



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2016 – 12:03 AM GMT

PDB ID : 9ICP  
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SIX BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF PYROPHOSPHATE (1 MILLIMOLAR) AND MGCL2 (5 MILLIMOLAR)  
Authors : Pelletier, H.; Sawaya, M.R.  
Deposited on : 1995-12-16  
Resolution : 3.10 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

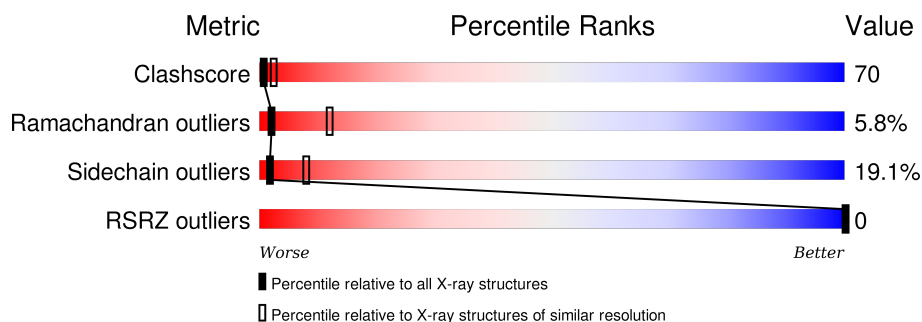
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	7	
2	P	6	
3	A	335	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3022 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
1	T	7	Total	C	N	O	P	0	0	0
			122	58	20	38	6			

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

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

- 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	116	Total	O	0	0
			116	116		
5	P	23	Total	O	0	0
			23	23		
5	T	10	Total	O	0	0
			10	10		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

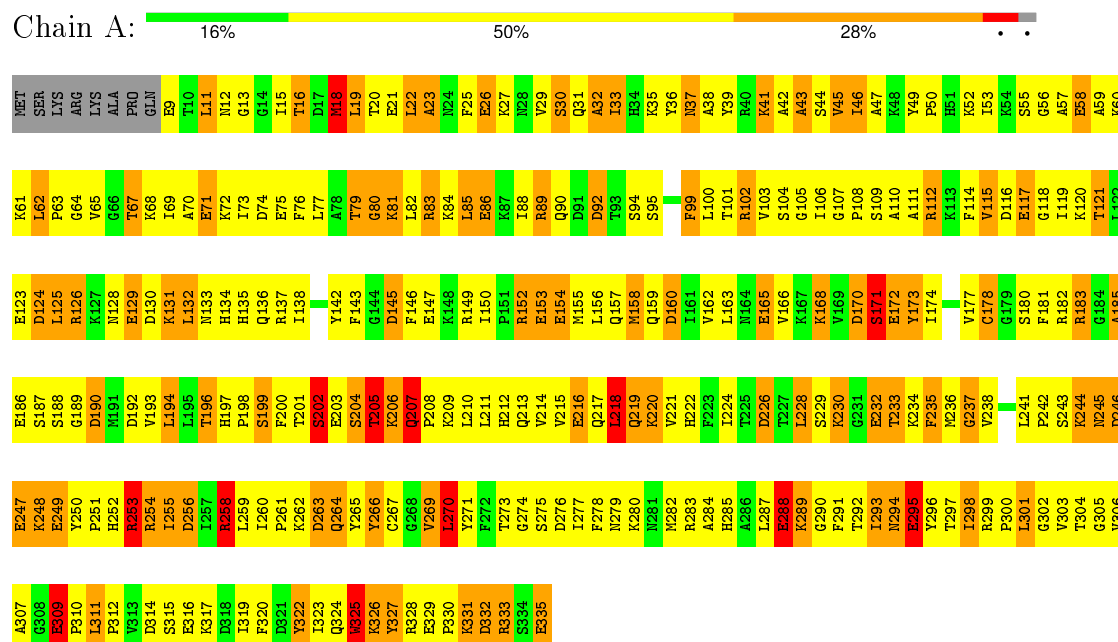
- Molecule 1: DNA (5'-D(\*CP\*AP\*TP\*CP\*TP\*GP\*T)-3')



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.66 Å   57.82 Å   48.49 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 3.10 10.60 – 2.68	Depositor EDS
% Data completeness (in resolution range)	91.0 (20.00-3.10) 85.8 (10.60-2.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 2.68 Å)	Xtriage
Refinement program	TNT V. 5-D	Depositor
R, $R_{free}$	0.165 , (Not available) 0.158 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	20.9	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.16 , 154.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 12625 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	3022	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	2.32	7/135 (5.2%)	2.67	19/207 (9.2%)
2	P	2.62	9/141 (6.4%)	3.93	25/214 (11.7%)
3	A	1.26	26/2672 (1.0%)	1.80	78/3590 (2.2%)
All	All	1.42	42/2948 (1.4%)	2.02	122/4011 (3.0%)

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 (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	5	DT	C1'-N1	9.60	1.61	1.49
2	P	5	DT	N1-C2	8.67	1.45	1.38
2	P	5	DT	C4-C5	8.15	1.52	1.45
1	T	7	DG	C1'-N9	-7.61	1.36	1.47
1	T	4	DT	C1'-N1	7.45	1.58	1.49
3	A	21	GLU	CD-OE1	7.26	1.33	1.25
3	A	147	GLU	CD-OE2	7.18	1.33	1.25
3	A	75	GLU	CD-OE1	7.14	1.33	1.25
3	A	153	GLU	CD-OE2	6.84	1.33	1.25
3	A	329	GLU	CD-OE2	6.79	1.33	1.25
1	T	7	DG	N9-C4	-6.75	1.32	1.38
2	P	5	DT	C2-N3	-6.71	1.32	1.37
3	A	71	GLU	CD-OE1	6.66	1.32	1.25
3	A	249	GLU	CD-OE2	6.65	1.32	1.25
2	P	4	DA	C3'-O3'	-6.62	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	2	DC	N1-C6	-6.42	1.33	1.37
3	A	117	GLU	CD-OE2	6.41	1.32	1.25
3	A	309	GLU	CD-OE2	6.40	1.32	1.25
3	A	203	GLU	CD-OE1	6.38	1.32	1.25
3	A	295	GLU	CD-OE1	6.30	1.32	1.25
3	A	58	GLU	CD-OE1	6.14	1.32	1.25
1	T	6	DT	C3'-O3'	-6.06	1.36	1.44
3	A	335	GLU	CD-OE2	6.04	1.32	1.25
1	T	6	DT	C1'-N1	-6.01	1.38	1.47
2	P	1	DC	N1-C6	-5.97	1.33	1.37
3	A	186	GLU	CD-OE1	5.91	1.32	1.25
3	A	165	GLU	CD-OE2	5.89	1.32	1.25
2	P	3	DG	C8-N7	5.88	1.34	1.30
