Full wwPDB X-ray Structure Validation Report (i)

Jul 25, 2023 – 02:03 AM EDT

PDB ID	:	9ICU
Title	:	DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SIX BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF DTTP (1 MILLIMOLAR) AND MNCL2 (5 MILLIMOLAR)
Authors	:	Pelletier, H.; Sawaya, M.R.
Deposited on	:	1995-12-16
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

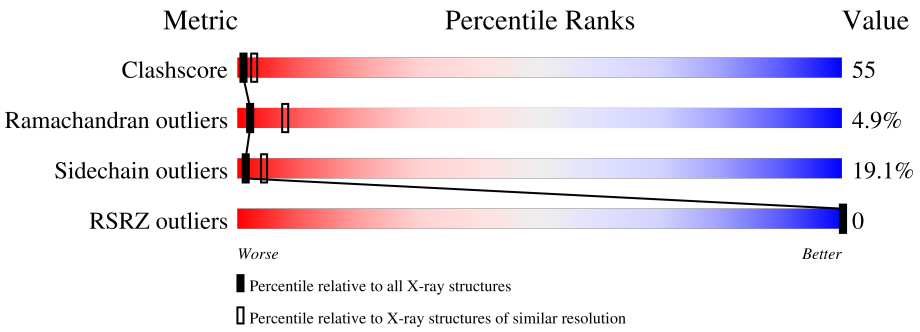
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	7	14% 57% 29%
2	P	6	100%
3	A	335	23% 47% 23% . .

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3029 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*CP*TP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	T	7	122	58	20	38	6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	P	6	126	59	25	36	6	0	0	0

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

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

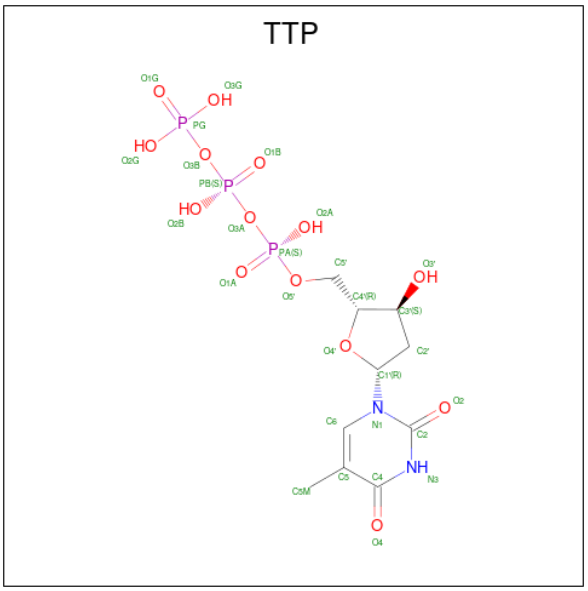
- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	T	11	11	11	0	0
			Total	O		
7	P	17	17	17	0	0
			Total	O		
7	A	107	107	107	0	0

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*CP*TP*GP*T)-3')

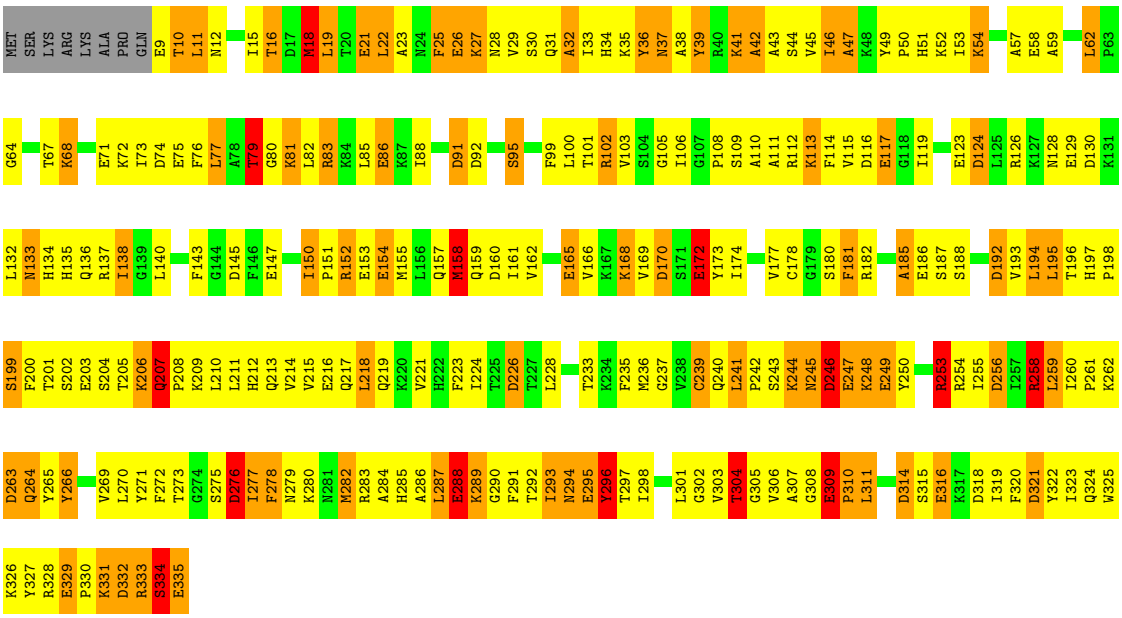
Chain T: 14% 57% 29%

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

Chain P: 100%

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

Chain A: 23% 47% 23%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	178.86Å 57.68Å 48.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 12.00 – 2.79	Depositor EDS
% Data completeness (in resolution range)	91.0 (20.00-2.90) 88.3 (12.00-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 2.78Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.167 , (Not available) 0.158 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	42.7	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.16 , 129.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3029	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: TTP, MN, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	T	1.52	1/135 (0.7%)	2.97	14/207 (6.8%)
2	P	1.41	0/141	3.03	18/214 (8.4%)
3	A	1.19	26/2672 (1.0%)	1.79	69/3590 (1.9%)
All	All	1.22	27/2948 (0.9%)	1.96	101/4011 (2.5%)

