Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:34 pm BST

PDB ID	:	8ICJ
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 following versions of software and data (see references ①) were used in the production of this report:

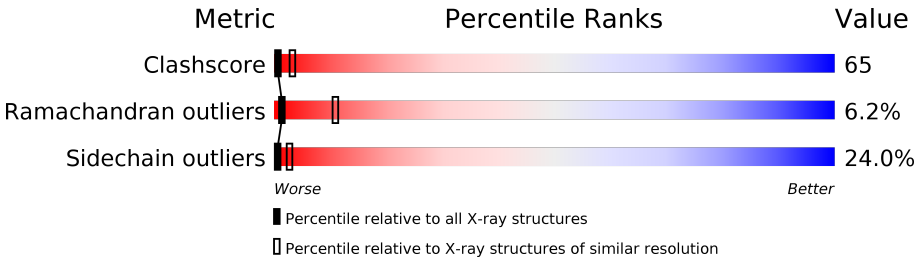
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (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 on 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	T	8	50% 50%
2	P	7	29% 71%
3	A	335	19% 48% 27%

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			

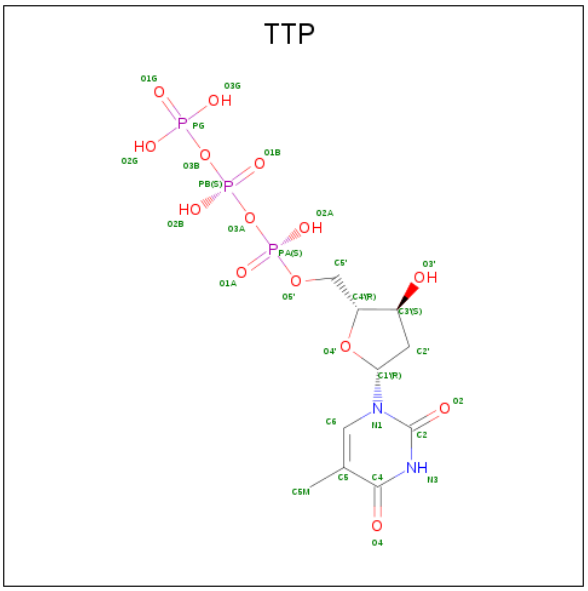
- Molecule 3 is a protein called PROTEIN (DNA POLYMERASE BETA (E.C.2.7.7.7)).

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 (three-letter code: NA) (formula: Na).

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

- Molecule 5 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



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

- 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

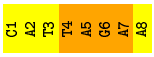
3 Residue-property plots (i)

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

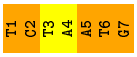
- Molecule 1: DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3')

Chain T:



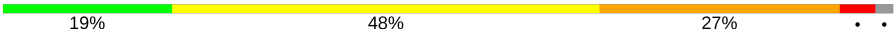
- Molecule 2: DNA (5'-D(*TP*CP*TP*AP*AP*TP*G)-3')

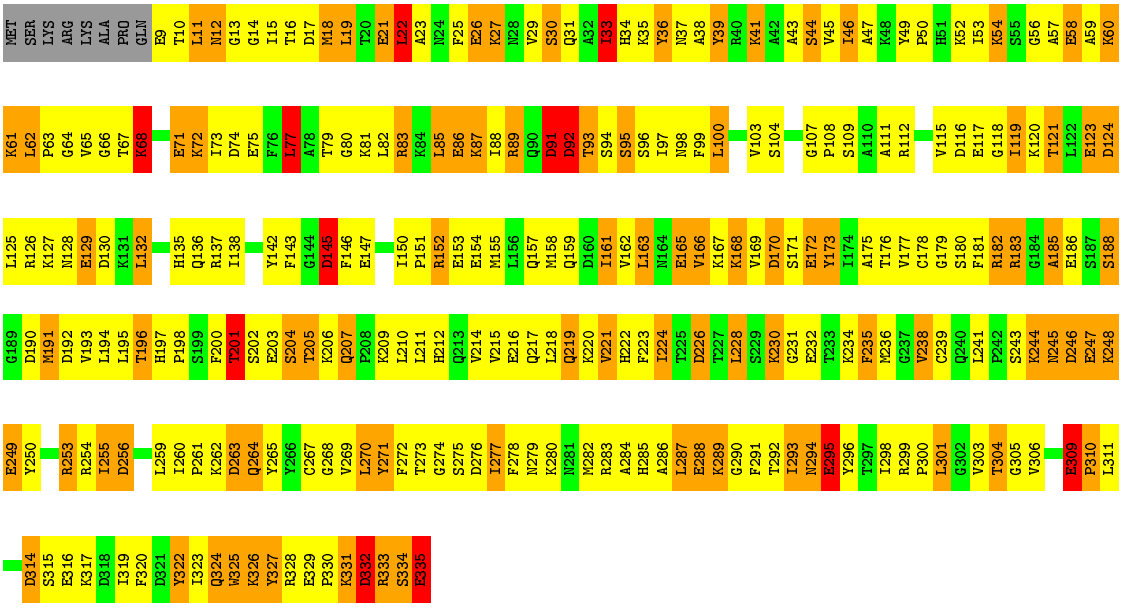
Chain P:



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

Chain A:





4 Data and refinement statistics (i)

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.96	2/162 (1.2%)	4.17	28/249 (11.2%)
2	P	2.79	10/160 (6.2%)	3.81	30/243 (12.3%)
3	A	1.32	27/2672 (1.0%)	1.80	58/3590 (1.6%)
All	All	1.48	39/2994 (1.3%)	2.18	116/4082 (2.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	2	0

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	2	DC	C1'-N1	10.59	1.63	1.49
2	P	3	DT	C1'-N1	10.32	1.62	1.49
3	A	147	GLU	CD-OE2	9.80	1.36	1.25
2	P	5	DA	N9-C4	9.31	1.43	1.37
1	T	1	DC	C3'-O3'	8.89	1.55	1.44
2	P	3	DT	N1-C2	8.37	1.44	1.38
3	A	75	GLU	CD-OE1	7.86	1.34	1.25
3	A	58	GLU	CD-OE1	7.72	1.34	1.25
3	A	86	GLU	CD-OE1	7.68	1.34	1.25
3	A	203	GLU	CD-OE1	7.39	1.33	1.25
3	A	271	TYR	CB-CG	-7.30	1.40	1.51
3	A	335	GLU	CD-OE2	7.06	1.33	1.25
3	A	329	GLU	CD-OE2	7.05	1.33	1.25
3	A	172	GLU	CD-OE2	6.99	1.33	1.25
3	A	117	GLU	CD-OE2	6.94	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	123	GLU	CD-OE1	6.81	1.33	1.25
3	A	71	GLU	CD-OE1	6.80	1.33	1.25
3	A	249	GLU	CD-OE2	6.75	1.33	1.25
3	A	288	GLU	CD-OE2	6.62	1.32	1.25
3	A	295	GLU	CD-OE2	6.50	1.32	1.25
3	A	26	GLU	CD-OE1	6.37	1.32	1.25
3	A	216	GLU	CD-OE2	6.29	1.32	1.25
3	A	232	GLU	CD-OE2	6.28	1.32	1.25
3	A	129	GLU	CD-OE1	6.18	1.32	1.25
2	P	1	DT	C5-C7	6.15	1.53	1.50
2	P	1	DT	C2-O2	6.13	1.27	1.22
3	A	309	GLU	CD-OE2	6.12	1.32	1.25
3	A	39	TYR	CB-CG	-6.07	1.42	1.51
2	P	6	DT	C4-C5	-5.81	1.39	1.45
2	P	5	DA	N7-C5	5.79	1.42	1.39
3	A	186	GLU	CD-OE1	5.76	1.31	1.25
3	A	247	GLU	CD-OE1	5.71	1.31	1.25
3	A	154	GLU	CD-OE2	5.65	1.31	1.25
2	P	5	DA	N3-C4	5.62	1.38	1.34
1	T	5	DA	N1-C2	5.35	1.39	1.34
3	A	326	LYS	CE-NZ	-5.32	1.35	1.49
2	P	3	DT	C5-C7	5.26	1.53	1.50
3	A	9	GLU	CD-OE2	5.24	1.31	1.25
3	A	153	GLU	CD-OE2	5.19	1.31	1.25

