



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:16 PM UTC

PDB ID : 8ICW / pdb_00008icw
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SEVEN BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF DTTP (1 MILLIMOLAR) AND MNCL2 (5 MILLIMOLAR)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1995-12-15
Resolution : 3.30 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

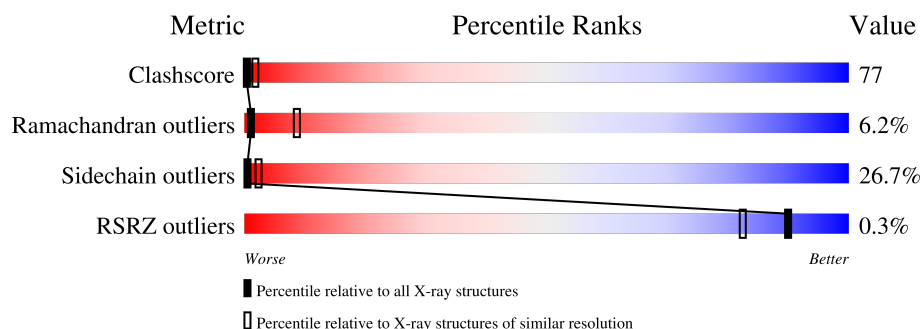
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

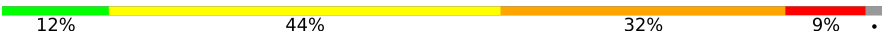
The reported resolution of this entry is 3.30 Å.

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	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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% 25% 62%
2	P	8	 12% 88%
3	A	335	 12% 44% 32% 9% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3071 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*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	8	Total	C	N	O	P	0	0	0
			150	70	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	17	0	0
			2623	1657	458	499	9			

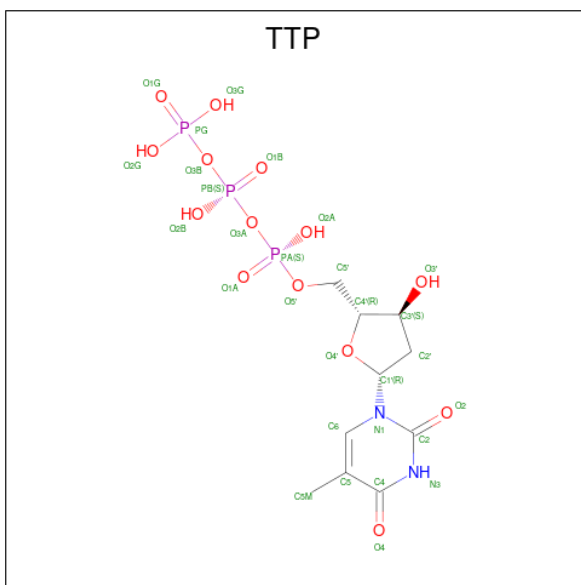
- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	P	0	0
			20	5	12	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	T	13	Total O 13 13	0	0
7	P	16	Total O 16 16	0	0
7	A	101	Total O 101 101	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	180.05Å 57.72Å 48.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 20.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	92.0 (20.00-3.30) 92.0 (20.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.79Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.164 , (Not available) 0.158 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 275.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3071	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.08	0/162	3.68	15/249 (6.0%)
2	P	1.17	1/165 (0.6%)	3.21	22/251 (8.8%)
3	A	1.59	19/2672 (0.7%)	2.23	140/3590 (3.9%)
All	All	1.55	20/2999 (0.7%)	2.41	177/4090 (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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	224	ILE	CA-C	-8.24	1.43	1.53
3	A	195	LEU	CA-C	-7.67	1.43	1.52
3	A	65	VAL	C-N	-7.51	1.25	1.33
2	P	1	DT	OP3-P	6.82	1.62	1.48
3	A	242	PRO	CA-C	-6.06	1.43	1.52
3	A	251	PRO	N-CA	-6.02	1.40	1.47
3	A	256	ASP	N-CA	5.93	1.53	1.46
3	A	139	GLY	C-N	-5.89	1.25	1.33
3	A	321	ASP	CG-OD2	5.78	1.36	1.25
3	A	177	VAL	N-CA	-5.60	1.39	1.46
3	A	161	ILE	CA-C	-5.55	1.46	1.52
3	A	106	ILE	CA-CB	-5.40	1.47	1.53
3	A	260	ILE	CA-C	-5.37	1.47	1.52
3	A	114	PHE	CA-C	-5.32	1.46	1.52
3	A	224	ILE	CA-CB	-5.28	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	247	GLU	CD-OE1	5.27	1.35	1.25
3	A	116	ASP	CA-C	-5.20	1.46	1.52
3	A	66	GLY	CA-C	-5.15	1.46	1.52
3	A	229	SER	N-CA	-5.09	1.39	1.46
3	A	176	THR	N-CA	-5.04	1.40	1.46