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 (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	147	GLU	CD-OE2	7.06	1.33	1.25
3	A	129	GLU	CD-OE1	6.85	1.33	1.25
3	A	203	GLU	CD-OE1	6.82	1.33	1.25
3	A	249	GLU	CD-OE2	6.56	1.32	1.25
3	A	86	GLU	CD-OE1	6.40	1.32	1.25
3	A	165	GLU	CD-OE2	6.39	1.32	1.25
3	A	172	GLU	CD-OE2	6.30	1.32	1.25
3	A	75	GLU	CD-OE1	6.28	1.32	1.25
3	A	21	GLU	CD-OE1	6.20	1.32	1.25
3	A	58	GLU	CD-OE1	6.02	1.32	1.25
3	A	154	GLU	CD-OE2	6.02	1.32	1.25
3	A	71	GLU	CD-OE1	6.00	1.32	1.25
3	A	123	GLU	CD-OE1	5.99	1.32	1.25
3	A	329	GLU	CD-OE2	5.97	1.32	1.25
3	A	309	GLU	CD-OE2	5.74	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	295	GLU	CD-OE1	5.65	1.31	1.25
3	A	117	GLU	CD-OE2	5.54	1.31	1.25
3	A	186	GLU	CD-OE1	5.47	1.31	1.25
1	T	3	DA	N9-C4	5.46	1.41	1.37
3	A	316	GLU	CD-OE2	5.45	1.31	1.25
3	A	326	LYS	CE-NZ	-5.44	1.35	1.49
3	A	153	GLU	CD-OE2	5.39	1.31	1.25
3	A	335	GLU	CD-OE2	5.37	1.31	1.25
3	A	247	GLU	CD-OE1	5.30	1.31	1.25
3	A	288	GLU	CD-OE2	5.25	1.31	1.25
3	A	9	GLU	CD-OE2	5.23	1.31	1.25
3	A	26	GLU	CD-OE1	5.10	1.31	1.25

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	5	DC	C2-N1-C1'	17.41	137.95	118.80
1	T	5	DC	C6-N1-C1'	-14.87	102.95	120.80
1	T	4	DT	C6-N1-C1'	-13.81	99.68	120.40
2	P	1	DC	C2-N1-C1'	13.40	133.54	118.80
1	T	4	DT	C2-N1-C1'	13.22	139.36	118.20
2	P	1	DC	C6-N1-C1'	-11.87	106.56	120.80
2	P	2	DA	C4'-C3'-C2'	-11.33	92.91	103.10
2	P	2	DA	O4'-C4'-C3'	-10.07	99.95	106.00
2	P	4	DA	O4'-C1'-N9	-9.83	101.12	108.00
3	A	92	ASP	CB-CG-OD2	-9.26	109.97	118.30
3	A	126	ARG	NE-CZ-NH2	-9.12	115.74	120.30
2	P	3	DG	C8-N9-C1'	8.92	138.60	127.00
1	T	7	DG	C4-N9-C1'	-8.87	114.98	126.50
2	P	5	DT	C2-N1-C1'	8.65	132.04	118.20
3	A	124	ASP	CB-CG-OD2	-8.54	110.62	118.30
2	P	5	DT	C6-N1-C1'	-8.41	107.78	120.40
1	T	7	DG	C8-N9-C1'	8.19	137.64	127.00
3	A	256	ASP	CB-CG-OD2	-8.01	111.09	118.30
2	P	3	DG	C4-N9-C1'	-7.96	116.14	126.50
3	A	258	ARG	NE-CZ-NH1	7.85	124.23	120.30
2	P	5	DT	O4'-C1'-N1	7.84	113.49	108.00
2	P	3	DG	O4'-C1'-N9	7.76	113.43	108.00
3	A	116	ASP	CB-CG-OD2	-7.64	111.43	118.30
3	A	192	ASP	CB-CG-OD2	-7.55	111.50	118.30
3	A	241	LEU	C-N-CD	-7.53	104.04	120.60
2	P	4	DA	P-O3'-C3'	7.52	128.73	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	92	ASP	N-CA-CB	7.43	123.97	110.60
2	P	1	DC	P-O3'-C3'	7.30	128.46	119.70
3	A	256	ASP	CB-CG-OD1	7.23	124.80	118.30
2	P	2	DA	O4'-C1'-N9	7.20	113.04	108.00
2	P	3	DG	P-O3'-C3'	7.14	128.26	119.70
3	A	253	ARG	NE-CZ-NH1	7.10	123.85	120.30
3	A	126	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	T	4	DT	C1'-O4'-C4'	-7.01	103.09	110.10
3	A	226	ASP	CB-CG-OD1	6.90	124.51	118.30
3	A	145	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	T	7	DG	O4'-C1'-N9	6.82	112.78	108.00
3	A	314	ASP	CB-CG-OD2	-6.81	112.17	118.30
3	A	263	ASP	CB-CG-OD2	-6.68	112.29	118.30
3	A	124	ASP	CB-CG-OD1	6.67	124.31	118.30
3	A	334	SER	N-CA-CB	6.65	120.48	110.50
3	A	314	ASP	CB-CG-OD1	6.57	124.21	118.30
3	A	333	ARG	NE-CZ-NH1	6.51	123.56	120.30
3	A	226	ASP	CB-CG-OD2	-6.50	112.45	118.30
3	A	145	ASP	CB-CG-OD1	6.33	124.00	118.30
1	T	3	DA	C8-N9-C1'	6.31	139.06	127.70
3	A	264	GLN	N-CA-CB	6.18	121.73	110.60
3	A	266	TYR	CA-CB-CG	-6.10	101.81	113.40
3	A	138	ILE	CB-CA-C	-6.08	99.44	111.60
1	T	4	DT	O4'-C1'-N1	6.06	112.25	108.00
3	A	246	ASP	CB-CG-OD1	-6.05	112.85	118.30
3	A	101	THR	N-CA-CB	-6.05	98.81	110.30
3	A	74	ASP	CB-CG-OD2	-6.05	112.86	118.30
3	A	137	ARG	NE-CZ-NH1	6.04	123.32	120.30
3	A	116	ASP	N-CA-CB	6.03	121.46	110.60
3	A	91	ASP	CB-CG-OD1	-6.02	112.88	118.30
3	A	18	MET	CG-SD-CE	-5.99	90.62	100.20
3	A	137	ARG	NE-CZ-NH2	-5.96	117.32	120.30
3	A	152	ARG	N-CA-CB	5.96	121.32	110.60
3	A	334	SER	CB-CA-C	5.90	121.32	110.10
3	A	304	THR	N-CA-CB	-5.86	99.17	110.30
3	A	39	TYR	CB-CG-CD1	-5.81	117.51	121.00
3	A	92	ASP	CB-CG-OD1	5.80	123.52	118.30
3	A	79	THR	CA-CB-CG2	-5.79	104.29	112.40
2	P	2	DA	C1'-O4'-C4'	-5.76	104.34	110.10
3	A	170	ASP	CB-CG-OD2	-5.67	113.19	118.30
3	A	199	SER	N-CA-CB	-5.62	102.06	110.50
3	A	74	ASP	CB-CG-OD1	5.59	123.33	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	181	PHE	CB-CA-C	-5.59	99.22	110.40
3	A	335	GLU	N-CA-CB	5.57	120.63	110.60
3	A	42	ALA	N-CA-CB	5.51	117.81	110.10
3	A	296	TYR	CB-CA-C	-5.49	99.42	110.40
3	A	276	ASP	CB-CG-OD2	-5.46	113.39	118.30
3	A	276	ASP	CB-CG-OD1	5.45	123.20	118.30
3	A	102	ARG	CD-NE-CZ	-5.45	115.98	123.60
3	A	57	ALA	N-CA-CB	-5.42	102.51	110.10
3	A	326	LYS	CD-CE-NZ	5.40	124.12	111.70
3	A	239	CYS	CA-CB-SG	-5.39	104.30	114.00
2	P	6	DG	C4'-C3'-C2'	-5.37	98.27	103.10
3	A	192	ASP	CB-CG-OD1	5.27	123.04	118.30
3	A	29	VAL	CA-CB-CG1	-5.25	103.02	110.90
1	T	6	DT	O4'-C1'-N1	-5.25	104.33	108.00
3	A	278	PHE	CB-CA-C	-5.23	99.94	110.40
3	A	91	ASP	CB-CG-OD2	5.21	122.99	118.30
3	A	153	GLU	N-CA-CB	5.21	119.98	110.60
3	A	158	MET	CG-SD-CE	5.20	108.53	100.20
3	A	253	ARG	NE-CZ-NH2	-5.20	117.70	120.30
3	A	92	ASP	CB-CA-C	5.19	120.79	110.40
1	T	3	DA	C8-N9-C4	-5.19	103.72	105.80
3	A	47	ALA	CB-CA-C	-5.19	102.32	110.10
3	A	332	ASP	CB-CG-OD2	5.17	122.95	118.30
3	A	195	LEU	CB-CG-CD1	-5.15	102.25	111.00
3	A	83	ARG	N-CA-CB	5.14	119.84	110.60
3	A	116	ASP	CB-CG-OD1	5.12	122.91	118.30
3	A	318	ASP	CB-CG-OD2	-5.12	113.69	118.30
3	A	195	LEU	CB-CA-C	-5.06	100.59	110.20
3	A	81	LYS	N-CA-CB	-5.05	101.50	110.60
1	T	3	DA	C4-N9-C1'	-5.04	117.22	126.30
1	T	6	DT	C6-N1-C2	5.01	123.81	121.30
3	A	321	ASP	CB-CG-OD2	-5.01	113.79	118.30
2	P	6	DG	C3'-C2'-C1'	-5.00	96.49	102.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	92	ASP	CA
3	A	334	SER	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	122	0	69	4	0
2	P	126	0	68	15	0
3	A	2623	0	2641	295	1
4	A	1	0	0	0	0
5	A	2	0	0	0	0
6	A	20	0	7	0	0
7	A	107	0	0	12	0
7	P	17	0	0	2	0
7	T	11	0	0	1	0
All	All	3029	0	2785	308	1