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	7	DA	C4-N9-C1'	-22.04	86.64	126.30
1	T	7	DA	C8-N9-C1'	21.80	166.93	127.70
1	T	6	DG	C8-N9-C1'	19.83	152.78	127.00
1	T	6	DG	C4-N9-C1'	-19.49	101.16	126.50
2	P	1	DT	C6-N1-C1'	-19.11	91.74	120.40
2	P	1	DT	C2-N1-C1'	17.13	145.61	118.20
1	T	4	DT	C6-N1-C1'	-16.70	95.34	120.40
1	T	4	DT	C2-N1-C1'	15.61	143.18	118.20
2	P	3	DT	C2-N1-C1'	14.96	142.13	118.20
2	P	2	DC	C2-N1-C1'	14.71	134.98	118.80
2	P	3	DT	C6-N1-C1'	-14.10	99.25	120.40
1	T	1	DC	P-O3'-C3'	11.63	133.65	119.70
1	T	3	DT	O4'-C1'-N1	11.15	115.81	108.00
2	P	2	DC	C6-N1-C1'	-10.54	108.16	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	3	DT	O4'-C1'-N1	10.32	115.23	108.00
1	T	5	DA	C8-N9-C1'	10.19	146.05	127.70
2	P	6	DT	C4-C5-C7	-10.16	112.90	119.00
2	P	5	DA	C4-N9-C1'	10.15	144.56	126.30
3	A	333	ARG	NE-CZ-NH1	10.13	125.37	120.30
3	A	77	LEU	N-CA-CB	10.02	130.43	110.40
2	P	5	DA	C8-N9-C1'	-9.97	109.75	127.70
1	T	5	DA	C4-N9-C1'	-9.71	108.83	126.30
3	A	130	ASP	CB-CG-OD2	-9.64	109.62	118.30
3	A	256	ASP	CB-CG-OD2	-9.62	109.64	118.30
1	T	5	DA	N1-C6-N6	9.28	124.17	118.60
3	A	256	ASP	CB-CG-OD1	9.23	126.61	118.30
2	P	6	DT	C2-N1-C1'	9.13	132.81	118.20
2	P	6	DT	C6-N1-C1'	-9.01	106.88	120.40
2	P	2	DC	C6-N1-C2	-8.64	116.84	120.30
3	A	333	ARG	NE-CZ-NH2	-8.35	116.12	120.30
3	A	39	TYR	CB-CG-CD1	-8.24	116.05	121.00
2	P	3	DT	N3-C2-O2	-8.18	117.39	122.30
2	P	2	DC	O4'-C1'-N1	8.05	113.64	108.00
3	A	124	ASP	CB-CG-OD2	-7.99	111.11	118.30
3	A	263	ASP	CB-CG-OD2	-7.93	111.16	118.30
3	A	192	ASP	CB-CG-OD1	7.88	125.39	118.30
3	A	192	ASP	CB-CG-OD2	-7.78	111.30	118.30
3	A	314	ASP	CB-CG-OD1	-7.73	111.34	118.30
3	A	224	ILE	CA-CB-CG1	-7.69	96.39	111.00
2	P	1	DT	O4'-C4'-C3'	-7.67	101.39	106.00
3	A	74	ASP	CB-CG-OD1	7.63	125.17	118.30
3	A	130	ASP	CB-CG-OD1	7.61	125.15	118.30
2	P	7	DG	P-O5'-C5'	-7.48	108.94	120.90
3	A	326	LYS	CD-CE-NZ	7.44	128.82	111.70
1	T	4	DT	O4'-C1'-C2'	-7.37	100.01	105.90
1	T	4	DT	C1'-O4'-C4'	-7.25	102.85	110.10
2	P	6	DT	C6-C5-C7	7.23	127.24	122.90
2	P	4	DA	C4-N9-C1'	-7.08	113.55	126.30
2	P	6	DT	C5-C4-O4	-7.06	119.96	124.90
1	T	5	DA	C5-C6-N1	-7.04	114.18	117.70
3	A	72	LYS	CB-CA-C	6.97	124.34	110.40
2	P	6	DT	O4'-C4'-C3'	-6.89	101.74	104.50
2	P	4	DA	C8-N9-C1'	6.89	140.10	127.70
1	T	2	DA	C8-N9-C1'	6.86	140.04	127.70
1	T	5	DA	C2-N3-C4	-6.77	107.21	110.60
3	A	91	ASP	CB-CG-OD1	-6.76	112.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	173	TYR	CB-CA-C	-6.52	97.36	110.40