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	7	DA	C4-N9-C1'	-28.99	83.56	127.05
1	T	7	DA	C8-N9-C1'	28.34	169.56	127.05
2	P	3	DT	C6-N1-C1'	-13.37	99.30	119.35
2	P	7	DG	P-O3'-C3'	13.03	139.75	120.20
1	T	4	DT	C6-N1-C1'	-12.95	99.92	119.35
2	P	5	DA	C4-N9-C1'	12.83	146.30	127.05
1	T	4	DT	C2-N1-C1'	12.80	138.55	119.35
1	T	6	DG	C4-N9-C1'	-12.79	107.82	127.00
2	P	6	DT	C6-N1-C1'	-12.44	100.70	119.35
2	P	6	DT	C2-N1-C1'	12.10	137.50	119.35
2	P	3	DT	C2-N1-C1'	12.06	137.45	119.35
1	T	6	DG	C8-N9-C1'	11.94	144.92	127.00
3	A	45	VAL	N-CA-CB	11.58	123.73	110.65
1	T	3	DT	C2-N1-C1'	11.40	136.45	119.35
2	P	5	DA	C8-N9-C1'	-11.13	110.35	127.05
2	P	4	DA	C4-N9-C1'	10.89	143.38	127.05
3	A	224	ILE	CB-CA-C	-10.75	99.62	111.23
2	P	2	DC	C2-N1-C1'	10.68	135.71	119.70
2	P	2	DC	C6-N1-C1'	-10.41	104.09	119.70
1	T	3	DT	C6-N1-C1'	-10.38	103.78	119.35
2	P	4	DA	C8-N9-C1'	-10.17	111.79	127.05
3	A	297	THR	N-CA-C	9.07	121.65	108.86
2	P	8	DT	P-O5'-C5'	-9.01	106.49	120.00
3	A	77	LEU	N-CA-CB	8.79	122.74	109.91
1	T	1	DC	P-O3'-C3'	8.79	133.38	120.20
3	A	286	ALA	CA-C-N	8.60	132.50	120.29
3	A	286	ALA	C-N-CA	8.60	132.50	120.29
3	A	116	ASP	CA-CB-CG	-8.47	104.13	112.60
2	P	1	DT	C2-N1-C1'	8.41	131.97	119.35
2	P	3	DT	O4'-C1'-N1	8.13	120.59	108.40
3	A	135	HIS	O-C-N	8.11	130.47	122.03
3	A	83	ARG	N-CA-CB	8.06	121.70	110.01
2	P	1	DT	C6-N1-C1'	-8.06	107.26	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	241	LEU	O-C-N	7.93	128.65	121.35
3	A	224	ILE	O-C-N	7.90	131.29	122.68
3	A	45	VAL	O-C-N	7.82	130.31	121.94
2	P	7	DG	C4-N9-C1'	-7.78	115.32	127.00
3	A	62	LEU	N-CA-C	7.74	119.83	110.07
3	A	214	VAL	N-CA-C	7.72	117.83	110.42
3	A	49	TYR	CA-C-N	7.71	129.47	119.84
3	A	49	TYR	C-N-CA	7.71	129.47	119.84
3	A	168	LYS	N-CA-CB	7.67	121.36	109.94
3	A	65	VAL	N-CA-CB	7.64	120.36	111.66
3	A	12	ASN	CA-CB-CG	7.63	120.23	112.60
3	A	114	PHE	CA-CB-CG	-7.61	106.19	113.80
3	A	266	TYR	CA-CB-CG	-7.59	100.24	113.90
3	A	157	GLN	CB-CA-C	7.57	122.76	110.88
3	A	157	GLN	N-CA-CB	7.55	120.95	110.01
3	A	162	VAL	N-CA-CB	7.48	118.81	110.51
3	A	17	ASP	CA-CB-CG	-7.47	105.13	112.60
3	A	107	GLY	O-C-N	7.39	129.16	121.77
1	T	6	DG	P-O3'-C3'	-7.33	109.20	120.20
3	A	291	PHE	CA-CB-CG	-7.33	106.47	113.80
3	A	193	VAL	N-CA-C	7.33	119.04	107.98
3	A	270	LEU	O-C-N	7.28	129.60	122.03
2	P	7	DG	O3'-P-O5'	-7.23	93.16	104.00
3	A	321	ASP	CA-CB-CG	7.21	119.81	112.60
3	A	313	VAL	N-CA-C	7.15	117.95	107.37
3	A	115	VAL	CB-CA-C	-7.12	102.85	111.97
3	A	77	LEU	CB-CA-C	7.07	121.84	110.96
3	A	207	GLN	CA-C-N	6.99	128.57	119.84
3	A	207	GLN	C-N-CA	6.99	128.57	119.84
3	A	177	VAL	N-CA-C	-6.98	97.55	108.23
2	P	7	DG	C8-N9-C1'	6.97	137.45	127.00
3	A	65	VAL	CA-C-O	6.96	129.18	121.04
3	A	107	GLY	CA-C-N	6.96	126.20	118.97
3	A	107	GLY	C-N-CA	6.96	126.20	118.97
3	A	66	GLY	N-CA-C	-6.83	103.21	112.57
3	A	24	ASN	N-CA-CB	6.81	120.09	109.94
3	A	270	LEU	CA-C-N	6.77	130.20	120.79
3	A	270	LEU	C-N-CA	6.77	130.20	120.79
3	A	192	ASP	N-CA-C	6.75	120.45	108.24
3	A	164	ASN	CA-C-N	-6.72	111.30	120.44
3	A	164	ASN	C-N-CA	-6.72	111.30	120.44
3	A	45	VAL	CA-C-O	-6.71	113.40	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	65	VAL	CA-CB-CG2	-6.67	99.05	110.40
3	A	215	VAL	O-C-N	6.67	128.61	121.94
3	A	235	PHE	N-CA-C	-6.62	99.13	109.72
3	A	223	PHE	CA-C-N	6.61	131.40	122.01
3	A	223	PHE	C-N-CA	6.61	131.40	122.01
3	A	207	GLN	C-N-CD	-6.60	97.96	125.00
3	A	285	HIS	N-CA-C	6.59	118.26	111.14
3	A	88	ILE	CB-CA-C	-6.42	102.68	112.05
1	T	1	DC	C6-N1-C1'	-6.40	110.10	119.70
1	T	5	DA	P-O3'-C3'	-6.39	110.61	120.20
3	A	219	GLN	N-CA-C	-6.35	103.88	111.69
3	A	68	LYS	N-CA-CB	6.25	119.08	110.01
1	T	1	DC	C2-N1-C1'	6.24	129.07	119.70
2	P	7	DG	P-O5'-C5'	-6.24	110.64	120.00
3	A	59	ALA	O-C-N	6.23	128.82	122.09
1	T	4	DT	P-O3'-C3'	-6.21	110.88	120.20
3	A	260	ILE	O-C-N	6.20	128.17	121.10
3	A	238	VAL	CB-CA-C	6.20	119.85	110.62
3	A	11	LEU	CA-C-N	-6.18	112.71	122.79
3	A	11	LEU	C-N-CA	-6.18	112.71	122.79
3	A	332	ASP	CA-CB-CG	6.14	118.74	112.60
3	A	65	VAL	CB-CA-C	6.12	119.77	111.88
3	A	120	LYS	N-CA-C	6.03	118.75	111.40
3	A	74	ASP	CB-CA-C	6.00	120.20	110.96
3	A	277	ILE	N-CA-CB	5.99	118.24	110.57
3	A	212	HIS	CA-CB-CG	-5.99	107.81	113.80
3	A	137	ARG	N-CA-C	-5.97	104.15	112.45
3	A	161	ILE	N-CA-CB	5.95	117.12	110.51
3	A	321	ASP	CB-CA-C	-5.94	100.88	110.74
3	A	316	GLU	CA-C-N	5.92	128.14	120.44
3	A	316	GLU	C-N-CA	5.92	128.14	120.44
3	A	228	LEU	N-CA-C	-5.84	105.82	113.12
3	A	256	ASP	N-CA-CB	5.82	121.55	111.13
3	A	39	TYR	CA-CB-CG	-5.79	103.48	113.90
3	A	241	LEU	CA-C-N	5.74	127.01	119.84
3	A	241	LEU	C-N-CA	5.74	127.01	119.84
3	A	18	MET	CA-C-N	5.73	127.96	120.28
3	A	18	MET	C-N-CA	5.73	127.96	120.28
3	A	91	ASP	N-CA-CB	5.72	120.16	110.49
3	A	200	PHE	N-CA-C	5.72	118.05	108.73
3	A	294	ASN	CA-CB-CG	5.70	118.30	112.60
3	A	235	PHE	CA-CB-CG	-5.69	108.11	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	222	HIS	N-CA-CB	5.69	120.10	110.49
2	P	3	DT	P-O3'-C3'	5.68	128.73	120.20
3	A	102	ARG	N-CA-C	5.65	118.21	111.71
3	A	41	LYS	N-CA-CB	5.63	118.40	110.12
3	A	195	LEU	O-C-N	5.59	130.41	123.15
3	A	124	ASP	O-C-N	5.54	127.77	122.07
3	A	246	ASP	N-CA-CB	5.54	119.85	110.49
3	A	309	GLU	CB-CA-C	5.53	121.06	110.17
3	A	49	TYR	O-C-N	5.50	127.65	121.32
2	P	3	DT	N1-C1'-C2'	5.49	121.73	113.50
3	A	92	ASP	CB-CA-C	5.49	119.89	110.79
3	A	234	LYS	CA-C-O	5.47	126.40	120.32
3	A	132	LEU	CB-CA-C	-5.45	100.80	109.80
3	A	76	PHE	N-CA-C	-5.40	105.42	112.23
3	A	40	ARG	N-CA-CB	5.40	117.90	110.07
3	A	158	MET	O-C-N	5.38	127.84	122.08
3	A	102	ARG	CA-CB-CG	-5.34	103.42	114.10
3	A	240	GLN	N-CA-C	5.34	116.52	108.46
3	A	76	PHE	CA-C-N	-5.33	113.61	120.65
3	A	76	PHE	C-N-CA	-5.33	113.61	120.65
3	A	161	ILE	O-C-N	5.33	127.27	121.94
3	A	215	VAL	CA-C-N	5.32	127.41	120.28
3	A	215	VAL	C-N-CA	5.32	127.41	120.28
3	A	122	LEU	N-CA-C	-5.32	105.39	111.14
3	A	320	PHE	CA-C-N	5.31	128.78	120.82
3	A	320	PHE	C-N-CA	5.31	128.78	120.82
3	A	191	MET	N-CA-CB	5.30	118.90	110.16
3	A	314	ASP	N-CA-CB	5.26	118.50	110.44
3	A	194	LEU	N-CA-CB	5.25	118.74	110.23
3	A	20	THR	CB-CA-C	5.25	119.77	110.85
3	A	309	GLU	CA-C-N	5.24	126.39	119.84
3	A	309	GLU	C-N-CA	5.24	126.39	119.84
3	A	299	ARG	N-CA-C	5.21	117.51	110.31
3	A	148	LYS	N-CA-C	5.21	118.19	110.48
3	A	190	ASP	CA-CB-CG	5.20	117.80	112.60
3	A	327	TYR	N-CA-CB	5.19	117.59	109.85
2	P	7	DG	C2'-C3'-O3'	-5.19	103.71	111.50
3	A	124	ASP	N-CA-C	-5.19	105.52	111.07
3	A	67	THR	N-CA-CB	-5.17	102.52	110.12
3	A	115	VAL	N-CA-CB	-5.16	104.51	110.55
3	A	63	PRO	CB-CA-C	-5.16	105.14	111.64
3	A	292	THR	CB-CA-C	5.15	118.59	109.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	320	PHE	CA-CB-CG	-5.11	108.69	113.80
1	T	3	DT	P-O5'-C5'	5.10	127.64	120.00
3	A	243	SER	CB-CA-C	5.10	118.42	110.67
3	A	138	ILE	N-CA-C	-5.09	104.62	111.44
3	A	326	LYS	CA-C-N	-5.09	113.83	120.95
3	A	326	LYS	C-N-CA	-5.09	113.83	120.95
3	A	272	PHE	CA-CB-CG	-5.08	108.72	113.80
3	A	223	PHE	O-C-N	5.08	128.00	122.11
3	A	267	CYS	O-C-N	5.08	127.52	122.03
3	A	99	PHE	CA-CB-CG	-5.07	108.73	113.80
3	A	303	VAL	N-CA-C	5.07	119.19	111.89
3	A	309	GLU	N-CA-C	5.06	120.99	109.81
3	A	271	TYR	N-CA-CB	-5.04	102.16	109.82
3	A	334	SER	N-CA-C	5.04	118.20	111.75
3	A	95	SER	O-C-N	5.03	127.32	122.09
3	A	266	TYR	N-CA-CB	-5.02	102.01	110.49
3	A	128	ASN	CA-CB-CG	-5.00	107.60	112.60
3	A	306	VAL	CB-CA-C	-5.00	101.85	110.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	246	ASP	CA
3	A	309	GLU	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	13	0
2	P	150	0	80	27	0
3	A	2623	0	2641	411	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
6	A	20	0	6	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	101	0	0	19	0
7	P	16	0	0	1	0
7	T	13	0	0	2	0
All	All	3071	0	2807	435	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 77.