3	A	326	LYS	CE-NZ	-5.78	1.34	1.49
2	P	5	DT	N3-C4	-5.75	1.34	1.38
3	A	172	GLU	CD-OE2	5.71	1.31	1.25
3	A	26	GLU	CD-OE1	5.70	1.31	1.25
3	A	232	GLU	CD-OE2	5.58	1.31	1.25
2	P	3	DG	C3'-O3'	-5.55	1.36	1.44
3	A	288	GLU	CD-OE2	5.50	1.31	1.25
3	A	129	GLU	CD-OE1	5.48	1.31	1.25
3	A	86	GLU	CD-OE1	5.46	1.31	1.25
3	A	216	GLU	CD-OE2	5.44	1.31	1.25
1	T	7	DG	O4'-C1'	-5.41	1.35	1.42
3	A	154	GLU	CD-OE2	5.40	1.31	1.25
3	A	247	GLU	CD-OE1	5.21	1.31	1.25
3	A	9	GLU	CD-OE2	5.20	1.31	1.25

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	5	DT	C6-N1-C1'	-19.66	90.91	120.40
2	P	5	DT	C2-N1-C1'	19.04	148.67	118.20
2	P	3	DG	C8-N9-C1'	16.61	148.59	127.00
2	P	3	DG	C4-N9-C1'	-13.93	108.39	126.50
3	A	253	ARG	NE-CZ-NH1	11.39	125.99	120.30
2	P	5	DT	O4'-C1'-N1	10.80	115.56	108.00
2	P	4	DA	P-O3'-C3'	10.58	132.40	119.70
2	P	2	DA	O4'-C4'-C3'	-10.49	99.71	106.00
3	A	253	ARG	NE-CZ-NH2	-10.12	115.24	120.30
2	P	5	DT	N3-C2-O2	-9.74	116.46	122.30
1	T	6	DT	O4'-C4'-C3'	-9.46	100.32	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	4	DA	O4'-C1'-N9	-9.38	101.44	108.00
2	P	4	DA	C8-N9-C1'	-8.82	111.83	127.70
2	P	3	DG	C8-N9-C4	-8.54	102.98	106.40
2	P	4	DA	C4-N9-C1'	8.52	141.64	126.30
2	P	5	DT	C6-C5-C7	-8.52	117.79	122.90
1	T	6	DT	C2-N1-C1'	-8.25	105.01	118.20
1	T	6	DT	C6-N1-C1'	8.23	132.75	120.40
2	P	5	DT	C5-C4-O4	8.04	130.53	124.90
2	P	2	DA	C4'-C3'-C2'	-7.99	95.91	103.10
3	A	190	ASP	CB-CG-OD1	7.97	125.47	118.30
3	A	121	THR	CA-CB-CG2	-7.88	101.37	112.40
2	P	5	DT	C1'-O4'-C4'	-7.86	102.24	110.10
3	A	126	ARG	NE-CZ-NH2	-7.86	116.37	120.30
2	P	5	DT	N3-C4-O4	-7.86	115.19	119.90
3	A	253	ARG	CD-NE-CZ	7.79	134.51	123.60
3	A	190	ASP	CB-CG-OD2	-7.77	111.31	118.30
3	A	145	ASP	CB-CG-OD2	-7.74	111.33	118.30
3	A	152	ARG	N-CA-CB	7.71	124.47	110.60
3	A	183	ARG	NE-CZ-NH1	7.67	124.14	120.30
3	A	256	ASP	CB-CG-OD1	7.58	125.12	118.30
3	A	43	ALA	CB-CA-C	7.56	121.44	110.10
2	P	2	DA	P-O5'-C5'	-7.55	108.82	120.90
2	P	1	DC	P-O3'-C3'	7.48	128.68	119.70
3	A	229	SER	N-CA-CB	7.47	121.71	110.50
1	T	3	DA	P-O3'-C3'	7.35	128.52	119.70
3	A	57	ALA	N-CA-CB	-7.34	99.82	110.10
3	A	92	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	T	6	DT	O4'-C1'-N1	-7.24	102.93	108.00
3	A	254	ARG	NE-CZ-NH2	-7.23	116.69	120.30
3	A	170	ASP	CB-CG-OD1	7.22	124.80	118.30
3	A	310	PRO	N-CA-CB	7.13	111.86	103.30
2	P	5	DT	N1-C1'-C2'	7.08	126.06	112.60
2	P	5	DT	P-O3'-C3'	6.91	128.00	119.70
3	A	266	TYR	CB-CG-CD1	-6.90	116.86	121.00
3	A	263	ASP	CB-CG-OD2	-6.89	112.10	118.30
3	A	170	ASP	CB-CG-OD2	-6.87	112.11	118.30
3	A	160	ASP	CB-CG-OD2	-6.87	112.12	118.30
3	A	126	ARG	NE-CZ-NH1	6.83	123.72	120.30
3	A	124	ASP	CB-CG-OD2	-6.80	112.18	118.30
3	A	160	ASP	CB-CG-OD1	6.80	124.42	118.30
3	A	116	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	T	2	DC	C6-N1-C1'	-6.70	112.76	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	332	ASP	CB-CG-OD1	-6.67	112.30	118.30
1	T	5	DC	P-O3'-C3'	6.67	127.70	119.70
3	A	74	ASP	CB-CG-OD1	6.56	124.20	118.30
3	A	254	ARG	NE-CZ-NH1	6.51	123.56	120.30
3	A	124	ASP	CB-CG-OD1	6.48	124.13	118.30
3	A	332	ASP	CB-CG-OD2	6.46	124.11	118.30