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 55.

All (308) 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	1.26	1.17
2:P:1:DC:H2"	2:P:2:DA:H5"	1.26	1.15
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.52	1.08
2:P:4:DA:H2"	2:P:5:DT:H5"	1.42	1.01
3:A:150:ILE:HD13	3:A:253:ARG:HG2	1.41	0.99
3:A:41:LYS:HE2	3:A:64:GLY:HA2	1.41	0.99
3:A:277:ILE:HG13	3:A:335:GLU:HB3	1.43	0.99
3:A:82:LEU:HD23	3:A:85:LEU:HB2	1.46	0.98
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.47	0.95
3:A:151:PRO:HG2	3:A:154:GLU:HG3	1.44	0.95
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.64	0.95
3:A:285:HIS:CE1	3:A:289:LYS:HE3	2.03	0.94
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.55	0.89
3:A:31:GLN:HE21	3:A:112:ARG:HH12	0.94	0.88
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.09	0.87
2:P:1:DC:C2'	2:P:2:DA:H5"	2.04	0.87
3:A:32:ALA:HB1	3:A:35:LYS:HB2	1.57	0.86
3:A:218:LEU:HB3	3:A:224:ILE:HD12	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:293:ILE:HD13	3:A:298:ILE:CG1	2.08	0.83
3:A:245:ASN:N	3:A:245:ASN:HD22	1.72	0.83
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.58	0.83
3:A:68:LYS:HB2	3:A:68:LYS:NZ	1.91	0.83
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.19	0.83
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.08	0.82
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.62	0.81
2:P:4:DA:H2"	2:P:5:DT:C5'	2.11	0.81
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.10	0.80
3:A:157:GLN:HE22	3:A:244:LYS:NZ	1.79	0.80
3:A:12:ASN:HB3	3:A:46:ILE:CD1	2.12	0.79
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.13	0.78
3:A:25:PHE:CE2	3:A:88:ILE:HG12	2.19	0.78
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.14	0.78
3:A:52:LYS:HG2	7:A:554:HOH:O	1.84	0.77
3:A:23:ALA:HB2	3:A:39:TYR:HB2	1.65	0.77
3:A:162:VAL:O	3:A:166:VAL:HG23	1.84	0.77
3:A:155:MET:CE	3:A:188:SER:HB2	2.14	0.76
3:A:286:ALA:HA	3:A:323:ILE:HG21	1.66	0.76
3:A:30:SER:HB3	7:A:561:HOH:O	1.85	0.76
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.23	0.74
3:A:177:VAL:HG22	3:A:193:VAL:HG22	1.69	0.73
3:A:278:PHE:HB2	3:A:333:ARG:O	1.89	0.72
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.38	0.72
3:A:172:GLU:HG2	3:A:198:PRO:HG2	1.71	0.71
3:A:218:LEU:CB	3:A:224:ILE:HD12	2.20	0.71
3:A:18:MET:HE3	3:A:76:PHE:CB	2.20	0.71
3:A:12:ASN:HD21	3:A:53:ILE:H	1.37	0.70
3:A:11:LEU:HD23	3:A:11:LEU:H	1.57	0.69
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.22	0.69
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.57	0.69
3:A:270:LEU:HA	3:A:316:GLU:OE2	1.94	0.68
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.76	0.68
3:A:68:LYS:O	3:A:72:LYS:HE3	1.94	0.67
3:A:212:HIS:HB3	7:A:541:HOH:O	1.95	0.67
3:A:157:GLN:HE22	3:A:244:LYS:HZ3	1.42	0.67
3:A:18:MET:O	3:A:22:LEU:HD22	1.95	0.67
3:A:30:SER:HA	7:A:558:HOH:O	1.94	0.67
1:T:6:DT:H5"	7:T:547:HOH:O	1.95	0.67
3:A:18:MET:HE3	3:A:76:PHE:CG	2.29	0.66
3:A:59:ALA:O	3:A:62:LEU:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:155:MET:HE2	3:A:188:SER:HB2	1.77	0.66
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.31	0.66
3:A:292:THR:O	3:A:298:ILE:HA	1.96	0.66
7:P:568:HOH:O	3:A:110:ALA:HB2	1.96	0.65
3:A:197:HIS:ND1	3:A:198:PRO:HD2	2.11	0.65
3:A:31:GLN:N	7:A:641:HOH:O	2.29	0.65
3:A:245:ASN:N	3:A:245:ASN:ND2	2.45	0.65
3:A:18:MET:HE3	3:A:76:PHE:HB2	1.79	0.64
3:A:15:ILE:HD11	3:A:77:LEU:CD1	2.23	0.64
3:A:261:PRO:HG2	3:A:264:GLN:HG3	1.79	0.64
3:A:275:SER:O	3:A:278:PHE:N	2.30	0.64