All (435) 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:285:HIS:HD2	3:A:323:ILE:HD12	1.18	1.06
2:P:1:DT:H2"	2:P:2:DC:H5'	1.41	1.02
2:P:6:DT:H2"	2:P:7:DG:H5"	1.39	1.02
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.45	0.99
3:A:12:ASN:HD21	3:A:53:ILE:H	1.02	0.96
3:A:245:ASN:N	3:A:245:ASN:HD22	1.60	0.96
3:A:253:ARG:HG3	3:A:253:ARG:HH11	1.30	0.95
3:A:245:ASN:HD22	3:A:245:ASN:H	1.01	0.95
3:A:311:LEU:HB3	3:A:322:TYR:HE2	1.30	0.94
1:T:6:DG:H2"	1:T:7:DA:C8	2.02	0.94
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.07	0.94
3:A:285:HIS:CD2	3:A:323:ILE:HD12	2.02	0.93
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.49	0.91
3:A:18:MET:HE2	3:A:82:LEU:HD22	1.52	0.90
3:A:245:ASN:H	3:A:245:ASN:ND2	1.68	0.90
3:A:27:LYS:HB3	3:A:36:TYR:CD2	2.08	0.87
3:A:313:VAL:HG11	3:A:319:ILE:HG13	1.59	0.85
3:A:29:VAL:HG13	3:A:97:ILE:HD12	1.59	0.84
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.74	0.83
3:A:282:MET:HB2	3:A:325:TRP:HZ3	1.44	0.83
3:A:60:LYS:HA	3:A:65:VAL:HG23	1.60	0.83
2:P:5:DA:H2"	2:P:6:DT:C5'	2.09	0.82
3:A:18:MET:HE1	3:A:76:PHE:CB	2.08	0.82
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.20	0.82
3:A:22:LEU:HD22	3:A:85:LEU:HD13	1.60	0.82
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.42	0.82
3:A:15:ILE:CG2	3:A:46:ILE:HD13	2.10	0.82
3:A:18:MET:HG2	3:A:19:LEU:N	1.96	0.81
3:A:142:TYR:CE2	3:A:238:VAL:HG11	2.15	0.81
3:A:128:ASN:N	3:A:128:ASN:HD22	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.16	0.81
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.10	0.81
3:A:73:ILE:CG2	3:A:77:LEU:HD13	2.12	0.80
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.64	0.80
3:A:128:ASN:N	3:A:128:ASN:ND2	2.29	0.80
3:A:155:MET:HE2	3:A:188:SER:CB	2.11	0.80
3:A:16:THR:HG23	3:A:46:ILE:HD11	1.64	0.80
3:A:12:ASN:ND2	3:A:53:ILE:H	1.79	0.80
3:A:108:PRO:O	3:A:112:ARG:HG3	1.82	0.80
3:A:155:MET:HE2	3:A:188:SER:HB2	1.63	0.79
3:A:172:GLU:HG3	3:A:198:PRO:HG2	1.66	0.78
3:A:270:LEU:HA	3:A:316:GLU:OE2	1.84	0.78
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.18	0.77
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.64	0.77
3:A:277:ILE:HD13	3:A:277:ILE:H	1.50	0.77
3:A:68:LYS:O	3:A:72:LYS:HE3	1.83	0.77
3:A:127:LYS:HB2	3:A:128:ASN:ND2	2.00	0.77
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.66	0.77
3:A:218:LEU:HB2	3:A:224:ILE:CD1	2.15	0.77
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.18	0.77
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.16	0.76
3:A:323:ILE:O	3:A:324:GLN:HG2	1.84	0.76
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.16	0.76
3:A:140:LEU:HD12	3:A:140:LEU:O	1.86	0.76
2:P:6:DT:C2'	2:P:7:DG:H5''	2.15	0.75
3:A:22:LEU:HD22	3:A:85:LEU:CD1	2.15	0.74
3:A:73:ILE:HG23	3:A:77:LEU:HD13	1.69	0.74
3:A:155:MET:HA	3:A:158:MET:CE	2.17	0.74
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.69	0.73
3:A:243:SER:HB3	3:A:249:GLU:HA	1.68	0.73
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.23	0.73
3:A:227:THR:HG21	3:A:230:LYS:HB2	1.71	0.72
1:T:4:DT:H5''	3:A:231:GLY:HA3	1.71	0.72
3:A:12:ASN:HD21	3:A:53:ILE:N	1.84	0.72
3:A:114:PHE:HB3	3:A:119:ILE:HB	1.70	0.72
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.20	0.72
3:A:123:GLU:O	3:A:127:LYS:HG2	1.89	0.71
3:A:11:LEU:HD23	3:A:12:ASN:H	1.56	0.71
3:A:19:LEU:HB3	3:A:43:ALA:HB2	1.71	0.71
3:A:112:ARG:O	3:A:115:VAL:HB	1.89	0.71
3:A:123:GLU:HG3	7:A:623:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:4:DT:C5'	3:A:231:GLY:HA3	2.21	0.70
3:A:22:LEU:CD2	3:A:85:LEU:HD13	2.20	0.70
3:A:83:ARG:HA	3:A:86:GLU:HG2	1.73	0.70
2:P:1:DT:H2''	2:P:2:DC:C5'	2.20	0.70
3:A:155:MET:HA	3:A:158:MET:HE3	1.73	0.70
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.08	0.69
3:A:165:GLU:HA	3:A:168:LYS:CG	2.23	0.68
3:A:133:ASN:H	3:A:136:GLN:HE21	1.40	0.68
2:P:5:DA:H2''	2:P:6:DT:H5''	1.73	0.68
3:A:323:ILE:C	3:A:324:GLN:HG2	2.19	0.68
3:A:75:GLU:OE1	3:A:82:LEU:HD12	1.93	0.68
3:A:44:SER:O	3:A:47:ALA:HB3	1.93	0.68
3:A:233:THR:HB	7:A:538:HOH:O	1.93	0.68
3:A:49:TYR:CE2	3:A:51:HIS:HB2	2.28	0.68
3:A:170:ASP:HB3	3:A:173:TYR:CE2	2.29	0.68
3:A:23:ALA:HB2	3:A:39:TYR:HB2	1.76	0.67
3:A:121:THR:O	3:A:124:ASP:HB2	1.95	0.67
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.88	0.67
3:A:52:LYS:HD3	3:A:54:LYS:HE3	1.77	0.67
3:A:56:GLY:O	3:A:59:ALA:HB3	1.95	0.67
3:A:152:ARG:HA	3:A:155:MET:HB2	1.74	0.67
3:A:169:VAL:HG22	3:A:170:ASP:N	2.10	0.67
3:A:121:THR:HG23	3:A:124:ASP:OD1	1.95	0.67
1:T:6:DG:N7	7:T:652:HOH:O	2.28	0.66
3:A:210:LEU:CB	3:A:259:LEU:HD21	2.25	0.66
3:A:289:LYS:HD3	3:A:289:LYS:N	2.10	0.66
3:A:155:MET:HE3	3:A:181:PHE:HB2	1.77	0.66
3:A:270:LEU:HD23	3:A:319:ILE:HG21	1.76	0.66
3:A:282:MET:HB2	3:A:325:TRP:CZ3	2.28	0.66
3:A:152:ARG:NH2	3:A:181:PHE:O	2.28	0.66
2:P:5:DA:H2''	2:P:6:DT:H5'	1.76	0.65
3:A:218:LEU:HB2	3:A:224:ILE:HD11	1.79	0.65
3:A:195:LEU:HB3	3:A:259:LEU:HA	1.79	0.65
3:A:266:TYR:O	3:A:270:LEU:N	2.29	0.65
3:A:79:THR:O	3:A:81:LYS:N	2.30	0.65
3:A:156:LEU:HD23	3:A:181:PHE:HE1	1.61	0.65
3:A:172:GLU:HB3	3:A:197:HIS:CD2	2.32	0.65
3:A:240:GLN:NE2	3:A:250:TYR:O	2.30	0.64
3:A:209:LYS:HA	3:A:212:HIS:HB2	1.79	0.64
3:A:16:THR:HG23	3:A:46:ILE:CD1	2.27	0.64
3:A:331:LYS:HG2	3:A:332:ASP:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:268:GLY:O	3:A:271:TYR:HB3	1.98	0.64
3:A:15:ILE:O	3:A:19:LEU:HD13	1.96	0.64
3:A:165:GLU:O	3:A:169:VAL:HG12	1.97	0.64
3:A:14:GLY:O	3:A:18:MET:N	2.30	0.63
3:A:144:GLY:N	7:A:590:HOH:O	2.28	0.63
3:A:73:ILE:HG22	3:A:77:LEU:HD13	1.80	0.63
3:A:134:HIS:HA	3:A:137:ARG:HB2	1.80	0.62
3:A:286:ALA:O	3:A:291:PHE:N	2.30	0.62
3:A:92:ASP:HA	3:A:95:SER:HB2	1.82	0.62
3:A:101:THR:HA	3:A:106:ILE:HG22	1.81	0.62
3:A:111:ALA:O	3:A:115:VAL:HG23	1.99	0.62
3:A:27:LYS:HB3	3:A:36:TYR:CG	2.33	0.62
3:A:58:GLU:O	3:A:61:LYS:HG3	1.99	0.62
2:P:5:DA:P	3:A:109:SER:HB3	2.40	0.62
3:A:11:LEU:HD23	3:A:12:ASN:N	2.14	0.62
3:A:33:ILE:O	3:A:37:ASN:HB2	1.99	0.62
3:A:149:ARG:NH2	3:A:188:SER:HA	2.14	0.61
3:A:60:LYS:HA	3:A:65:VAL:CG2	2.30	0.61
3:A:266:TYR:HA	3:A:269:VAL:HB	1.83	0.61
3:A:122:LEU:C	3:A:122:LEU:HD23	2.25	0.61
3:A:122:LEU:HD21	3:A:126:ARG:CZ	2.31	0.61
3:A:285:HIS:CE1	3:A:289:LYS:HG2	2.36	0.61
3:A:277:ILE:HG12	3:A:335:GLU:HA	1.83	0.61
3:A:309:GLU:N	3:A:309:GLU:OE1	2.35	0.60
3:A:21:GLU:OE1	3:A:85:LEU:HG	2.01	0.60
3:A:216:GLU:HA	3:A:219:GLN:OE1	2.01	0.60
3:A:328:ARG:HB3	3:A:332:ASP:OD1	2.00	0.60
3:A:313:VAL:HG13	3:A:318:ASP:HB2	1.83	0.60