3	A	271	TYR	CB-CG-CD1	-6.47	117.12	121.00
1	T	7	DA	P-O5'-C5'	-6.38	110.69	120.90
3	A	68	LYS	N-CA-CB	6.34	122.02	110.60
2	P	5	DA	C2-N3-C4	6.33	113.76	110.60
1	T	2	DA	C4-N9-C1'	-6.29	114.97	126.30
1	T	3	DT	C2-N1-C1'	6.27	128.23	118.20
3	A	116	ASP	CB-CG-OD2	-6.25	112.67	118.30
2	P	1	DT	C1'-O4'-C4'	-6.23	103.87	110.10
2	P	4	DA	O4'-C1'-N9	-6.20	103.66	108.00
1	T	3	DT	C6-N1-C1'	-6.19	111.11	120.40
3	A	315	SER	N-CA-CB	6.17	119.75	110.50
3	A	74	ASP	CB-CG-OD2	-6.08	112.83	118.30
3	A	322	TYR	CB-CG-CD1	-6.07	117.36	121.00
3	A	183	ARG	NE-CZ-NH1	6.05	123.33	120.30
3	A	219	GLN	CB-CA-C	-6.04	98.32	110.40
3	A	256	ASP	N-CA-CB	5.99	121.38	110.60
3	A	116	ASP	CB-CG-OD1	5.98	123.68	118.30
3	A	271	TYR	CA-CB-CG	-5.97	102.05	113.40
1	T	5	DA	O4'-C4'-C3'	5.90	109.54	106.00
3	A	92	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	T	5	DA	C6-C5-N7	-5.87	128.19	132.30
3	A	17	ASP	CB-CG-OD2	5.86	123.58	118.30
1	T	4	DT	C6-C5-C7	-5.70	119.48	122.90
3	A	170	ASP	CB-CG-OD1	5.69	123.42	118.30
2	P	6	DT	O4'-C1'-N1	5.65	111.95	108.00
3	A	246	ASP	CB-CG-OD1	-5.64	113.22	118.30
3	A	151	PRO	N-CA-CB	5.64	110.06	103.30
3	A	92	ASP	CB-CG-OD2	5.63	123.37	118.30
3	A	332	ASP	CB-CG-OD2	5.59	123.33	118.30
3	A	314	ASP	CB-CG-OD2	5.54	123.28	118.30
3	A	12	ASN	CB-CA-C	5.46	121.33	110.40
3	A	332	ASP	CB-CG-OD1	-5.45	113.39	118.30
3	A	334	SER	CB-CA-C	5.42	120.40	110.10
3	A	163	LEU	CA-CB-CG	-5.41	102.86	115.30
3	A	91	ASP	CB-CG-OD2	5.40	123.16	118.30
1	T	6	DG	N1-C6-O6	5.39	123.14	119.90
2	P	3	DT	C6-N1-C2	-5.38	118.61	121.30
1	T	5	DA	P-O5'-C5'	-5.36	112.32	120.90
2	P	3	DT	N1-C2-O2	5.29	127.33	123.10
3	A	145	ASP	CB-CG-OD2	-5.25	113.57	118.30
3	A	263	ASP	CB-CG-OD1	5.25	123.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	116	ASP	CB-CA-C	5.25	120.89	110.40
2	P	3	DT	O4'-C1'-C2'	-5.24	101.70	105.90
2	P	1	DT	P-O3'-C3'	5.24	125.99	119.70
3	A	196	THR	N-CA-CB	5.19	120.16	110.30
3	A	17	ASP	N-CA-CB	5.19	119.94	110.60
3	A	183	ARG	NE-CZ-NH2	-5.18	117.71	120.30
3	A	77	LEU	CB-CA-C	5.17	120.01	110.20
3	A	226	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	T	6	DG	C5-C6-O6	-5.14	125.51	128.60
1	T	6	DG	P-O3'-C3'	5.14	125.87	119.70
3	A	175	ALA	N-CA-CB	5.11	117.25	110.10
1	T	3	DT	C4-C5-C7	5.07	122.04	119.00
3	A	98	ASN	CB-CA-C	5.07	120.53	110.40
3	A	238	VAL	CA-CB-CG1	5.06	118.49	110.90
3	A	271	TYR	N-CA-CB	-5.06	101.49	110.60
3	A	201	THR	CA-CB-CG2	-5.06	105.32	112.40
3	A	22	LEU	CB-CG-CD1	-5.02	102.47	111.00
3	A	246	ASP	CB-CG-OD2	5.02	122.82	118.30