3:A:210:LEU:HB3	3:A:259:LEU:HD21	1.79	0.64
3:A:302:GLY:H	3:A:307:ALA:HB3	1.62	0.64
3:A:329:GLU:O	3:A:333:ARG:HG2	1.98	0.64
3:A:151:PRO:HG2	3:A:154:GLU:CG	2.24	0.64
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.30	0.64
3:A:27:LYS:HB3	3:A:36:TYR:CD2	2.32	0.63
3:A:180:SER:HB2	3:A:185:ALA:CB	2.28	0.63
3:A:207:GLN:O	3:A:210:LEU:HB2	1.99	0.63
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.33	0.63
3:A:18:MET:CE	3:A:76:PHE:HB2	2.29	0.63
3:A:201:THR:HA	3:A:261:PRO:CB	2.29	0.63
3:A:166:VAL:O	3:A:169:VAL:HG12	1.98	0.63
3:A:271:TYR:HB2	7:A:592:HOH:O	1.96	0.63
3:A:245:ASN:HD22	3:A:245:ASN:H	1.44	0.63
2:P:6:DG:OP1	3:A:105:GLY:N	2.30	0.62
3:A:288:GLU:OE1	3:A:288:GLU:HA	1.91	0.62
3:A:259:LEU:HD12	3:A:260:ILE:H	1.65	0.62
3:A:73:ILE:HG22	3:A:77:LEU:HD13	1.81	0.62
3:A:150:ILE:N	3:A:188:SER:O	2.29	0.62
2:P:2:DA:C8	2:P:2:DA:H5'	2.35	0.61
3:A:19:LEU:HB3	3:A:43:ALA:HB2	1.82	0.61
3:A:180:SER:HB2	3:A:185:ALA:HB2	1.82	0.61
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.83	0.61
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.82	0.61
3:A:201:THR:HA	3:A:261:PRO:HB3	1.82	0.61
3:A:194:LEU:HD21	3:A:272:PHE:HD2	1.66	0.60
3:A:253:ARG:HH11	3:A:253:ARG:CG	2.14	0.60
3:A:277:ILE:CG1	3:A:335:GLU:HB3	2.28	0.60
3:A:52:LYS:HD3	3:A:54:LYS:HE3	1.82	0.60
3:A:277:ILE:HG13	3:A:335:GLU:CB	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:33:ILE:HG23	3:A:34:HIS:N	2.16	0.59
3:A:41:LYS:HD3	3:A:42:ALA:N	2.16	0.59
3:A:218:LEU:HB3	3:A:224:ILE:CD1	2.32	0.59
3:A:16:THR:HG23	3:A:46:ILE:HG12	1.84	0.59
3:A:15:ILE:O	3:A:19:LEU:HB2	2.03	0.58
3:A:286:ALA:O	3:A:291:PHE:HB2	2.03	0.58
3:A:23:ALA:CB	3:A:39:TYR:HB2	2.32	0.58
3:A:73:ILE:HG22	3:A:77:LEU:CD1	2.33	0.58
3:A:166:VAL:HG12	3:A:173:TYR:CB	2.32	0.58
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.68	0.58
3:A:11:LEU:H	3:A:11:LEU:CD2	2.15	0.57
3:A:157:GLN:O	3:A:160:ASP:HB3	2.04	0.57
3:A:321:ASP:O	3:A:324:GLN:N	2.34	0.57
3:A:241:LEU:HB3	3:A:242:PRO:HD2	1.86	0.57
3:A:282:MET:HG2	7:A:555:HOH:O	2.04	0.57
3:A:41:LYS:O	3:A:45:VAL:HG13	2.04	0.57
3:A:330:PRO:HA	3:A:333:ARG:CG	2.35	0.57
3:A:26:GLU:OE1	3:A:26:GLU:HA	2.05	0.57
3:A:308:GLY:O	3:A:309:GLU:HB2	2.04	0.57
3:A:68:LYS:HB2	3:A:68:LYS:HZ1	1.70	0.57
2:P:5:DT:OP2	3:A:108:PRO:HD2	2.05	0.56
3:A:16:THR:HG23	3:A:46:ILE:CG1	2.35	0.56
3:A:140:LEU:HD12	3:A:140:LEU:O	2.05	0.56
3:A:306:VAL:HG23	3:A:307:ALA:N	2.18	0.56
3:A:124:ASP:O	3:A:128:ASN:ND2	2.38	0.56
3:A:23:ALA:O	3:A:36:TYR:HD2	1.88	0.56
3:A:32:ALA:CB	3:A:35:LYS:HB2	2.32	0.56
3:A:259:LEU:O	3:A:260:ILE:HD13	2.04	0.56
3:A:165:GLU:OE1	3:A:168:LYS:NZ	2.30	0.56
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.40	0.56
3:A:111:ALA:O	3:A:115:VAL:HG23	2.06	0.55
3:A:27:LYS:HB3	3:A:36:TYR:CG	2.41	0.55
3:A:253:ARG:HH11	3:A:253:ARG:HG3	1.71	0.55
3:A:197:HIS:CE1	3:A:199:SER:HB2	2.42	0.55
3:A:217:GLN:O	3:A:221:VAL:HG22	2.06	0.55
3:A:150:ILE:HG21	3:A:158:MET:CE	2.38	0.54
3:A:303:VAL:C	3:A:305:GLY:H	2.09	0.54
3:A:244:LYS:CB	3:A:245:ASN:HD22	2.20	0.54
3:A:298:ILE:O	3:A:311:LEU:HB2	2.07	0.54
3:A:262:LYS:O	3:A:262:LYS:HG3	2.07	0.54
3:A:277:ILE:HG12	3:A:335:GLU:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:259:LEU:HD12	3:A:260:ILE:N	2.23	0.54
3:A:113:LYS:O	3:A:117:GLU:HG3	2.07	0.54
3:A:302:GLY:N	3:A:307:ALA:HB3	2.24	0.53
3:A:331:LYS:HD2	3:A:332:ASP:N	2.23	0.53
3:A:132:LEU:HB3	3:A:136:GLN:HB3	1.91	0.53
3:A:255:ILE:HG12	3:A:256:ASP:N	2.22	0.53
3:A:25:PHE:CD2	3:A:88:ILE:HG12	2.43	0.53
