU:HG	2.19	0.42
3:A:28:ASN:ND2	3:A:108:PRO:HG3	2.34	0.42
3:A:304:THR:H	3:A:304:THR:HG23	1.31	0.42
3:A:315:SER:O	3:A:317:LYS:N	2.52	0.42
1:T:4:DT:N3	2:P:4:DA:C2	2.77	0.42
3:A:223:PHE:CZ	3:A:239:CYS:HB2	2.54	0.42
3:A:287:LEU:HD13	3:A:287:LEU:HA	1.48	0.42
3:A:303:VAL:C	3:A:305:GLY:N	2.75	0.42
3:A:157:GLN:O	3:A:161:ILE:HG12	2.18	0.42
3:A:36:TYR:CD2	3:A:37:ASN:N	2.88	0.42
3:A:196:THR:OG1	3:A:262:LYS:HA	2.19	0.42
3:A:122:LEU:CD2	3:A:126:ARG:CZ	2.97	0.42
3:A:195:LEU:HB3	3:A:258:ARG:O	2.19	0.42
3:A:243:SER:O	3:A:244:LYS:O	2.38	0.42
3:A:293:ILE:HD13	3:A:298:ILE:CD1	2.49	0.42
3:A:99:PHE:HD1	3:A:100:LEU:HD13	1.85	0.42
3:A:253:ARG:CG	3:A:253:ARG:NH1	2.79	0.41
3:A:26:GLU:O	3:A:30:SER:O	2.38	0.41
3:A:204:SER:O	3:A:204:SER:OG	2.29	0.41
3:A:230:LYS:HB3	3:A:230:LYS:HE2	1.20	0.41
3:A:205:THR:HG23	3:A:205:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:25:PHE:CD1	3:A:25:PHE:C	2.98	0.41
3:A:127:LYS:HB2	3:A:128:ASN:ND2	2.36	0.41
3:A:133:ASN:HD22	3:A:133:ASN:C	2.28	0.41
3:A:178:CYS:SG	3:A:194:LEU:CD2	3.09	0.41
3:A:40:ARG:HE	3:A:40:ARG:HB2	1.46	0.41
3:A:183:ARG:NH1	3:A:275:SER:HA	2.35	0.41
3:A:11:LEU:CD2	3:A:11:LEU:N	2.81	0.41
3:A:119:ILE:CG2	3:A:124:ASP:CB	2.97	0.41
3:A:241:LEU:HB2	3:A:250:TYR:CD2	2.56	0.41
3:A:151:PRO:C	3:A:153:GLU:N	2.77	0.41
3:A:244:LYS:H	3:A:244:LYS:HG2	1.48	0.41
3:A:302:GLY:H	3:A:307:ALA:HB3	1.81	0.41
3:A:273:THR:HB	7:A:584:HOH:O	2.21	0.41
3:A:135:HIS:HB2	7:A:596:HOH:O	2.20	0.40
3:A:159:GLN:O	3:A:163:LEU:HG	2.21	0.40
3:A:201:THR:OG1	3:A:202:SER:N	2.54	0.40
3:A:279:ASN:O	3:A:283:ARG:N	2.43	0.40
3:A:25:PHE:CD2	3:A:88:ILE:HD13	2.56	0.40
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.54	0.40
3:A:320:PHE:O	3:A:323:ILE:HG13	2.22	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%)	262 (81%)	40 (12%)	23 (7%)	1 4

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	205	THR

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Mol	Chain	Res	Type
3	A	244	LYS
3	A	246	ASP
3	A	265	TYR
3	A	295	GLU
3	A	309	GLU
3	A	10	THR
3	A	78	ALA
3	A	80	GLY
3	A	204	SER
3	A	206	LYS
3	A	247	GLU
3	A	266	TYR
3	A	304	THR
3	A	60	LYS
3	A	202	SER
3	A	279	ASN
3	A	316	GLU
3	A	185	ALA
3	A	50	PRO
3	A	91	ASP
3	A	13	GLY
3	A	207	GLN

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%)	211 (73%)	77 (27%)	0 3

All (77) 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

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Mol	Chain	Res	Type
3	A	20	THR
3	A	22	LEU
3	A	27	LYS
3	A	30	SER
3	A	33	ILE
3	A	37	ASN
3	A	40	ARG
3	A	41	LYS
3	A	45	VAL
3	A	46	ILE
3	A	52	LYS
3	A	62	LEU
3	A	67	THR
3	A	68	LYS
3	A	72	LYS
3	A	77	LEU
3	A	79	THR
3	A	81	LYS
3	A	85	LEU
3	A	88	ILE
3	A	89	ARG
3	A	92	ASP
3	A	94	SER
3	A	100	LEU
3	A	101	THR
3	A	119	ILE
3	A	121	THR
3	A	127	LYS
3	A	128	ASN
3	A	133	ASN
3	A	136	GLN
3	A	138	ILE
3	A	157	GLN
3	A	161	ILE
3	A	167	LYS
3	A	168	LYS
3	A	169	VAL
3	A	174	ILE
3	A	180	SER
3	A	182	ARG
3	A	188	SER
3	A	194	LEU