3	A	192	ASP	CB-CG-OD2	-6.45	112.50	118.30
3	A	130	ASP	CB-CG-OD1	6.44	124.10	118.30
3	A	115	VAL	CA-CB-CG1	-6.41	101.28	110.90
2	P	1	DC	C6-N1-C1'	-6.38	113.14	120.80
3	A	333	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	T	5	DC	O4'-C1'-N1	6.30	112.41	108.00
3	A	276	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	T	6	DT	C4'-C3'-C2'	6.04	108.54	103.10
3	A	23	ALA	N-CA-CB	6.03	118.54	110.10
3	A	230	LYS	N-CA-CB	5.99	121.38	110.60
1	T	5	DC	C6-N1-C1'	5.98	127.98	120.80
1	T	2	DC	O4'-C1'-N1	-5.97	103.82	108.00
3	A	152	ARG	CD-NE-CZ	-5.95	115.28	123.60
3	A	202	SER	N-CA-CB	-5.92	101.62	110.50
2	P	1	DC	C2-N1-C1'	5.90	125.29	118.80
3	A	83	ARG	NE-CZ-NH1	5.88	123.24	120.30
3	A	326	LYS	CD-CE-NZ	5.88	125.24	111.70
3	A	229	SER	CB-CA-C	5.88	121.28	110.10
3	A	276	ASP	CB-CG-OD1	5.88	123.59	118.30
3	A	152	ARG	NE-CZ-NH1	-5.86	117.37	120.30
3	A	74	ASP	CB-CG-OD2	-5.84	113.05	118.30
3	A	246	ASP	CB-CG-OD1	-5.84	113.04	118.30
3	A	266	TYR	CA-CB-CG	-5.84	102.31	113.40
2	P	5	DT	C4-C5-C7	5.83	122.50	119.00
1	T	4	DT	P-O3'-C3'	5.75	126.60	119.70
3	A	228	LEU	CA-CB-CG	-5.69	102.21	115.30
1	T	4	DT	P-O5'-C5'	-5.67	111.83	120.90
3	A	325	TRP	N-CA-CB	-5.66	100.42	110.60
2	P	3	DG	N7-C8-N9	5.65	115.92	113.10
3	A	256	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	T	7	DG	C8-N9-C4	5.62	108.65	106.40
3	A	152	ARG	NE-CZ-NH2	5.60	123.10	120.30
3	A	322	TYR	CB-CG-CD1	-5.60	117.64	121.00
3	A	18	MET	CG-SD-CE	-5.60	91.25	100.20
3	A	99	PHE	CA-CB-CG	-5.59	100.48	113.90
1	T	2	DC	C2-N1-C1'	5.58	124.94	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	192	ASP	CB-CG-OD1	5.58	123.33	118.30
3	A	89	ARG	NE-CZ-NH1	5.57	123.09	120.30
3	A	327	TYR	N-CA-CB	5.53	120.55	110.60
1	T	5	DC	C2-N1-C1'	-5.51	112.74	118.80
3	A	116	ASP	CB-CG-OD1	5.51	123.26	118.30
3	A	333	ARG	NE-CZ-NH2	-5.49	117.55	120.30
3	A	83	ARG	N-CA-CB	5.48	120.46	110.60
1	T	4	DT	O4'-C4'-C3'	5.48	109.29	106.00
3	A	258	ARG	NE-CZ-NH1	5.46	123.03	120.30
3	A	171	SER	N-CA-CB	5.46	118.69	110.50
3	A	222	HIS	CB-CA-C	-5.46	99.48	110.40
3	A	246	ASP	CB-CG-OD2	5.45	123.20	118.30
3	A	314	ASP	CB-CG-OD2	-5.40	113.44	118.30
3	A	173	TYR	CB-CG-CD1	-5.34	117.80	121.00
3	A	270	LEU	CA-C-N	-5.33	105.47	117.20
3	A	226	ASP	CB-CG-OD2	5.32	123.09	118.30
3	A	102	ARG	CD-NE-CZ	-5.26	116.23	123.60
3	A	269	VAL	CA-CB-CG1	-5.25	103.02	110.90
3	A	71	GLU	N-CA-CB	-5.24	101.16	110.60
3	A	237	GLY	O-C-N	5.24	131.08	122.70
1	T	4	DT	C2-N1-C1'	5.23	126.57	118.20
3	A	310	PRO	N-CA-C	5.20	125.63	112.10
3	A	218	LEU	CB-CA-C	5.19	120.07	110.20
1	T	6	DT	P-O3'-C3'	-5.18	113.48	119.70
3	A	196	THR	N-CA-CB	5.17	120.11	110.30
3	A	295	GLU	CB-CA-C	5.16	120.73	110.40
3	A	130	ASP	CB-CG-OD2	-5.15	113.67	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	152	ARG	CA
3	A	310	PRO	CA

There are no planarity outliers.

## 5.2 Too-close contacts

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	7	0
2	P	126	0	67	20	0
3	A	2623	0	2641	368	1
4	A	2	0	0	0	0
5	A	116	0	0	22	0
5	P	23	0	0	4	0
5	T	10	0	0	3	0
All	All	3022	0	2777	386	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 70.