3:A:296:TYR:HB2	3:A:297:THR:HG23	1.91	0.53
3:A:182:ARG:NH1	3:A:182:ARG:HG2	2.23	0.53
3:A:285:HIS:NE2	3:A:289:LYS:HE3	2.24	0.53
3:A:332:ASP:C	3:A:334:SER:H	2.11	0.53
3:A:242:PRO:HG2	7:A:589:HOH:O	2.07	0.53
3:A:194:LEU:HD21	3:A:272:PHE:CD2	2.44	0.52
3:A:83:ARG:HA	3:A:86:GLU:HG2	1.91	0.52
3:A:155:MET:HA	3:A:158:MET:HG3	1.91	0.52
2:P:5:DT:OP1	3:A:110:ALA:N	2.30	0.52
3:A:286:ALA:HA	3:A:323:ILE:CG2	2.36	0.52
3:A:316:GLU:O	3:A:320:PHE:HD1	1.92	0.52
2:P:6:DG:H2'	2:P:6:DG:O5'	2.10	0.52
3:A:243:SER:OG	3:A:249:GLU:HG3	2.10	0.52
3:A:41:LYS:HD3	3:A:42:ALA:H	1.75	0.52
3:A:285:HIS:NE2	3:A:289:LYS:HG3	2.24	0.52
3:A:200:PHE:O	3:A:262:LYS:N	2.39	0.52
3:A:157:GLN:HE22	3:A:244:LYS:HZ1	1.54	0.51
3:A:33:ILE:O	3:A:37:ASN:HB2	2.10	0.51
3:A:266:TYR:HA	3:A:269:VAL:HB	1.92	0.51
3:A:244:LYS:HB2	3:A:245:ASN:HD22	1.75	0.51
3:A:248:LYS:O	3:A:248:LYS:HG2	2.09	0.51
1:T:3:DA:N6	2:P:4:DA:N6	2.58	0.51
3:A:41:LYS:O	3:A:44:SER:HB3	2.10	0.51
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.40	0.51
3:A:22:LEU:HD13	3:A:85:LEU:CD1	2.40	0.51
3:A:261:PRO:HG2	3:A:264:GLN:CG	2.41	0.51
3:A:196:THR:OG1	3:A:197:HIS:N	2.43	0.50
3:A:133:ASN:HD22	3:A:134:HIS:N	2.09	0.50
3:A:275:SER:OG	3:A:334:SER:O	2.28	0.50
3:A:114:PHE:CD1	3:A:119:ILE:HD12	2.46	0.50
3:A:205:THR:O	3:A:206:LYS:O	2.29	0.50
3:A:150:ILE:HD13	3:A:253:ARG:CG	2.28	0.50
3:A:91:ASP:O	3:A:95:SER:OG	2.29	0.50
3:A:27:LYS:HG3	3:A:28:ASN:N	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:100:LEU:HD12	3:A:100:LEU:N	2.27	0.49
3:A:288:GLU:C	3:A:290:GLY:H	2.14	0.49
3:A:12:ASN:CB	3:A:46:ILE:HD12	2.36	0.49
3:A:204:SER:O	3:A:204:SER:OG	2.30	0.49
3:A:200:PHE:HB2	3:A:210:LEU:CD1	2.43	0.49
3:A:18:MET:HG2	3:A:22:LEU:HD22	1.94	0.49
3:A:100:LEU:N	3:A:100:LEU:CD1	2.77	0.48
3:A:79:THR:O	3:A:81:LYS:N	2.46	0.48
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.28	0.48
3:A:277:ILE:HD13	3:A:277:ILE:H	1.78	0.48
3:A:223:PHE:O	3:A:239:CYS:HB2	2.14	0.48
3:A:157:GLN:O	3:A:161:ILE:HG13	2.13	0.48
3:A:208:PRO:O	3:A:212:HIS:HD2	1.97	0.48
3:A:32:ALA:O	3:A:36:TYR:N	2.29	0.48
3:A:279:ASN:O	3:A:283:ARG:HG3	2.14	0.48
3:A:26:GLU:HA	3:A:30:SER:OG	2.14	0.47
3:A:152:ARG:HA	3:A:155:MET:HB2	1.96	0.47
3:A:331:LYS:CD	3:A:332:ASP:N	2.77	0.47
3:A:36:TYR:CD1	3:A:37:ASN:N	2.82	0.47
3:A:99:PHE:HD2	3:A:100:LEU:HD12	1.79	0.47
3:A:285:HIS:CD2	3:A:289:LYS:HG3	2.50	0.47
3:A:322:TYR:HD1	3:A:322:TYR:HA	1.49	0.47
3:A:158:MET:HG2	3:A:241:LEU:HD21	1.96	0.47
3:A:177:VAL:HG12	3:A:181:PHE:HD2	1.80	0.47
3:A:206:LYS:O	3:A:207:GLN:HB2	2.15	0.47
3:A:285:HIS:NE2	3:A:289:LYS:CG	2.78	0.47
3:A:81:LYS:NZ	3:A:86:GLU:OE1	2.47	0.47
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.29	0.47
3:A:172:GLU:CG	3:A:198:PRO:HG2	2.42	0.47
3:A:295:GLU:HA	7:A:592:HOH:O	2.14	0.47
3:A:301:LEU:HD12	3:A:301:LEU:HA	1.64	0.47
3:A:200:PHE:O	3:A:261:PRO:HA	2.15	0.46
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.12	0.46
3:A:12:ASN:HB3	3:A:46:ILE:HD11	1.94	0.46
3:A:44:SER:O	3:A:47:ALA:HB3	2.15	0.46
3:A:194:LEU:HD11	3:A:258:ARG:HD3	1.98	0.46
3:A:32:ALA:O	3:A:36:TYR:HB3	2.15	0.46
3:A:26:GLU:HG3	3:A:35:LYS:HB3	1.97	0.46
3:A:114:PHE:HB3	3:A:119:ILE:HB	1.96	0.46
3:A:26:GLU:OE1	3:A:30:SER:OG	2.28	0.45
3:A:315:SER:OG	3:A:316:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:319:ILE:O	3:A:322:TYR:HB2	2.16	0.45
1:T:3:DA:N1	2:P:5:DT:C4	2.84	0.45
3:A:49:TYR:CZ	3:A:51:HIS:HB2	2.51	0.45
3:A:169:VAL:HG13	3:A:170:ASP:N	2.31	0.45
3:A:244:LYS:CB	3:A:245:ASN:ND2	2.80	0.45