1:T:4:DT:H5''	3:A:231:GLY:CA	2.31	0.60
3:A:217:GLN:O	3:A:220:LYS:N	2.35	0.60
3:A:127:LYS:HB2	3:A:128:ASN:HD21	1.65	0.60
3:A:286:ALA:HB2	3:A:323:ILE:HG21	1.84	0.60
3:A:114:PHE:HD1	3:A:119:ILE:HG13	1.65	0.60
3:A:19:LEU:CB	3:A:43:ALA:HB2	2.32	0.60
3:A:115:VAL:HG12	3:A:116:ASP:N	2.16	0.60
3:A:177:VAL:HG11	3:A:191:MET:HE2	1.83	0.60
3:A:214:VAL:O	3:A:218:LEU:HD13	2.01	0.60
3:A:249:GLU:HG3	3:A:250:TYR:H	1.66	0.59
3:A:316:GLU:HB2	3:A:327:TYR:OH	2.02	0.59
3:A:18:MET:O	3:A:21:GLU:HB2	2.02	0.59
3:A:272:PHE:CD1	6:A:338:TTP:H4'	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:18:MET:HE3	3:A:76:PHE:CD2	2.37	0.59
3:A:291:PHE:CD1	3:A:300:PRO:HA	2.37	0.59
3:A:201:THR:OG1	3:A:202:SER:N	2.31	0.59
3:A:53:ILE:C	3:A:54:LYS:HD2	2.27	0.59
3:A:158:MET:CG	3:A:241:LEU:HD21	2.33	0.59
3:A:306:VAL:HG22	7:A:650:HOH:O	2.03	0.59
3:A:270:LEU:HD12	3:A:270:LEU:O	2.04	0.58
3:A:254:ARG:CZ	3:A:254:ARG:HB3	2.34	0.58
3:A:327:TYR:HD1	3:A:328:ARG:N	2.01	0.58
2:P:1:DT:C2'	2:P:2:DC:H5'	2.26	0.58
3:A:128:ASN:HD22	3:A:128:ASN:H	1.47	0.58
3:A:180:SER:HB2	3:A:185:ALA:CB	2.34	0.58
3:A:279:ASN:O	3:A:283:ARG:N	2.31	0.58
3:A:158:MET:HG3	3:A:241:LEU:HD21	1.86	0.58
3:A:103:VAL:HA	7:A:600:HOH:O	2.04	0.57
3:A:249:GLU:HG3	3:A:250:TYR:N	2.20	0.57
3:A:210:LEU:HB2	3:A:259:LEU:HD21	1.85	0.57
3:A:100:LEU:HD21	3:A:119:ILE:O	2.04	0.57
3:A:142:TYR:CD2	3:A:238:VAL:HG11	2.40	0.57
3:A:59:ALA:O	3:A:62:LEU:HB2	2.04	0.57
3:A:152:ARG:O	3:A:155:MET:N	2.38	0.57
1:T:4:DT:OP1	3:A:231:GLY:HA3	2.04	0.57
2:P:5:DA:H3'	7:P:648:HOH:O	2.05	0.57
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.85	0.57
3:A:73:ILE:O	3:A:77:LEU:N	2.38	0.56
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.87	0.56
2:P:1:DT:H2'	2:P:2:DC:C6	2.41	0.56
3:A:280:LYS:O	3:A:284:ALA:N	2.37	0.56
3:A:311:LEU:CB	3:A:322:TYR:HE2	2.13	0.56
3:A:295:GLU:HA	7:A:592:HOH:O	2.06	0.56
3:A:180:SER:C	3:A:185:ALA:HB3	2.31	0.56
3:A:245:ASN:N	3:A:245:ASN:ND2	2.34	0.56
3:A:16:THR:CG2	3:A:46:ILE:HD11	2.36	0.56
3:A:218:LEU:HB3	3:A:224:ILE:HG13	1.88	0.56
2:P:5:DA:P	3:A:107:GLY:HA3	2.47	0.55
3:A:73:ILE:HG23	3:A:77:LEU:CD1	2.36	0.55
3:A:45:VAL:HG21	3:A:63:PRO:O	2.06	0.55
3:A:93:THR:O	3:A:97:ILE:HG13	2.07	0.55
3:A:146:PHE:HZ	3:A:238:VAL:CG2	2.19	0.55
2:P:6:DT:H5'	2:P:6:DT:H6	1.72	0.55
3:A:207:GLN:HG2	3:A:207:GLN:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:8:DT:C5'	3:A:272:PHE:HE1	2.20	0.55
3:A:15:ILE:HB	3:A:46:ILE:CD1	2.37	0.55
3:A:149:ARG:HH21	3:A:188:SER:HA	1.70	0.55
3:A:41:LYS:O	3:A:44:SER:HB3	2.07	0.54
3:A:278:PHE:HB2	3:A:333:ARG:O	2.07	0.54
3:A:15:ILE:CD1	3:A:77:LEU:HD11	2.36	0.54
3:A:124:ASP:O	3:A:128:ASN:ND2	2.39	0.54
3:A:218:LEU:CB	3:A:224:ILE:HG13	2.37	0.54
3:A:270:LEU:HD12	3:A:270:LEU:C	2.31	0.54
3:A:57:ALA:O	3:A:60:LYS:HB3	2.08	0.54
3:A:218:LEU:H	3:A:218:LEU:CD1	2.20	0.54
3:A:286:ALA:HB1	3:A:323:ILE:HG21	1.87	0.54
3:A:84:LYS:O	3:A:88:ILE:HG13	2.07	0.54
3:A:236:MET:HG3	3:A:256:ASP:OD1	2.07	0.54
3:A:241:LEU:O	3:A:250:TYR:HB2	2.08	0.54
3:A:253:ARG:NH1	7:A:503:HOH:O	2.40	0.54
3:A:282:MET:HE3	7:A:555:HOH:O	2.07	0.54
2:P:7:DG:H2'	2:P:8:DT:C5'	2.38	0.53
3:A:140:LEU:HD12	3:A:140:LEU:C	2.31	0.53
3:A:322:TYR:C	3:A:324:GLN:H	2.14	0.53
3:A:237:GLY:O	3:A:254:ARG:NH1	2.40	0.53
1:T:5:DA:H1'	7:T:564:HOH:O	2.08	0.53
2:P:5:DA:H2'	2:P:6:DT:H71	1.91	0.53
3:A:166:VAL:HG13	3:A:173:TYR:HB3	1.91	0.53
3:A:298:ILE:HG23	3:A:298:ILE:O	2.08	0.53
3:A:326:LYS:HE3	3:A:328:ARG:HH21	1.72	0.53
3:A:18:MET:HG2	3:A:19:LEU:HD12	1.91	0.53
3:A:156:LEU:CD2	3:A:181:PHE:HE1	2.21	0.53
3:A:243:SER:CB	3:A:249:GLU:HA	2.38	0.53
3:A:288:GLU:OE1	3:A:288:GLU:HA	2.05	0.53
3:A:278:PHE:HE1	3:A:328:ARG:HD3	1.75	0.52
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.90	0.52
3:A:330:PRO:O	3:A:333:ARG:HG2	2.08	0.52
3:A:74:ASP:O	3:A:77:LEU:N	2.41	0.52
3:A:122:LEU:O	3:A:125:LEU:HB2	2.10	0.52
3:A:59:ALA:C	3:A:65:VAL:HG21	2.34	0.52
3:A:155:MET:HE2	3:A:188:SER:OG	2.09	0.52
3:A:180:SER:HB3	3:A:183:ARG:HH21	1.75	0.52
3:A:205:THR:HA	7:A:624:HOH:O	2.09	0.52
3:A:145:ASP:OD2	3:A:252:HIS:N	2.32	0.52
3:A:149:ARG:HH21	3:A:188:SER:CA	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:182:ARG:NH2	3:A:316:GLU:OE1	2.31	0.52
3:A:272:PHE:O	6:A:338:TTP:O3'	2.28	0.52
2:P:8:DT:OP2	6:A:338:TTP:O1A	2.28	0.51
3:A:294:ASN:O	3:A:296:TYR:N	2.43	0.51
3:A:18:MET:HE1	3:A:76:PHE:CG	2.45	0.51
3:A:34:HIS:O	3:A:38:ALA:N	2.43	0.51
3:A:53:ILE:O	3:A:54:LYS:HD2	2.10	0.51
3:A:15:ILE:HG22	3:A:46:ILE:HD13	1.89	0.51
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.40	0.51
3:A:41:LYS:HD3	3:A:42:ALA:N	2.26	0.51
3:A:164:ASN:O	3:A:168:LYS:HG2	2.10	0.51
3:A:170:ASP:HB3	3:A:173:TYR:CD2	2.45	0.51
3:A:235:PHE:HZ	3:A:237:GLY:HA3	1.72	0.51
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.92	0.51
3:A:106:ILE:HG22	3:A:106:ILE:O	2.09	0.51
3:A:203:GLU:O	3:A:205:THR:N	2.43	0.51
3:A:333:ARG:NH1	7:A:584:HOH:O	2.44	0.51
3:A:16:THR:HG22	3:A:46:ILE:HG13	1.93	0.51
3:A:248:LYS:O	3:A:248:LYS:HG2	2.11	0.51
3:A:165:GLU:O	3:A:168:LYS:N	2.44	0.51
2:P:8:DT:OP2	3:A:190:ASP:OD2	2.29	0.50
3:A:181:PHE:HA	7:A:530:HOH:O	2.10	0.50
3:A:270:LEU:HD12	7:A:584:HOH:O	2.11	0.50
3:A:284:ALA:O	3:A:287:LEU:HB2	2.11	0.50
3:A:276:ASP:O	3:A:280:LYS:HG3	2.12	0.50
3:A:332:ASP:C	3:A:334:SER:H	2.20	0.50
3:A:172:GLU:HB3	3:A:197:HIS:NE2	2.26	0.50
3:A:222:HIS:HB3	7:A:520:HOH:O	2.12	0.50
3:A:286:ALA:HB1	3:A:291:PHE:HB2	1.93	0.50
3:A:35:LYS:O	3:A:38:ALA:HB3	2.11	0.50
3:A:263:ASP:O	3:A:264:GLN:HG2	2.12	0.50
3:A:253:ARG:HG3	3:A:253:ARG:NH1	2.06	0.50
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.26	0.50
3:A:15:ILE:HG21	3:A:46:ILE:HD13	1.91	0.49
3:A:26:GLU:O	3:A:30:SER:O	2.29	0.49
3:A:218:LEU:HD22	3:A:224:ILE:HD11	1.94	0.49
3:A:79:THR:O	3:A:79:THR:OG1	2.29	0.49
3:A:213:GLN:HG3	7:A:644:HOH:O	2.10	0.49
3:A:264:GLN:NE2	3:A:296:TYR:HB3	2.27	0.49
3:A:218:LEU:CD2	3:A:224:ILE:HD11	2.43	0.49
3:A:75:GLU:O	3:A:75:GLU:HG2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:163:LEU:HD22	3:A:175:ALA:HB3	1.94	0.49
3:A:182:ARG:HH22	3:A:316:GLU:CD	2.19	0.49
3:A:317:LYS:HE3	3:A:321:ASP:OD1	2.12	0.49
3:A:46:ILE:HG13	3:A:47:ALA:N	2.28	0.49
3:A:157:GLN:O	3:A:160:ASP:HB3	2.12	0.49
3:A:212:HIS:N	3:A:212:HIS:CD2	2.79	0.49
3:A:165:GLU:HB3	3:A:217:GLN:CG	2.43	0.49
3:A:294:ASN:HB3	7:A:580:HOH:O	2.13	0.49
3:A:179:GLY:O	3:A:182:ARG:HB3	2.12	0.48
3:A:197:HIS:HD2	3:A:198:PRO:HD2	1.71	0.48
3:A:212:HIS:HB3	7:A:541:HOH:O	2.12	0.48