All (386) 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:23:ALA:HB2	3:A:39:TYR:HB2	1.27	1.08
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.50	1.07
3:A:301:LEU:HD11	3:A:306:VAL:HA	1.41	1.02
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.41	1.02
3:A:177:VAL:HG22	3:A:193:VAL:HG22	1.46	0.97
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.07	0.97
3:A:62:LEU:HD12	3:A:63:PRO:HD2	1.46	0.97
3:A:285:HIS:CE1	3:A:289:LYS:HE3	2.00	0.96
3:A:245:ASN:N	3:A:245:ASN:HD22	1.57	0.95
3:A:201:THR:HA	3:A:261:PRO:HB2	1.50	0.94
3:A:245:ASN:H	3:A:245:ASN:HD22	1.12	0.93
2:P:2:DA:C8	2:P:2:DA:H5'	2.05	0.92
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.02	0.88
3:A:16:THR:HG23	3:A:46:ILE:HG12	1.55	0.86
3:A:201:THR:HA	3:A:261:PRO:CB	2.04	0.86
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.57	0.85
3:A:101:THR:HA	3:A:106:ILE:HG22	1.59	0.85
3:A:157:GLN:HE22	3:A:244:LYS:NZ	1.77	0.83
3:A:150:ILE:HB	3:A:155:MET:HE3	1.59	0.82
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.60	0.82
3:A:12:ASN:HB3	3:A:46:ILE:CD1	2.10	0.82
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.77	0.80
3:A:197:HIS:CE1	3:A:198:PRO:HD2	2.17	0.80
3:A:16:THR:HG23	3:A:46:ILE:CG1	2.11	0.80
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.17	0.80
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.29	0.80
3:A:68:LYS:HB2	3:A:68:LYS:NZ	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:245:ASN:N	3:A:245:ASN:ND2	2.31	0.79
3:A:157:GLN:HE22	3:A:244:LYS:HZ1	1.28	0.79
3:A:18:MET:HG2	3:A:19:LEU:N	1.96	0.78
3:A:157:GLN:NE2	3:A:244:LYS:NZ	2.31	0.78
3:A:294:ASN:HB2	3:A:295:GLU:OE2	1.83	0.77
3:A:278:PHE:HB2	3:A:333:ARG:O	1.83	0.77
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.12	0.77
3:A:41:LYS:HE2	3:A:64:GLY:HA2	1.66	0.77
3:A:202:SER:HB2	3:A:263:ASP:CG	2.04	0.77
3:A:111:ALA:O	3:A:115:VAL:HG23	1.84	0.77
3:A:128:ASN:HB3	3:A:131:LYS:HD2	1.65	0.77
3:A:293:ILE:HD13	3:A:298:ILE:CG1	2.13	0.76
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.20	0.76
3:A:49:TYR:CE2	3:A:53:ILE:HG13	2.20	0.76
3:A:15:ILE:O	3:A:19:LEU:HD22	1.86	0.76
3:A:15:ILE:CG2	3:A:46:ILE:HD13	2.16	0.76
3:A:218:LEU:HB2	3:A:224:ILE:HD12	1.67	0.76
3:A:298:ILE:O	3:A:311:LEU:HB2	1.86	0.75
3:A:197:HIS:ND1	3:A:198:PRO:HD2	2.00	0.75
3:A:218:LEU:CB	3:A:224:ILE:HD12	2.16	0.75
3:A:244:LYS:HB2	3:A:245:ASN:HD22	1.51	0.75
3:A:44:SER:O	3:A:47:ALA:HB3	1.87	0.75
2:P:3:DG:H1'	5:P:511:HOH:O	1.86	0.75
3:A:260:ILE:HG22	3:A:261:PRO:HD2	1.69	0.74
3:A:150:ILE:HG21	3:A:158:MET:CE	2.17	0.74
3:A:197:HIS:HE1	3:A:199:SER:HB2	1.52	0.74
3:A:38:ALA:O	3:A:41:LYS:HD3	1.88	0.74
3:A:271:TYR:HB2	5:A:592:HOH:O	1.88	0.74
3:A:157:GLN:NE2	3:A:244:LYS:HZ1	1.86	0.73
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.68	0.73
3:A:41:LYS:O	3:A:45:VAL:HG13	1.88	0.73
3:A:68:LYS:O	3:A:72:LYS:HE3	1.89	0.73
3:A:182:ARG:HG2	3:A:273:THR:CG2	2.19	0.73
3:A:328:ARG:HB3	3:A:332:ASP:OD1	1.89	0.72
3:A:18:MET:O	3:A:22:LEU:HD22	1.90	0.72
3:A:289:LYS:HD2	3:A:324:GLN:OE1	1.89	0.72
3:A:59:ALA:O	3:A:62:LEU:HB2	1.90	0.72
3:A:15:ILE:HG21	3:A:46:ILE:HD13	1.71	0.71
3:A:182:ARG:HG2	3:A:273:THR:HG23	1.71	0.70
3:A:162:VAL:O	3:A:166:VAL:HG23	1.90	0.70
3:A:99:PHE:HD2	3:A:100:LEU:HD12	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:285:HIS:HE1	3:A:289:LYS:HE3	1.56	0.70