3:A:201:THR:OG1	3:A:263:ASP:OD1	2.28	0.45
3:A:294:ASN:C	3:A:294:ASN:HD22	2.19	0.45
3:A:79:THR:C	3:A:81:LYS:H	2.20	0.44
3:A:298:ILE:O	3:A:298:ILE:HG23	2.16	0.44
3:A:174:ILE:HG22	3:A:265:TYR:CE2	2.51	0.44
3:A:280:LYS:O	3:A:283:ARG:HB2	2.17	0.44
3:A:331:LYS:HD3	3:A:332:ASP:HB3	1.98	0.44
3:A:11:LEU:CD2	3:A:11:LEU:N	2.78	0.44
3:A:33:ILE:CG2	3:A:34:HIS:N	2.81	0.44
3:A:210:LEU:CB	3:A:259:LEU:HD21	2.47	0.44
3:A:289:LYS:HD2	3:A:324:GLN:OE1	2.18	0.44
3:A:292:THR:O	3:A:298:ILE:HG13	2.18	0.44
2:P:4:DA:H5"	7:P:614:HOH:O	2.17	0.44
3:A:135:HIS:HB2	7:A:596:HOH:O	2.16	0.44
3:A:276:ASP:O	3:A:280:LYS:HG3	2.18	0.44
3:A:154:GLU:HB3	7:A:521:HOH:O	2.18	0.44
3:A:197:HIS:ND1	3:A:198:PRO:CD	2.79	0.44
3:A:18:MET:HG2	3:A:22:LEU:CD2	2.47	0.44
3:A:280:LYS:O	3:A:284:ALA:N	2.45	0.44
3:A:103:VAL:HG22	3:A:143:PHE:CE2	2.53	0.43
3:A:270:LEU:HD13	3:A:316:GLU:OE2	2.18	0.43
3:A:303:VAL:O	3:A:305:GLY:N	2.51	0.43
3:A:293:ILE:HD13	3:A:298:ILE:CD1	2.48	0.43
3:A:150:ILE:O	3:A:187:SER:HA	2.19	0.43
3:A:172:GLU:HG2	3:A:198:PRO:CG	2.46	0.43
3:A:195:LEU:HA	3:A:195:LEU:HD12	1.66	0.43
3:A:323:ILE:O	3:A:324:GLN:HG3	2.19	0.43
3:A:152:ARG:HB3	7:A:530:HOH:O	2.19	0.43
3:A:205:THR:O	3:A:205:THR:HG23	2.17	0.43
3:A:194:LEU:HD12	3:A:194:LEU:HA	1.73	0.43
3:A:103:VAL:HB	3:A:106:ILE:HD12	2.00	0.43
3:A:165:GLU:HB2	3:A:218:LEU:HD11	2.00	0.43
2:P:2:DA:H5'	2:P:2:DA:H2'	1.27	0.42
3:A:103:VAL:HG22	3:A:143:PHE:CD2	2.53	0.42
1:T:2:DC:H2"	1:T:3:DA:C8	2.54	0.42
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:244:LYS:HB2	3:A:245:ASN:H	1.58	0.42
3:A:49:TYR:CE2	3:A:51:HIS:HB2	2.54	0.42
3:A:133:ASN:HD21	3:A:135:HIS:HB3	1.84	0.42
3:A:287:LEU:HA	3:A:287:LEU:HD13	1.47	0.42
3:A:255:ILE:O	3:A:255:ILE:HG23	2.18	0.42
3:A:280:LYS:O	3:A:283:ARG:N	2.53	0.42
2:P:5:DT:P	3:A:109:SER:HB3	2.60	0.42
3:A:327:TYR:CD1	3:A:328:ARG:N	2.87	0.42
3:A:82:LEU:CD2	3:A:85:LEU:HB2	2.33	0.42
3:A:150:ILE:HG13	3:A:188:SER:O	2.20	0.42
3:A:249:GLU:CG	3:A:250:TYR:N	2.83	0.42
3:A:260:ILE:HG22	3:A:261:PRO:HD2	2.01	0.42
2:P:2:DA:H2"	2:P:3:DG:OP2	2.20	0.42
3:A:22:LEU:CD1	3:A:85:LEU:CD1	2.98	0.42
3:A:212:HIS:H	3:A:212:HIS:CD2	2.38	0.42
3:A:28:ASN:N	3:A:28:ASN:HD22	2.17	0.41
3:A:211:LEU:HD12	3:A:211:LEU:O	2.19	0.41
3:A:280:LYS:HG3	3:A:280:LYS:H	1.63	0.41
3:A:73:ILE:CG2	3:A:77:LEU:CD1	2.97	0.41
3:A:239:CYS:O	3:A:240:GLN:HB2	2.20	0.41
3:A:213:GLN:O	3:A:216:GLU:HB3	2.21	0.41
3:A:200:PHE:CE2	3:A:261:PRO:HD3	2.56	0.41
3:A:68:LYS:HB2	3:A:68:LYS:HZ2	1.80	0.41
3:A:211:LEU:O	3:A:215:VAL:HG23	2.20	0.41
3:A:215:VAL:O	3:A:219:GLN:HG3	2.19	0.41
3:A:309:GLU:HA	3:A:310:PRO:HD2	1.65	0.41
3:A:26:GLU:O	3:A:30:SER:OG	2.39	0.41
3:A:49:TYR:CE2	3:A:53:ILE:HG13	2.56	0.41
3:A:132:LEU:N	3:A:132:LEU:HD23	2.35	0.41
3:A:138:ILE:O	3:A:138:ILE:HG22	2.21	0.41
3:A:259:LEU:HD12	3:A:259:LEU:HA	1.36	0.41
3:A:177:VAL:HG12	3:A:181:PHE:CD2	2.56	0.41
3:A:21:GLU:HB2	3:A:85:LEU:HD11	2.03	0.41
3:A:31:GLN:O	3:A:33:ILE:N	2.54	0.41
3:A:102:ARG:HH11	3:A:102:ARG:HD3	1.52	0.41
3:A:197:HIS:CE1	3:A:199:SER:CB	3.04	0.40
3:A:209:LYS:HA	3:A:209:LYS:HD3	1.36	0.40
3:A:237:GLY:O	3:A:254:ARG:NH1	2.54	0.40
3:A:35:LYS:O	3:A:38:ALA:HB3	2.20	0.40
3:A:273:THR:HG22	3:A:273:THR:O	2.21	0.40
3:A:271:TYR:CD2	3:A:272:PHE:N	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:309:GLU:HA	3:A:309:GLU:OE1	2.19	0.40
3:A:79:THR:O	3:A:79:THR:OG1	2.38	0.40
3:A:206:LYS:HA	3:A:206:LYS:HD3	1.64	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:83:ARG:NH1	3:A:117:GLU:CB[3_558]	2.14	0.06