1:T:2:DA:N6	2:P:5:DA:N6	2.61	0.48
1:T:4:DT:O2	2:P:4:DA:H2	1.95	0.48
3:A:176:THR:HG22	3:A:178:CYS:SG	2.53	0.48
3:A:41:LYS:HE2	3:A:64:GLY:HA2	1.94	0.48
1:T:7:DA:H61	2:P:1:DT:H3	1.62	0.48
3:A:260:ILE:HG23	3:A:261:PRO:CD	2.41	0.48
3:A:16:THR:CG2	3:A:46:ILE:HG13	2.44	0.48
2:P:8:DT:C5'	3:A:272:PHE:CE1	2.96	0.48
2:P:5:DA:C2'	2:P:6:DT:H5"	2.41	0.47
3:A:204:SER:O	3:A:206:LYS:N	2.47	0.47
3:A:207:GLN:HB3	7:A:625:HOH:O	2.14	0.47
3:A:218:LEU:N	3:A:218:LEU:HD12	2.29	0.47
3:A:15:ILE:HB	3:A:46:ILE:HD13	1.96	0.47
3:A:256:ASP:C	3:A:257:ILE:HG13	2.39	0.47
3:A:294:ASN:ND2	3:A:297:THR:OG1	2.48	0.47
3:A:330:PRO:HA	3:A:333:ARG:CG	2.44	0.47
3:A:25:PHE:CD2	3:A:88:ILE:HG23	2.49	0.47
3:A:210:LEU:HB3	3:A:259:LEU:HD21	1.95	0.47
2:P:5:DA:O5'	3:A:107:GLY:HA3	2.14	0.47
3:A:62:LEU:CD1	3:A:62:LEU:N	2.77	0.47
3:A:300:PRO:HD2	3:A:308:GLY:O	2.14	0.47
3:A:11:LEU:N	3:A:11:LEU:CD2	2.78	0.47
3:A:214:VAL:CG2	3:A:215:VAL:N	2.78	0.47
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.40	0.47
3:A:286:ALA:O	3:A:291:PHE:HB2	2.15	0.47
3:A:288:GLU:C	3:A:289:LYS:HD3	2.40	0.47
3:A:315:SER:OG	3:A:316:GLU:N	2.48	0.47
3:A:121:THR:HG23	3:A:124:ASP:CG	2.39	0.47
3:A:145:ASP:OD2	3:A:252:HIS:HB2	2.15	0.47
3:A:146:PHE:HZ	3:A:238:VAL:HG22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:263:ASP:C	3:A:264:GLN:HG2	2.40	0.47
3:A:285:HIS:CE1	3:A:289:LYS:CG	2.98	0.47
3:A:334:SER:O	3:A:335:GLU:HB3	2.13	0.47
3:A:15:ILE:CB	3:A:46:ILE:HD13	2.44	0.47
3:A:182:ARG:HH11	3:A:273:THR:HG21	1.80	0.47
3:A:196:THR:HB	3:A:265:TYR:CD1	2.50	0.46
3:A:114:PHE:O	3:A:119:ILE:N	2.30	0.46
3:A:146:PHE:CZ	3:A:238:VAL:HG22	2.50	0.46
3:A:251:PRO:HB2	3:A:253:ARG:CZ	2.45	0.46
3:A:145:ASP:HB3	3:A:252:HIS:O	2.16	0.46
3:A:277:ILE:HG13	3:A:335:GLU:CB	2.45	0.46
3:A:114:PHE:O	3:A:119:ILE:HG12	2.14	0.46
3:A:218:LEU:CD1	3:A:218:LEU:N	2.79	0.46
3:A:81:LYS:NZ	3:A:86:GLU:HB3	2.30	0.46
3:A:207:GLN:O	3:A:209:LYS:N	2.49	0.46
3:A:291:PHE:HD1	3:A:300:PRO:HA	1.80	0.46
3:A:275:SER:OG	3:A:277:ILE:HD13	2.14	0.46
3:A:329:GLU:O	3:A:333:ARG:HG2	2.15	0.46
3:A:18:MET:CE	3:A:76:PHE:CG	2.99	0.46
3:A:27:LYS:HG3	3:A:28:ASN:N	2.25	0.46
3:A:95:SER:HA	7:A:563:HOH:O	2.15	0.46
3:A:285:HIS:NE2	3:A:289:LYS:CG	2.79	0.46
3:A:290:GLY:O	3:A:301:LEU:N	2.36	0.46
3:A:16:THR:HG22	3:A:46:ILE:CG1	2.45	0.46
3:A:68:LYS:HB2	3:A:68:LYS:NZ	2.30	0.46
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.97	0.46
3:A:230:LYS:HB2	3:A:230:LYS:HE2	1.86	0.46
3:A:249:GLU:CG	3:A:250:TYR:N	2.79	0.46
3:A:271:TYR:HB2	7:A:592:HOH:O	2.15	0.46
3:A:22:LEU:HD22	3:A:85:LEU:HD11	1.98	0.45
3:A:150:ILE:HD13	3:A:253:ARG:HG2	1.94	0.45
1:T:4:DT:N3	2:P:4:DA:C2	2.77	0.45
3:A:162:VAL:CG2	3:A:223:PHE:CE2	2.99	0.45
3:A:214:VAL:O	3:A:217:GLN:N	2.49	0.45
3:A:272:PHE:HD1	6:A:338:TTP:H4'	1.78	0.45
3:A:128:ASN:HB3	3:A:131:LYS:HG3	1.98	0.45
3:A:260:ILE:CG2	3:A:261:PRO:N	2.80	0.45
3:A:282:MET:CB	3:A:325:TRP:CZ3	2.98	0.45
3:A:11:LEU:HD23	3:A:11:LEU:N	2.31	0.45
3:A:162:VAL:HG23	3:A:223:PHE:CE2	2.51	0.45
3:A:149:ARG:NH2	3:A:188:SER:CA	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:194:LEU:HD12	3:A:194:LEU:HA	1.45	0.45
3:A:228:LEU:HD12	3:A:228:LEU:HA	1.57	0.45
3:A:287:LEU:HD13	3:A:287:LEU:HA	1.62	0.45
1:T:3:DT:O2	2:P:5:DA:H2	1.99	0.45
3:A:182:ARG:HH12	3:A:273:THR:HG21	1.82	0.44
3:A:270:LEU:HD23	3:A:319:ILE:HD13	1.98	0.44
3:A:292:THR:HG22	3:A:301:LEU:HD22	2.00	0.44
3:A:309:GLU:N	3:A:310:PRO:CD	2.80	0.44
3:A:11:LEU:CD2	3:A:11:LEU:H	2.31	0.44
3:A:232:GLU:O	3:A:233:THR:HG23	2.16	0.44
3:A:18:MET:CE	3:A:76:PHE:CD2	3.00	0.44
3:A:253:ARG:NH1	3:A:253:ARG:CG	2.79	0.44
3:A:313:VAL:HG13	3:A:318:ASP:CB	2.46	0.44
3:A:182:ARG:NH1	3:A:273:THR:CG2	2.78	0.44
3:A:210:LEU:CD1	3:A:259:LEU:HD21	2.47	0.44
3:A:151:PRO:HG2	3:A:154:GLU:HG3	2.00	0.44
3:A:122:LEU:CD2	3:A:126:ARG:NH1	2.81	0.44
3:A:83:ARG:O	3:A:83:ARG:HG3	2.14	0.43
3:A:146:PHE:CZ	3:A:238:VAL:CG2	3.00	0.43
3:A:155:MET:HB3	3:A:181:PHE:CD1	2.53	0.43
3:A:262:LYS:C	3:A:264:GLN:H	2.26	0.43
3:A:45:VAL:O	3:A:48:LYS:N	2.51	0.43
3:A:22:LEU:HD13	3:A:22:LEU:HA	1.60	0.43
3:A:266:TYR:O	3:A:270:LEU:HB2	2.18	0.43
3:A:50:PRO:O	3:A:51:HIS:ND1	2.52	0.43
3:A:85:LEU:HD12	3:A:88:ILE:HD12	2.00	0.43
3:A:67:THR:H	3:A:67:THR:HG22	1.27	0.43
3:A:165:GLU:CA	3:A:168:LYS:HG2	2.36	0.43
3:A:91:ASP:OD2	3:A:93:THR:HB	2.19	0.43
3:A:152:ARG:C	3:A:155:MET:H	2.27	0.43
3:A:169:VAL:HG22	3:A:173:TYR:HE2	1.83	0.43
3:A:182:ARG:HH11	3:A:182:ARG:HG2	1.84	0.43
3:A:160:ASP:OD1	3:A:161:ILE:N	2.53	0.42
3:A:243:SER:OG	3:A:249:GLU:HG3	2.20	0.42
3:A:16:THR:N	3:A:46:ILE:HD11	2.35	0.42
3:A:251:PRO:O	3:A:253:ARG:HD2	2.19	0.42
3:A:182:ARG:HH11	3:A:273:THR:CG2	2.33	0.42
3:A:299:ARG:HA	3:A:300:PRO:HD3	1.95	0.42
3:A:177:VAL:HG13	3:A:193:VAL:HG22	2.02	0.42
3:A:260:ILE:HG22	3:A:261:PRO:N	2.34	0.42
3:A:209:LYS:HA	3:A:209:LYS:HD3	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:261:PRO:HG2	3:A:264:GLN:HG3	2.02	0.42
3:A:150:ILE:CG1	3:A:253:ARG:HG2	2.50	0.42
3:A:150:ILE:HG12	3:A:253:ARG:HG2	2.01	0.42
3:A:56:GLY:H	3:A:74:ASP:CG	2.28	0.41
3:A:183:ARG:HH11	3:A:275:SER:HA	1.85	0.41
3:A:270:LEU:HD11	3:A:282:MET:HE1	2.02	0.41
3:A:99:PHE:HD2	3:A:100:LEU:HD13	1.86	0.41
3:A:285:HIS:C	3:A:287:LEU:N	2.77	0.41
3:A:25:PHE:CD1	3:A:25:PHE:C	2.97	0.41
3:A:172:GLU:HB3	3:A:197:HIS:HE2	1.84	0.41
3:A:209:LYS:O	3:A:213:GLN:N	2.42	0.41
3:A:303:VAL:C	3:A:305:GLY:H	2.29	0.41
3:A:60:LYS:C	3:A:62:LEU:N	2.78	0.41
3:A:125:LEU:HA	3:A:125:LEU:HD23	1.40	0.41
3:A:163:LEU:N	3:A:163:LEU:HD23	2.34	0.41
3:A:49:TYR:CZ	3:A:51:HIS:HB2	2.55	0.41
3:A:330:PRO:HA	3:A:333:ARG:HG3	2.02	0.41
2:P:5:DA:C2'	2:P:6:DT:H71	2.50	0.41
3:A:260:ILE:CG2	3:A:261:PRO:CD	2.99	0.41
3:A:270:LEU:O	3:A:273:THR:HB	2.20	0.41
3:A:293:ILE:HG23	3:A:293:ILE:HD12	1.66	0.41
3:A:294:ASN:HB2	3:A:295:GLU:OE2	2.21	0.41
3:A:195:LEU:HD12	3:A:195:LEU:HA	1.81	0.41
3:A:241:LEU:HA	3:A:242:PRO:HD2	1.68	0.41
3:A:322:TYR:C	3:A:324:GLN:N	2.77	0.41
3:A:152:ARG:O	3:A:155:MET:HB2	2.21	0.40
1:T:4:DT:H5'	3:A:231:GLY:HA3	1.98	0.40
3:A:217:GLN:O	3:A:220:LYS:HB3	2.20	0.40
3:A:250:TYR:HA	3:A:251:PRO:HD3	1.88	0.40
3:A:16:THR:CG2	3:A:46:ILE:CG1	2.98	0.40
3:A:99:PHE:CD2	3:A:99:PHE:C	2.98	0.40
3:A:277:ILE:CG1	3:A:335:GLU:CB	3.00	0.40
3:A:25:PHE:CD2	3:A:29:VAL:HG21	2.56	0.40
3:A:250:TYR:HD1	3:A:251:PRO:HD2	1.86	0.40
3:A:150:ILE:HD11	3:A:253:ARG:HG2	1.98	0.40
3:A:303:VAL:C	3:A:305:GLY:N	2.78	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%)	249 (77%)	56 (17%)	20 (6%)	1 9