3:A:119:ILE:HG21	3:A:125:LEU:HD23	1.73	0.69
3:A:89:ARG:HB2	5:A:645:HOH:O	1.92	0.69
3:A:26:GLU:OE1	3:A:32:ALA:HB3	1.91	0.69
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.73	0.69
2:P:5:DT:OP2	3:A:109:SER:HB3	1.90	0.69
3:A:244:LYS:HB2	3:A:245:ASN:ND2	2.08	0.69
1:T:6:DT:H5"	5:T:547:HOH:O	1.92	0.68
2:P:5:DT:H2"	2:P:6:DG:H5'	1.75	0.68
3:A:114:PHE:HD1	3:A:119:ILE:HD12	1.57	0.68
3:A:31:GLN:N	5:A:641:HOH:O	2.27	0.68
3:A:81:LYS:HZ3	3:A:86:GLU:HB3	1.58	0.67
3:A:295:GLU:HA	5:A:592:HOH:O	1.93	0.67
3:A:291:PHE:CD1	3:A:300:PRO:HA	2.30	0.67
3:A:114:PHE:CD1	3:A:119:ILE:HD12	2.30	0.67
3:A:241:LEU:HB2	3:A:250:TYR:CD2	2.30	0.67
5:P:568:HOH:O	3:A:110:ALA:HB2	1.95	0.66
3:A:119:ILE:HG22	3:A:124:ASP:HB3	1.76	0.66
3:A:251:PRO:HG2	3:A:253:ARG:NH2	2.11	0.66
2:P:2:DA:N7	5:P:598:HOH:O	2.29	0.66
3:A:292:THR:O	3:A:298:ILE:HA	1.95	0.66
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.25	0.65
2:P:3:DG:N3	5:P:511:HOH:O	2.29	0.65
3:A:43:ALA:O	3:A:47:ALA:HB2	1.96	0.65
3:A:92:ASP:O	3:A:95:SER:HB2	1.96	0.65
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.29	0.65
3:A:266:TYR:N	5:A:508:HOH:O	2.29	0.65
3:A:285:HIS:O	3:A:288:GLU:N	2.30	0.64
3:A:52:LYS:HE2	5:A:554:HOH:O	1.96	0.64
3:A:157:GLN:O	3:A:160:ASP:HB3	1.98	0.64
3:A:11:LEU:CD2	3:A:11:LEU:H	2.11	0.64
3:A:120:LYS:N	3:A:124:ASP:OD2	2.29	0.63
3:A:279:ASN:O	3:A:283:ARG:N	2.29	0.63
3:A:278:PHE:HZ	3:A:320:PHE:CZ	2.15	0.63
3:A:81:LYS:NZ	3:A:86:GLU:HB3	2.13	0.63
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.39	0.63
3:A:12:ASN:HA	5:A:642:HOH:O	1.97	0.63
3:A:319:ILE:O	3:A:322:TYR:HB2	1.99	0.63
3:A:35:LYS:O	3:A:38:ALA:HB3	1.99	0.63
3:A:250:TYR:HB3	5:A:577:HOH:O	1.98	0.62
3:A:165:GLU:HA	3:A:168:LYS:HG3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:180:SER:HB2	3:A:185:ALA:HB2	1.82	0.62
3:A:11:LEU:HD23	3:A:12:ASN:H	1.65	0.62
2:P:5:DT:P	3:A:109:SER:HB3	2.39	0.62
3:A:259:LEU:O	3:A:260:ILE:HD13	1.98	0.62
3:A:33:ILE:HG21	5:A:616:HOH:O	2.00	0.61
3:A:100:LEU:HD11	3:A:120:LYS:O	1.99	0.61
3:A:100:LEU:O	3:A:106:ILE:HG21	2.01	0.61
3:A:243:SER:OG	3:A:249:GLU:HA	2.00	0.61
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.82	0.61
3:A:158:MET:O	3:A:162:VAL:HG23	1.99	0.60
3:A:183:ARG:HH11	3:A:275:SER:HA	1.66	0.60
3:A:280:LYS:O	3:A:284:ALA:N	2.32	0.60
3:A:212:HIS:HB3	5:A:541:HOH:O	2.01	0.60
3:A:282:MET:HG3	3:A:323:ILE:CD1	2.32	0.60
3:A:217:GLN:HE22	3:A:220:LYS:HD3	1.66	0.60
3:A:42:ALA:O	3:A:45:VAL:N	2.32	0.60
3:A:11:LEU:HD23	3:A:11:LEU:H	1.67	0.60
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.32	0.60
3:A:255:ILE:HG12	3:A:256:ASP:N	2.15	0.60
3:A:60:LYS:HE2	3:A:67:THR:CA	2.32	0.60
1:T:2:DC:H2"	1:T:3:DA:C8	2.37	0.60
3:A:197:HIS:CE1	3:A:199:SER:HB2	2.37	0.60
3:A:182:ARG:NH2	3:A:316:GLU:OE1	2.34	0.60
3:A:266:TYR:HA	3:A:269:VAL:HB	1.84	0.60
2:P:1:DC:H2"	2:P:2:DA:H5"	1.84	0.59
3:A:331:LYS:HD2	3:A:332:ASP:N	2.17	0.59
3:A:234:LYS:HB2	5:A:538:HOH:O	2.02	0.59
3:A:126:ARG:O	3:A:129:GLU:HB2	2.02	0.59
3:A:228:LEU:HB2	3:A:236:MET:O	2.02	0.59
3:A:16:THR:CG2	3:A:46:ILE:HG12	2.31	0.58
3:A:301:LEU:HD11	3:A:306:VAL:CA	2.27	0.58
3:A:293:ILE:HG23	3:A:298:ILE:HB	1.85	0.58
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.25	0.58
3:A:253:ARG:NH2	5:A:620:HOH:O	2.36	0.58
2:P:2:DA:H8	2:P:2:DA:H5'	1.66	0.58
3:A:23:ALA:O	3:A:36:TYR:HD2	1.87	0.58