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%)	271 (83%)	38 (12%)	16 (5%)	2 8

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	32	ALA
3	A	185	ALA
3	A	202	SER
3	A	206	LYS
3	A	244	LYS
3	A	247	GLU
3	A	309	GLU
3	A	10	THR
3	A	80	GLY
3	A	289	LYS
3	A	304	THR
3	A	246	ASP
3	A	334	SER

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Mol	Chain	Res	Type
3	A	276	ASP
3	A	310	PRO
3	A	207	GLN

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%)	233 (81%)	55 (19%)	1 4

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

Mol	Chain	Res	Type
3	A	10	THR
3	A	11	LEU
3	A	16	THR
3	A	18	MET
3	A	19	LEU
3	A	22	LEU
3	A	25	PHE
3	A	27	LYS
3	A	36	TYR
3	A	37	ASN
3	A	41	LYS
3	A	46	ILE
3	A	54	LYS
3	A	62	LEU
3	A	67	THR
3	A	68	LYS
3	A	77	LEU
3	A	79	THR
3	A	95	SER
3	A	113	LYS
3	A	130	ASP
3	A	133	ASN
3	A	150	ILE

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Mol	Chain	Res	Type
3	A	158	MET
3	A	159	GLN
3	A	168	LYS
3	A	172	GLU
3	A	192	ASP
3	A	194	LEU
3	A	207	GLN
3	A	214	VAL
3	A	218	LEU
3	A	226	ASP
3	A	228	LEU
3	A	233	THR
3	A	236	MET
3	A	245	ASN
3	A	246	ASP
3	A	248	LYS
3	A	253	ARG
3	A	258	ARG
3	A	259	LEU
3	A	277	ILE
3	A	282	MET
3	A	287	LEU
3	A	288	GLU
3	A	293	ILE
3	A	294	ASN
3	A	296	TYR
3	A	304	THR
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	325	TRP
3	A	331	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) 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

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Mol	Chain	Res	Type
3	A	133	ASN
3	A	136	GLN
3	A	157	GLN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	240	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 monosaccharides 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	16,20,30	1.55	1 (6%)	22,31,47	1.13	1 (4%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	338	TTP	O4'-C4'	4.37	1.51	1.44

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	338	TTP	O3G-PG-O3B	-2.49	96.30	104.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