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	134	HIS
3	A	204	SER
3	A	205	THR
3	A	208	PRO
3	A	244	LYS
3	A	245	ASN
3	A	246	ASP
3	A	262	LYS
3	A	264	GLN
3	A	295	GLU
3	A	80	GLY
3	A	145	ASP
3	A	207	GLN
3	A	222	HIS
3	A	266	TYR
3	A	324	GLN
3	A	91	ASP
3	A	233	THR
3	A	202	SER
3	A	310	PRO

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	288/295 (98%)	211 (73%)	77 (27%)	0 2

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	THR
3	A	18	MET
3	A	20	THR
3	A	22	LEU
3	A	27	LYS
3	A	30	SER
3	A	33	ILE
3	A	36	TYR
3	A	37	ASN
3	A	41	LYS
3	A	46	ILE
3	A	52	LYS
3	A	60	LYS
3	A	61	LYS
3	A	62	LEU
3	A	65	VAL
3	A	67	THR
3	A	68	LYS
3	A	72	LYS
3	A	73	ILE
3	A	79	THR
3	A	81	LYS
3	A	85	LEU
3	A	89	ARG
3	A	92	ASP
3	A	93	THR
3	A	94	SER
3	A	100	LEU
3	A	101	THR
3	A	104	SER
3	A	115	VAL
3	A	121	THR
3	A	122	LEU
3	A	128	ASN
3	A	133	ASN
3	A	136	GLN