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Mol	Chain	Res	Type
3	A	201	THR
3	A	205	THR
3	A	213	GLN
3	A	214	VAL
3	A	216	GLU
3	A	226	ASP
3	A	228	LEU
3	A	230	LYS
3	A	236	MET
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE
3	A	264	GLN
3	A	277	ILE
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	303	VAL
3	A	306	VAL
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	325	TRP
3	A	328	ARG
3	A	329	GLU
3	A	331	LYS
3	A	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) 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	128	ASN

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Mol	Chain	Res	Type
3	A	133	ASN
3	A	134	HIS
3	A	136	GLN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	245	ASN
3	A	264	GLN
3	A	279	ASN
3	A	294	ASN
3	A	324	GLN

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	DTP	A	338	4	10,12,32	2.31	2 (20%)	17,20,50	1.21	1 (5%)

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	DTP	A	338	4	-	6/12/12/34	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	338	DTP	PB-O3A	4.94	1.64	1.59
6	A	338	DTP	PB-O3B	-4.16	1.55	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	338	DTP	O2B-PB-O3A	2.05	112.82	107.27

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	338	DTP	PB-O3B-PG-O3G
6	A	338	DTP	PA-O3A-PB-O2B
6	A	338	DTP	PG-O3B-PB-O1B
6	A	338	DTP	PB-O3B-PG-O2G
6	A	338	DTP	PG-O3B-PB-O2B
6	A	338	DTP	PA-O3A-PB-O1B

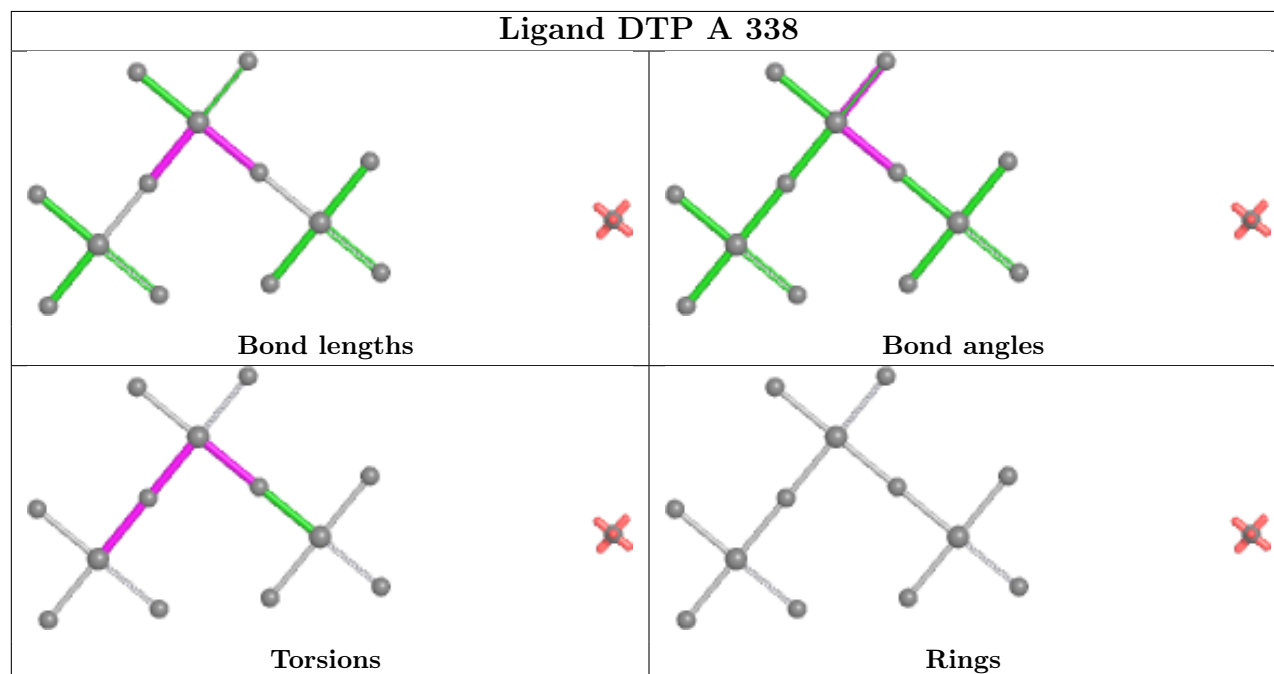
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	338	DTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	8/8 (100%)	-0.36	1 (12%) 8 5	17, 41, 98, 100	0
2	P	8/8 (100%)	-0.45	1 (12%) 8 5	17, 27, 67, 100	1 (12%)
3	A	325/335 (97%)	-1.04	1 (0%) 90 79	3, 31, 85, 100	0
All	All	341/351 (97%)	-1.01	3 (0%) 81 61	3, 31, 87, 100	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	1	DC	2.5
3	A	246	ASP	2.0
2	P	7	DG	2.0