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	352	0
4	A	2	0	0	0	0
5	A	5	0	0	1	0
6	A	109	0	0	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	P	18	0	0	2	0
6	T	12	0	0	0	0
All	All	3058	0	2802	365	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 65.

All (365) 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
3:A:73:ILE:HG23	3:A:77:LEU:HD11	1.52	0.89
2:P:5:DA:H2"	2:P:6:DT:H5'	1.54	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	3:A:245:ASN:HD22	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:155:MET:HA	3:A:158:MET:HE3	1.70	0.73
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: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:NH1	3:A:182:ARG:HG2	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: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:155:MET:HE1	3:A:188:SER:HB2	1.77	0.67
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.30	0.67
3:A:83:ARG:O	3:A:86:GLU:HG2	1.95	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:253:ARG:HG3	3:A:253:ARG:HH11	1.60	0.66
3:A:268:GLY:O	3:A:271:TYR:HB3	1.97	0.65
3:A:12:ASN:ND2	3:A:53:ILE:H	1.91	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: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:CD2	3:A:11:LEU:H	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:121:THR:HG23	3:A:124:ASP:CG	2.22	0.60
3:A:163:LEU:N	3:A:163:LEU:HD23	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:92:ASP:HA	3:A:95:SER:HB2	1.86	0.58
3:A:218:LEU:CB	3:A:224:ILE:HD12	2.34	0.58
3:A:83:ARG:O	3:A:87:LYS:N	2.28	0.58
3:A:77:LEU:N	3:A:77:LEU:HD13	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: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: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:HA	3:A:217:GLN:NE2	2.19	0.57
3:A:253:ARG:NH1	6:A:503:HOH:O	2.37	0.57
1:T:5:DA:H2"	1:T:6:DG:O5'	2.05	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:292:THR:O	3:A:293:ILE:HD13	2.06	0.56
3:A:11:LEU:HA	3:A:52:LYS:HZ1	1.69	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:183:ARG:HD3	3:A:273:THR:O	2.05	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