3:A:202:SER:HB2	3:A:263:ASP:OD2	2.03	0.58
3:A:99:PHE:HD2	3:A:100:LEU:CD1	2.16	0.58
3:A:183:ARG:NH1	3:A:275:SER:HA	2.19	0.58
3:A:159:GLN:O	3:A:163:LEU:HG	2.03	0.58
3:A:103:VAL:HG22	3:A:143:PHE:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:282:MET:HE3	3:A:323:ILE:HD11	1.86	0.58
3:A:18:MET:HE1	3:A:82:LEU:HD13	1.84	0.57
3:A:200:PHE:O	3:A:262:LYS:N	2.30	0.57
3:A:132:LEU:HD23	3:A:132:LEU:N	2.18	0.57
3:A:133:ASN:O	3:A:137:ARG:HG3	2.04	0.57
3:A:233:THR:HG22	3:A:259:LEU:HB3	1.86	0.57
2:P:4:DA:H2'	2:P:5:DT:H71	1.84	0.57
3:A:326:LYS:HG3	3:A:326:LYS:O	2.04	0.57
3:A:254:ARG:HH11	3:A:255:ILE:N	2.02	0.57
3:A:327:TYR:HD1	3:A:328:ARG:N	2.02	0.57
3:A:60:LYS:HE2	3:A:67:THR:N	2.20	0.57
3:A:182:ARG:HH22	3:A:316:GLU:CD	2.08	0.57
3:A:215:VAL:O	3:A:219:GLN:HG3	2.05	0.57
3:A:18:MET:HG3	3:A:22:LEU:CD2	2.35	0.56
3:A:294:ASN:HD22	3:A:294:ASN:H	1.53	0.56
3:A:86:GLU:O	3:A:90:GLN:HG3	2.05	0.56
3:A:106:ILE:HD11	3:A:125:LEU:HD11	1.86	0.56
3:A:172:GLU:HB3	3:A:198:PRO:CD	2.34	0.56
3:A:295:GLU:H	3:A:295:GLU:CD	2.09	0.56
3:A:150:ILE:N	3:A:188:SER:O	2.29	0.56
3:A:68:LYS:O	3:A:71:GLU:HB3	2.05	0.56
3:A:79:THR:O	3:A:81:LYS:N	2.29	0.56
3:A:81:LYS:NZ	3:A:86:GLU:OE1	2.34	0.56
3:A:254:ARG:NH2	3:A:256:ASP:OD1	2.36	0.56
1:T:3:DA:H1'	5:T:617:HOH:O	2.04	0.55
3:A:212:HIS:CE1	3:A:230:LYS:HD2	2.41	0.55
3:A:218:LEU:HB3	3:A:224:ILE:HD12	1.88	0.55
2:P:5:DT:OP2	3:A:108:PRO:HD2	2.07	0.55
3:A:29:VAL:HG21	3:A:94:SER:OG	2.07	0.55
3:A:248:LYS:HG2	3:A:248:LYS:O	2.06	0.55
3:A:154:GLU:O	3:A:158:MET:HG2	2.07	0.55
3:A:44:SER:HB2	5:A:608:HOH:O	2.06	0.55
2:P:5:DT:H2''	2:P:6:DG:C5'	2.35	0.55
3:A:152:ARG:CA	3:A:155:MET:HB2	2.37	0.55
2:P:4:DA:H5''	3:A:109:SER:OG	2.06	0.55
3:A:157:GLN:NE2	3:A:244:LYS:HZ3	2.04	0.54
3:A:63:PRO:C	3:A:65:VAL:H	2.09	0.54
3:A:150:ILE:HG12	3:A:253:ARG:HG2	1.89	0.54
3:A:129:GLU:O	3:A:129:GLU:HG2	2.08	0.54
3:A:33:ILE:O	3:A:37:ASN:HB2	2.07	0.54
3:A:134:HIS:CE1	3:A:138:ILE:HD11	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:254:ARG:NH1	3:A:255:ILE:N	2.56	0.54
3:A:132:LEU:HB3	3:A:136:GLN:HB3	1.90	0.53
3:A:201:THR:HG23	3:A:204:SER:HB3	1.90	0.53
3:A:270:LEU:HD23	3:A:319:ILE:HD13	1.89	0.53
3:A:150:ILE:HB	3:A:155:MET:CE	2.33	0.53
3:A:331:LYS:C	3:A:331:LYS:HD2	2.29	0.53
3:A:68:LYS:HB2	3:A:68:LYS:HZ1	1.70	0.53
2:P:5:DT:P	3:A:107:GLY:HA3	2.48	0.53
3:A:108:PRO:O	3:A:112:ARG:HG2	2.08	0.53
3:A:103:VAL:HG12	3:A:104:SER:N	2.24	0.53
3:A:65:VAL:HG13	3:A:69:ILE:HG21	1.90	0.53
3:A:197:HIS:CE1	3:A:199:SER:H	2.27	0.53
2:P:1:DC:H2''	2:P:2:DA:C5'	2.39	0.52
3:A:101:THR:HA	3:A:106:ILE:CG2	2.37	0.52
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.44	0.52
3:A:309:GLU:HA	3:A:309:GLU:OE1	2.10	0.52
3:A:115:VAL:O	3:A:118:GLY:N	2.41	0.52
3:A:36:TYR:CD1	3:A:37:ASN:N	2.78	0.52
3:A:278:PHE:HZ	3:A:320:PHE:CE1	2.27	0.52
3:A:282:MET:CE	3:A:323:ILE:HD11	2.40	0.52
3:A:294:ASN:HD22	3:A:294:ASN:N	2.05	0.52
3:A:76:PHE:O	3:A:79:THR:O	2.28	0.52
3:A:177:VAL:HG12	3:A:177:VAL:O	2.09	0.52
3:A:173:TYR:OH	3:A:213:GLN:NE2	2.43	0.52
3:A:19:LEU:HD23	3:A:43:ALA:HB2	1.93	0.51
3:A:155:MET:CE	3:A:188:SER:HB2	2.40	0.51
3:A:262:LYS:HG3	3:A:262:LYS:O	2.10	0.51
3:A:241:LEU:HB2	3:A:250:TYR:CG	2.46	0.51
3:A:189:GLY:HA2	5:A:523:HOH:O	2.11	0.51
3:A:55:SER:O	3:A:58:GLU:HB3	2.10	0.51
3:A:60:LYS:HE2	3:A:67:THR:HA	1.93	0.51