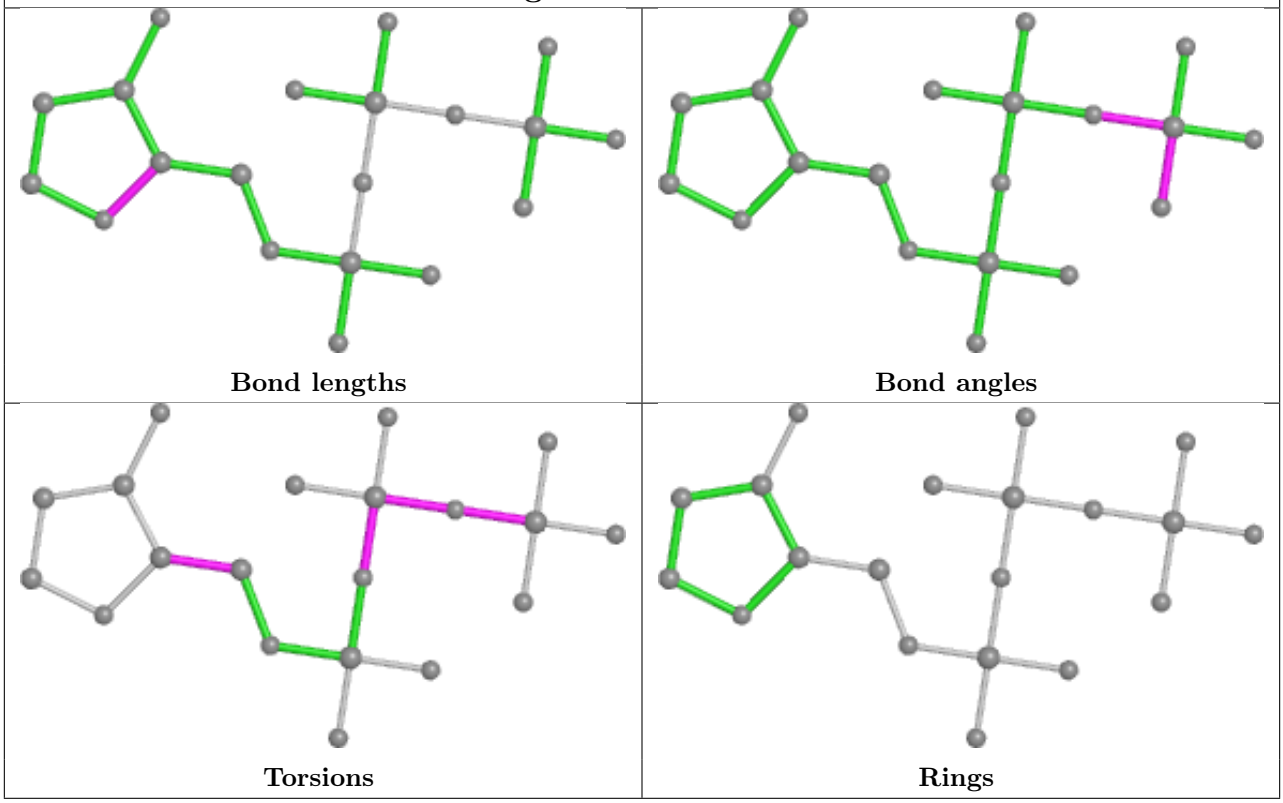
Mol	Chain	Res	Type	Atoms
6	A	338	TTP	PB-O3B-PG-O2G
6	A	338	TTP	PB-O3B-PG-O3G
6	A	338	TTP	O4'-C4'-C5'-O5'
6	A	338	TTP	PA-O3A-PB-O2B
6	A	338	TTP	PG-O3B-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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.

Ligand TTP A 338



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	7/7 (100%)	-1.27	0	100	100	24, 48, 67, 100	0
2	P	6/6 (100%)	-1.62	0	100	100	32, 38, 42, 43	0
3	A	324/335 (96%)	-1.17	0	100	100	7, 41, 88, 99	0
All	All	337/348 (96%)	-1.18	0	100	100	7, 41, 89, 100	0

There are no RSRZ outliers to report.

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 monosaccharides 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.

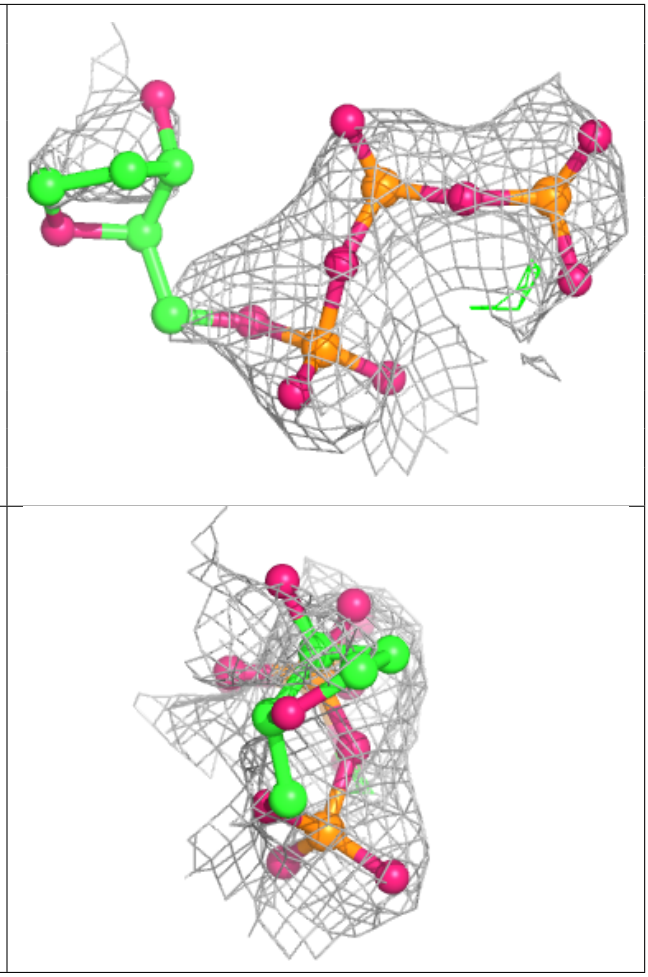
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	TTP	A	338	20/29	0.89	0.22	68,87,91,91	20
5	NA	A	342	1/1	0.97	0.23	59,59,59,59	0
4	MN	A	339	1/1	0.98	0.09	30,30,30,30	1
5	NA	A	341	1/1	0.98	0.10	39,39,39,39	0

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.

Electron density around TTP A 338:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.