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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	0.56
3:A:44:SER:O	3:A:47:ALA:HB3	2.06	0.56
2:P:5:DA:H2'	6:P:648:HOH:O	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:331:LYS:HG2	3:A:332:ASP:N	2.06	0.55
3:A:179:GLY:O	3:A:182:ARG:HB3	2.07	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
2:P:1:DT:H2'	2:P:2:DC:C6	2.43	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:323:ILE:C	3:A:324:GLN:HG2	2.28	0.53
3:A:11:LEU:N	3:A:11:LEU:HD23	2.14	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:73:ILE:O	3:A:77:LEU:HD22	2.08	0.53
3:A:115:VAL:C	3:A:118:GLY:H	2.12	0.53
3:A:183:ARG:HG3	3:A:273:THR:HG22	1.91	0.53
3:A:172:GLU:HB3	3:A:197:HIS:NE2	2.23	0.53
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.90	0.53
3:A:178:CYS:SG	3:A:269:VAL:HG22	2.48	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
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:155:MET:HE2	3:A:181:PHE:HB2	1.92	0.52
3:A:218:LEU:HB3	3:A:224:ILE:CD1	2.40	0.52
3:A:212:HIS:CD2	3:A:212:HIS:N	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:O	3:A:326:LYS:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:270:LEU:HD21	3:A:282:MET:HE1	1.91	0.52
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: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: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:196:THR:OG1	3:A:197:HIS:N	2.43	0.51
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.55	0.51
3:A:288:GLU:O	3:A:290:GLY:N	2.39	0.51
3:A:287:LEU:HA	3:A:291:PHE:O	2.10	0.51
3:A:298:ILE:HG22	6:A:578:HOH:O	2.10	0.51
3:A:25:PHE:CE2	3:A:88:ILE:HG12	2.46	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:292:THR:C	3:A:293:ILE:HD13	2.32	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:278:PHE:CE1	3:A:325:TRP:HZ3	2.30	0.50
3:A:123:GLU:O	3:A:126:ARG:N	2.45	0.50
3:A:19:LEU:HD23	3:A:43:ALA:HA	1.93	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
3:A:167:LYS:O	3:A:170:ASP:O	2.31	0.49
2:P:6:DT:H2"	2:P:7:DG:C8	2.48	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:204:SER:OG	3:A:204:SER:O	2.29	0.48
3:A:214:VAL:CG2	3:A:215:VAL:N	2.76	0.48
3:A:91:ASP:O	3:A:95:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:15:ILE:HD11	3:A:77:LEU:HD12	1.94	0.48
3:A:263:ASP:C	3:A:264:GLN:HG2	2.34	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:N	3:A:128:ASN:ND2	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:259:LEU:O	3:A:260:ILE:HD13	2.13	0.47
3:A:57:ALA:O	3:A:60:LYS:HB3	2.14	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:162:VAL:HG12	3:A:162:VAL:O	2.14	0.47
3:A:15:ILE:HG22	3:A:46:ILE:CD1	2.45	0.47
3:A:182:ARG:NE	6:A:576:HOH:O	2.45	0.47
3:A:182:ARG:NH1	3:A:273:THR:CG2	2.77	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
1:T:4:DT:H2"	1:T:5:DA:C8	2.49	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:59:ALA:O	3:A:62:LEU:N	2.43	0.47
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.96	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:190:ASP:OD1	3:A:190:ASP:N	2.48	0.46
3:A:303:VAL:C	3:A:305:GLY:H	2.19	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:165:GLU:CD	3:A:168:LYS:HD3	2.36	0.46
3:A:152:ARG:CA	3:A:155:MET:HB2	2.36	0.46
3:A:211:LEU:HD12	3:A:211:LEU:O	2.16	0.46
3:A:16:THR:CG2	3:A:47:ALA:HB2	2.45	0.46