3:A:298:ILE:O	3:A:298:ILE:HG23	2.11	0.51
3:A:300:PRO:HD3	3:A:311:LEU:HD13	1.93	0.51
3:A:182:ARG:HG2	3:A:273:THR:HG21	1.92	0.51
3:A:282:MET:HG3	3:A:323:ILE:HD11	1.93	0.51
3:A:22:LEU:HB3	3:A:39:TYR:CE2	2.46	0.51
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.41	0.50
3:A:316:GLU:CD	3:A:333:ARG:HH12	2.14	0.50
3:A:283:ARG:NH2	3:A:294:ASN:HA	2.26	0.50
3:A:327:TYR:CD1	3:A:328:ARG:N	2.79	0.50
3:A:206:LYS:O	3:A:207:GLN:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:172:GLU:HB3	3:A:198:PRO:HD3	1.94	0.50
3:A:196:THR:OG1	3:A:197:HIS:N	2.44	0.50
1:T:3:DA:C2	2:P:5:DT:N3	2.79	0.50
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.93	0.49
3:A:201:THR:HA	3:A:261:PRO:HB3	1.90	0.49
3:A:241:LEU:O	3:A:250:TYR:HD2	1.96	0.49
3:A:205:THR:O	3:A:206:LYS:O	2.30	0.49
3:A:65:VAL:HG13	3:A:69:ILE:CG2	2.42	0.49
3:A:106:ILE:HG22	3:A:106:ILE:O	2.10	0.49
3:A:282:MET:CE	3:A:319:ILE:HG22	2.42	0.49
3:A:237:GLY:O	3:A:254:ARG:NH1	2.46	0.49
3:A:265:TYR:O	3:A:269:VAL:N	2.35	0.49
3:A:297:THR:HG22	5:A:626:HOH:O	2.12	0.49
3:A:73:ILE:CG2	3:A:77:LEU:HD13	2.42	0.49
3:A:149:ARG:NH2	3:A:187:SER:O	2.36	0.49
3:A:261:PRO:HG2	3:A:264:GLN:HG3	1.95	0.49
3:A:26:GLU:HG3	3:A:35:LYS:HB3	1.93	0.49
3:A:170:ASP:OD1	3:A:171:SER:N	2.46	0.49
3:A:114:PHE:HD1	3:A:119:ILE:CD1	2.26	0.48
3:A:235:PHE:HZ	3:A:237:GLY:HA3	1.70	0.48
3:A:173:TYR:CE1	3:A:197:HIS:CD2	3.01	0.48
3:A:209:LYS:O	3:A:213:GLN:HG3	2.13	0.48
3:A:123:GLU:HG3	5:A:623:HOH:O	2.12	0.48
3:A:326:LYS:HD2	5:A:657:HOH:O	2.12	0.48
3:A:12:ASN:HB3	3:A:46:ILE:HD11	1.90	0.48
3:A:299:ARG:HB3	3:A:300:PRO:HD2	1.95	0.48
3:A:201:THR:CG2	3:A:204:SER:HB3	2.43	0.48
3:A:142:TYR:O	3:A:146:PHE:HB2	2.13	0.48
3:A:12:ASN:O	3:A:46:ILE:HD11	2.14	0.48
3:A:333:ARG:HD3	5:A:584:HOH:O	2.13	0.48
3:A:108:PRO:HA	3:A:111:ALA:HB3	1.96	0.48
3:A:31:GLN:O	3:A:33:ILE:N	2.48	0.47
3:A:177:VAL:CG2	3:A:193:VAL:HG22	2.33	0.47
3:A:285:HIS:CD2	3:A:325:TRP:CD1	3.02	0.47
3:A:270:LEU:HA	3:A:316:GLU:OE2	2.15	0.47
3:A:60:LYS:CE	3:A:67:THR:HB	2.43	0.47
3:A:267:CYS:HB2	3:A:295:GLU:O	2.14	0.47
3:A:288:GLU:O	3:A:290:GLY:N	2.47	0.47
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.97	0.47
3:A:288:GLU:HA	3:A:288:GLU:OE1	2.04	0.47
3:A:55:SER:OG	3:A:58:GLU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:6:DG:OP1	3:A:105:GLY:N	2.47	0.47
3:A:291:PHE:HD1	3:A:300:PRO:HA	1.75	0.47
3:A:261:PRO:HG2	3:A:264:GLN:CG	2.45	0.47
3:A:19:LEU:CB	3:A:43:ALA:HB2	2.45	0.47
3:A:173:TYR:CD1	3:A:197:HIS:HB2	2.50	0.47
3:A:115:VAL:C	3:A:118:GLY:H	2.18	0.47
3:A:16:THR:O	3:A:20:THR:HG23	2.15	0.47
1:T:3:DA:H2	2:P:5:DT:O2	1.98	0.46
2:P:1:DC:H2'	2:P:2:DA:C8	2.50	0.46
3:A:103:VAL:HG22	3:A:143:PHE:CD1	2.50	0.46
1:T:6:DT:H2''	1:T:7:DG:C8	2.50	0.46
3:A:152:ARG:O	3:A:156:LEU:HD12	2.15	0.46
3:A:58:GLU:O	3:A:61:LYS:HG3	2.15	0.46
3:A:145:ASP:CG	3:A:252:HIS:H	2.19	0.46
3:A:80:GLY:O	3:A:81:LYS:HG2	2.15	0.46
3:A:315:SER:OG	3:A:316:GLU:N	2.49	0.46
3:A:32:ALA:HB1	3:A:35:LYS:HB2	1.98	0.46
3:A:67:THR:O	3:A:70:ALA:HB3	2.16	0.46
3:A:212:HIS:ND1	3:A:230:LYS:HD3	2.31	0.45
3:A:100:LEU:CD1	3:A:100:LEU:N	2.79	0.45
3:A:114:PHE:CD1	3:A:119:ILE:CD1	2.99	0.45
3:A:194:LEU:HA	3:A:194:LEU:HD12	1.44	0.45
1:T:4:DT:H5'	5:T:617:HOH:O	2.16	0.45
3:A:172:GLU:HG2	3:A:198:PRO:HG3	1.98	0.45
3:A:303:VAL:O	3:A:305:GLY:N	2.49	0.45
3:A:212:HIS:CE1	3:A:230:LYS:CD	2.98	0.45