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.

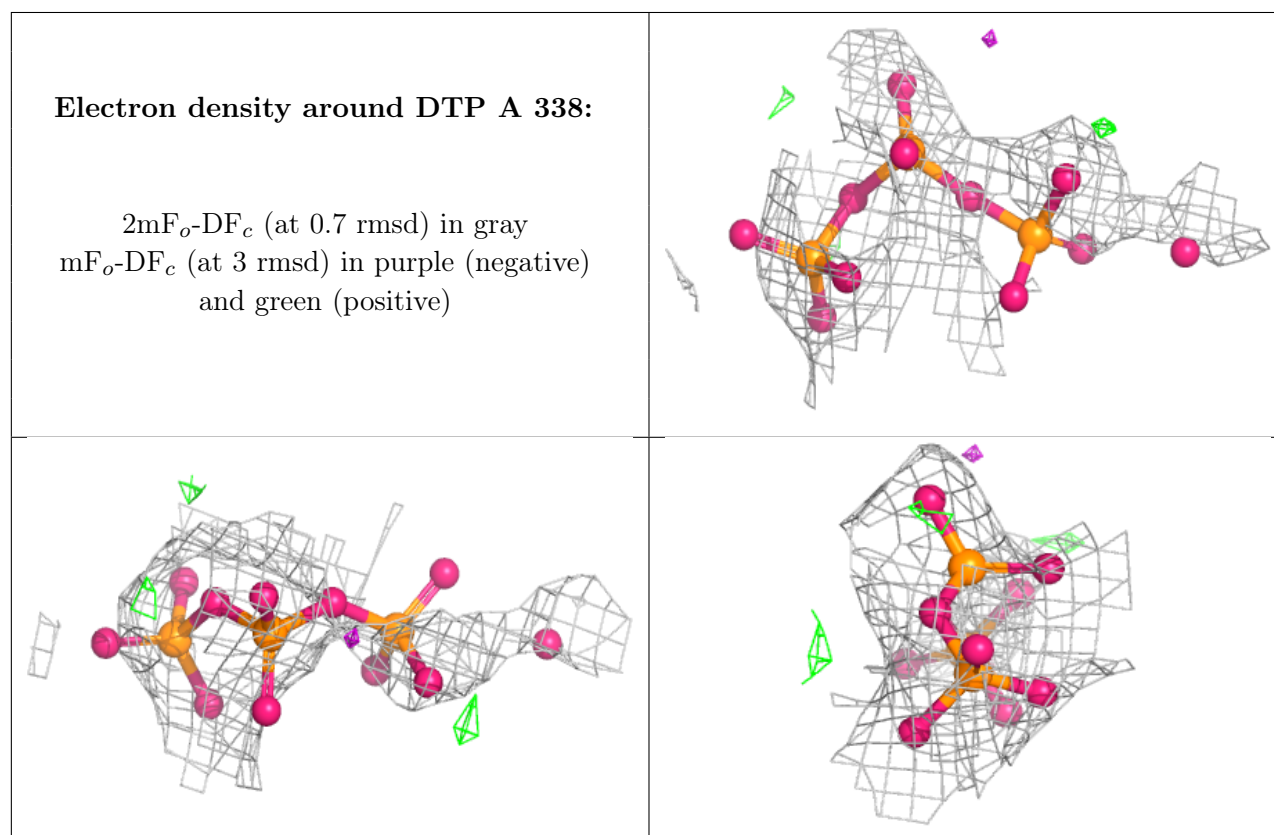
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NA	A	342	1/1	0.91	0.05	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	DTP	A	338	14/30	0.92	0.15	1,70,90,93	14
4	ZN	A	339	1/1	0.98	0.02	30,30,30,30	1
4	ZN	A	343	1/1	0.98	0.03	30,30,30,30	1
5	NA	A	341	1/1	0.99	0.02	9,9,9,9	0

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



6.5 Other polymers ⓘ

There are no such residues in this entry.