3:A:230:LYS:NZ	3:A:230:LYS:CB	2.77	0.46
2:P:6:DT:H2"	2:P:7:DG:H5"	1.98	0.46
3:A:270:LEU:HD21	3:A:282:MET:HE2	1.97	0.46
1:T:7:DA:O5'	1:T:8:DA:OP2	2.34	0.46
3:A:125:LEU:HD23	3:A:125:LEU:HA	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:289:LYS:HA	3:A:289:LYS:HD3	1.52	0.46
3:A:62:LEU:CD1	3:A:63:PRO:HD2	2.42	0.46
3:A:254:ARG:HB3	3:A:254:ARG:CZ	2.47	0.45
3:A:278:PHE:O	3:A:282:MET:HB3	2.16	0.45
3:A:99:PHE:HD2	3:A:100:LEU:CD1	2.27	0.45
3:A:155:MET:HE1	3:A:188:SER:CB	2.44	0.45
3:A:193:VAL:HG23	3:A:193:VAL:H	1.35	0.45
3:A:115:VAL:HG13	3:A:120:LYS:HE2	1.98	0.45
3:A:60:LYS:HE3	3:A:66:GLY:C	2.37	0.45
3:A:209:LYS:HA	3:A:209:LYS:HD3	1.64	0.45
3:A:62:LEU:HA	3:A:62:LEU:HD12	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: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:214:VAL:HG22	3:A:215:VAL:N	2.33	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:250:TYR:HB3	6:A:577:HOH:O	2.18	0.44
3:A:180:SER:OG	5:A:338:TTP:O2G	2.32	0.44
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.32	0.44
3:A:138:ILE:HG21	3:A:228:LEU:HD11	2.00	0.43
1:T:4:DT:O5'	3:A:231:GLY:HA3	2.17	0.43
3:A:142:TYR:CE2	3:A:238:VAL:HG11	2.52	0.43
3:A:85:LEU:HA	3:A:85:LEU:HD12	1.21	0.43
3:A:177:VAL:HG11	3:A:191:MET:CE	2.48	0.43
3:A:45:VAL:HG21	3:A:63:PRO:O	2.18	0.43
3:A:103:VAL:CG2	3:A:143:PHE:CE2	3.02	0.43
3:A:68:LYS:O	3:A:72:LYS:HE2	2.19	0.43
3:A:292:THR:O	3:A:298:ILE:HA	2.19	0.43
3:A:27:LYS:CB	3:A:36:TYR:CD1	2.98	0.43
3:A:183:ARG:HB2	3:A:183:ARG:HE	1.07	0.43
3:A:194:LEU:HD21	3:A:272:PHE:CD2	2.53	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:82:LEU:HB3	3:A:85:LEU:CB	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:270:LEU:HD23	3:A:319:ILE:HD13	2.01	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:157:GLN:O	3:A:161:ILE:HG13	2.18	0.42
3:A:27:LYS:HB3	3:A:36:TYR:CG	2.53	0.42
3:A:26:GLU:O	3:A:30:SER:O	2.36	0.42
3:A:267:CYS:HA	3:A:319:ILE:HD11	2.01	0.42
3:A:83:ARG:O	3:A:86:GLU:N	2.52	0.42
3:A:277:ILE:CG1	3:A:335:GLU:CB	2.98	0.42
3:A:223:PHE:O	3:A:239:CYS:HA	2.19	0.42
3:A:79:THR:C	3:A:81:LYS:H	2.23	0.42
3:A:93:THR:HG22	3:A:94:SER:N	2.35	0.42
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.54	0.42
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.43	0.42
3:A:248:LYS:HG2	3:A:248:LYS:O	2.20	0.42
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
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
3:A:332:ASP:C	3:A:334:SER:H	2.24	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:155:MET:HE2	3:A:188:SER:OG	2.21	0.41
3:A:330:PRO:O	3:A:333:ARG:HG2	2.20	0.41
3:A:119:ILE:HG23	3:A:124:ASP:HB2	2.00	0.41
3:A:270:LEU:CD2	3:A:282:MET:HE2	2.51	0.41
3:A:200:PHE:HE1	3:A:260:ILE:C	2.25	0.41
3:A:54:LYS:HD2	3:A:54:LYS:HA	1.29	0.41
3:A:177:VAL:CG1	3:A:191:MET:HE2	2.51	0.41
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.86	0.41
3:A:135:HIS:CD2	3:A:135:HIS:C	2.94	0.40
3:A:68:LYS:O	3:A:71:GLU:HB3	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:34:HIS:O	3:A:38:ALA:N	2.54	0.40
3:A:163:LEU:HA	3:A:163:LEU:HD23	1.44	0.40
3:A:159:GLN:O	3:A:159:GLN:HG3	2.21	0.40
3:A:19:LEU:HA	3:A:19:LEU:HD12	1.78	0.40
3:A:23:ALA:HB2	3:A:39:TYR:HB3	2.02	0.40
3:A:295:GLU:H	3:A:295:GLU:CD	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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 11