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Mol	Chain	Res	Type
3	A	140	LEU
3	A	153	GLU
3	A	161	ILE
3	A	166	VAL
3	A	168	LYS
3	A	169	VAL
3	A	174	ILE
3	A	177	VAL
3	A	188	SER
3	A	191	MET
3	A	192	ASP
3	A	194	LEU
3	A	204	SER
3	A	213	GLN
3	A	214	VAL
3	A	218	LEU
3	A	219	GLN
3	A	225	THR
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	270	LEU
3	A	277	ILE
3	A	287	LEU
3	A	293	ILE
3	A	294	ASN
3	A	295	GLU
3	A	301	LEU
3	A	303	VAL
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	324	GLN
3	A	325	TRP
3	A	328	ARG
3	A	331	LYS

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	28	ASN
3	A	31	GLN
3	A	98	ASN
3	A	128	ASN
3	A	133	ASN
3	A	136	GLN
3	A	159	GLN
3	A	207	GLN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	245	ASN
3	A	264	GLN
3	A	294	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 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	TTP	A	338	4	19,20,30	1.48	2 (10%)	25,31,47	1.71	4 (16%)

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	TTP	A	338	4	-	5/18/28/34	0/1/1/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	338	TTP	PB-O3A	3.83	1.63	1.59
6	A	338	TTP	O3'-C3'	-3.72	1.35	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	338	TTP	O3'-C3'-C2'	-4.94	99.85	111.43
6	A	338	TTP	O3A-PA-O1A	-3.46	100.28	110.70
6	A	338	TTP	O3'-C3'-C4'	-2.47	100.71	110.07
6	A	338	TTP	O2B-PB-O3A	2.29	113.45	107.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