All (20) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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 (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%)	219 (76%)	69 (24%)	0 3

All (69) 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
3	A	36	TYR
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

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Mol	Chain	Res	Type
3	A	83	ARG
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	145	ASP
3	A	152	ARG
3	A	161	ILE
3	A	165	GLU
3	A	168	LYS
3	A	182	ARG
3	A	188	SER
3	A	191	MET
3	A	201	THR
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	287	LEU
3	A	293	ILE
3	A	294	ASN
3	A	295	GLU
3	A	301	LEU
3	A	304	THR
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP

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Mol	Chain	Res	Type
3	A	324	GLN
3	A	325	TRP
3	A	327	TYR
3	A	331	LYS
3	A	332	ASP
3	A	335	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) 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	133	ASN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	245	ASN
3	A	294	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	1.72	2 (50%)	6,6,47	1.41	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	-2.13	1.48	1.54
5	A	338	TTP	PG-O3B	2.09	1.60	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	338	TTP	O3G-PG-O3B	-2.37	100.37	107.97
5	A	338	TTP	O2G-PG-O1G	2.10	118.57	110.89

There are no chirality outliers.

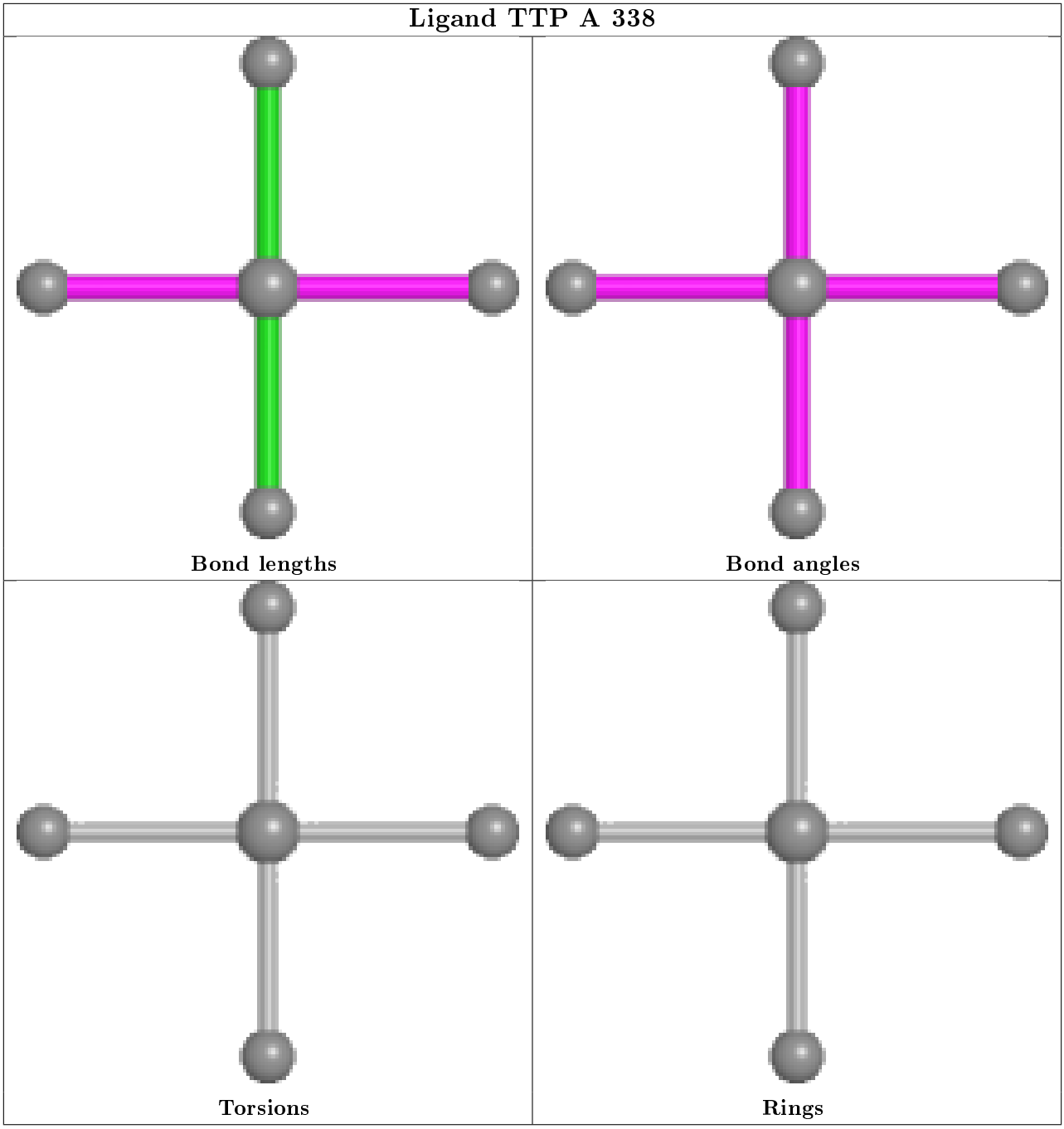
There are no torsion outliers.

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 then 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.