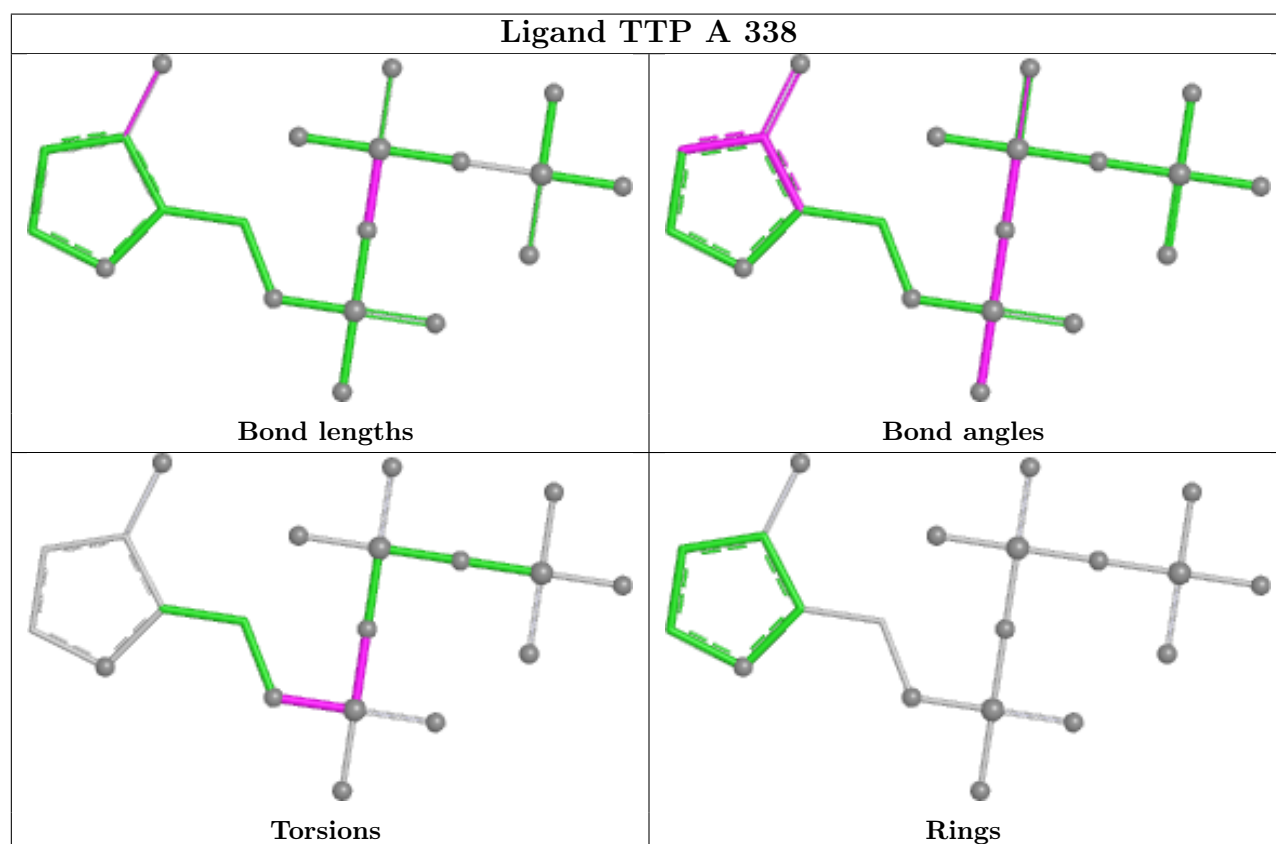
Mol	Chain	Res	Type	Atoms
6	A	338	TTP	C5'-O5'-PA-O2A
6	A	338	TTP	C5'-O5'-PA-O3A
6	A	338	TTP	C5'-O5'-PA-O1A
6	A	338	TTP	PB-O3A-PA-O5'
6	A	338	TTP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	338	TTP	4	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%)	-0.60	0 100 100	14, 37, 99, 99	0
2	P	8/8 (100%)	-0.40	1 (12%) 8 6	11, 30, 71, 100	0
3	A	325/335 (97%)	-0.77	0 100 100	1, 32, 87, 100	0
All	All	341/351 (97%)	-0.75	1 (0%) 90 82	1, 32, 87, 100	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	8	DT	3.0

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.

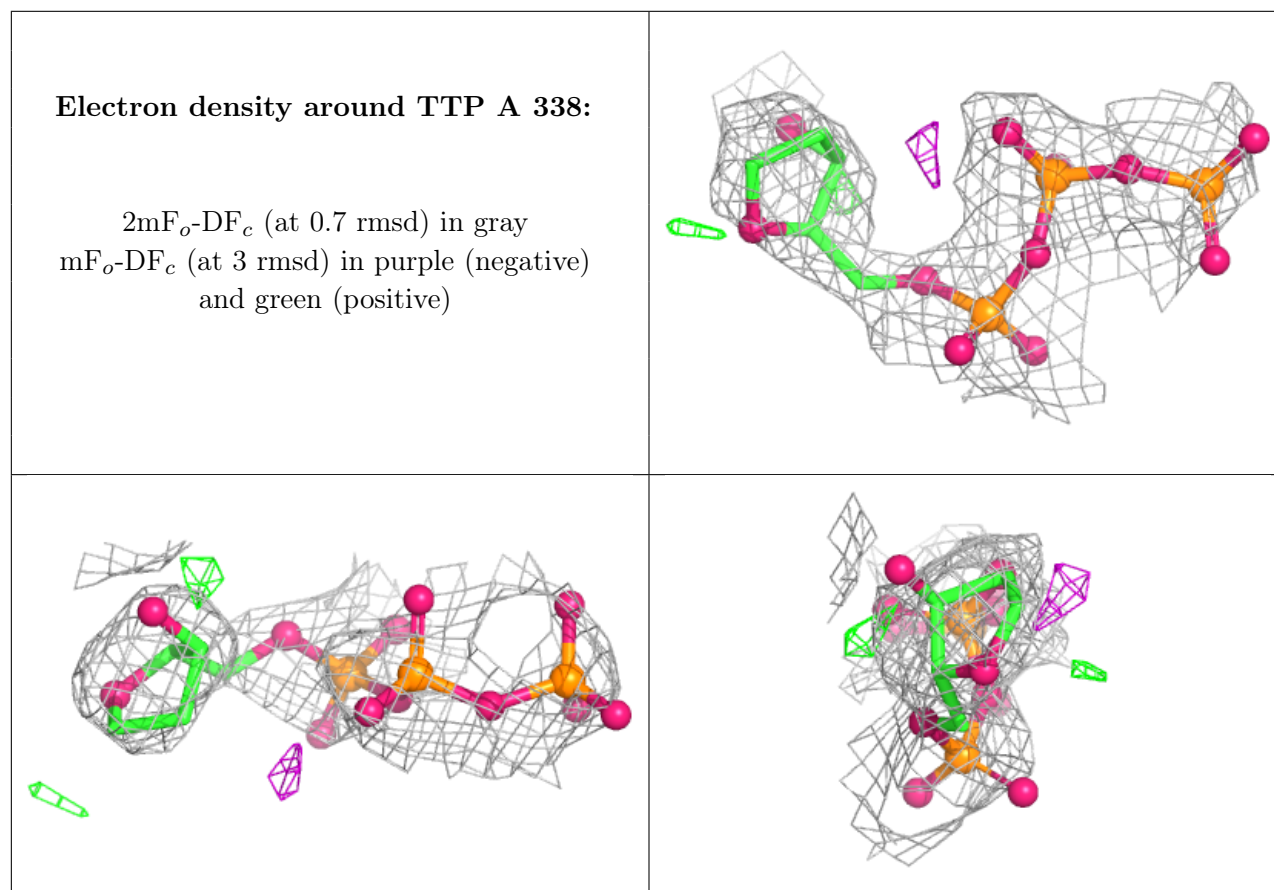
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	TTP	A	338	20/29	0.84	0.17	63,74,78,81	20
4	MN	A	339	1/1	0.90	0.07	30,30,30,30	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NA	A	342	1/1	0.97	0.04	37,37,37,37	0
5	NA	A	341	1/1	0.98	0.05	6,6,6,6	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.