3:A:208:PRO:HB3	3:A:232:GLU:HB2	1.98	0.45
3:A:259:LEU:HA	3:A:259:LEU:HD12	1.34	0.45
3:A:49:TYR:HE2	3:A:53:ILE:HG13	1.74	0.45
3:A:264:GLN:HB3	3:A:296:TYR:O	2.17	0.45
3:A:183:ARG:NH1	3:A:275:SER:CB	2.79	0.45
3:A:211:LEU:HB2	3:A:259:LEU:HD22	1.98	0.45
3:A:132:LEU:N	3:A:132:LEU:CD2	2.79	0.45
3:A:49:TYR:CD2	3:A:53:ILE:HG13	2.52	0.45
3:A:68:LYS:HB2	3:A:68:LYS:HZ2	1.80	0.45
3:A:274:GLY:HA3	3:A:275:SER:HA	1.78	0.45
3:A:18:MET:HG3	3:A:22:LEU:HD21	1.99	0.44
3:A:73:ILE:HG22	3:A:77:LEU:HD13	1.99	0.44
3:A:258:ARG:HG2	3:A:260:ILE:HD11	1.99	0.44
3:A:155:MET:HE1	3:A:188:SER:HB2	1.99	0.44
3:A:84:LYS:HD2	5:A:524:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:37:ASN:HA	3:A:37:ASN:HD22	1.44	0.44
3:A:166:VAL:HG12	3:A:173:TYR:HB2	1.98	0.44
3:A:182:ARG:CG	3:A:273:THR:HG23	2.43	0.44
3:A:132:LEU:HA	3:A:136:GLN:HE21	1.82	0.44
3:A:49:TYR:CE2	3:A:53:ILE:CG1	2.98	0.44
3:A:165:GLU:OE2	3:A:168:LYS:HD3	2.18	0.44
3:A:303:VAL:C	3:A:305:GLY:H	2.21	0.44
3:A:81:LYS:NZ	3:A:86:GLU:CB	2.81	0.44
3:A:201:THR:OG1	3:A:202:SER:N	2.51	0.44
3:A:278:PHE:CZ	3:A:320:PHE:HZ	2.36	0.44
3:A:206:LYS:HE3	3:A:232:GLU:OE2	2.18	0.44
3:A:181:PHE:HA	5:A:530:HOH:O	2.17	0.44
3:A:224:ILE:HA	3:A:238:VAL:O	2.18	0.44
3:A:60:LYS:HE3	3:A:67:THR:HB	1.99	0.44
3:A:115:VAL:O	3:A:115:VAL:HG12	2.17	0.44
3:A:198:PRO:C	3:A:200:PHE:H	2.20	0.44
3:A:25:PHE:CE2	3:A:88:ILE:HG12	2.53	0.44
3:A:11:LEU:HD23	3:A:12:ASN:N	2.32	0.43
3:A:27:LYS:HB3	3:A:36:TYR:CD2	2.53	0.43
3:A:301:LEU:HD12	3:A:302:GLY:N	2.33	0.43
3:A:183:ARG:HD3	3:A:273:THR:O	2.18	0.43
3:A:228:LEU:HD23	3:A:228:LEU:HA	1.26	0.43
3:A:82:LEU:HA	3:A:82:LEU:HD12	1.80	0.43
3:A:244:LYS:CB	3:A:245:ASN:ND2	2.78	0.43
3:A:243:SER:OG	3:A:249:GLU:HG3	2.19	0.43
3:A:99:PHE:CD2	3:A:100:LEU:HD12	2.44	0.43
3:A:233:THR:HB	5:A:538:HOH:O	2.19	0.43
3:A:49:TYR:HA	3:A:50:PRO:HD2	1.39	0.43
3:A:261:PRO:HB2	3:A:263:ASP:OD1	2.18	0.43
3:A:207:GLN:O	3:A:210:LEU:HB2	2.19	0.43
3:A:317:LYS:HG3	5:A:501:HOH:O	2.18	0.43
3:A:241:LEU:HA	3:A:242:PRO:HD3	1.86	0.43
3:A:301:LEU:CD1	3:A:306:VAL:HA	2.30	0.42
3:A:238:VAL:HA	3:A:253:ARG:O	2.19	0.42
3:A:271:TYR:CE1	3:A:283:ARG:NH2	2.88	0.42
3:A:11:LEU:N	3:A:11:LEU:CD2	2.78	0.42
3:A:311:LEU:HA	3:A:312:PRO:HD3	1.74	0.42
3:A:285:HIS:O	3:A:288:GLU:HB2	2.18	0.42
3:A:103:VAL:CG1	3:A:104:SER:N	2.83	0.42
3:A:206:LYS:HA	3:A:206:LYS:HD3	1.81	0.42
3:A:121:THR:H	3:A:121:THR:HG23	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:306:VAL:O	3:A:307:ALA:HB2	2.19	0.42
3:A:166:VAL:HG12	3:A:173:TYR:CB	2.49	0.42
3:A:216:GLU:O	3:A:220:LYS:N	2.52	0.42
3:A:102:ARG:HH11	3:A:102:ARG:HD3	1.58	0.42
3:A:244:LYS:HG2	3:A:244:LYS:H	1.69	0.42
3:A:278:PHE:CZ	3:A:320:PHE:CZ	3.02	0.42
3:A:183:ARG:NH1	3:A:275:SER:HB3	2.35	0.42
3:A:210:LEU:HA	3:A:210:LEU:HD23	1.38	0.42
3:A:145:ASP:HB3	3:A:252:HIS:H	1.85	0.42
3:A:16:THR:HG22	3:A:43:ALA:O	2.19	0.41
3:A:18:MET:CE	3:A:76:PHE:HB2	2.51	0.41
3:A:241:LEU:CB	3:A:250:TYR:CD2	3.01	0.41
3:A:12:ASN:HD21	3:A:53:ILE:H	1.68	0.41
3:A:16:THR:HG22	3:A:43:ALA:HA	2.03	0.41
3:A:131:LYS:HG3	3:A:131:LYS:H	1.48	0.41
3:A:327:TYR:CD1	3:A:327:TYR:C	2.94	0.41
3:A:132:LEU:HA	3:A:136:GLN:NE2	2.35	0.41
3:A:112:ARG:HG2	3:A:112:ARG:H	1.55	0.41
3:A:22:LEU:HD13	3:A:85:LEU:HD12	2.03	0.41
3:A:125:LEU:HD23	3:A:125:LEU:HA	1.62	0.41
3:A:197:HIS:ND1	3:A:198:PRO:CD	2.79	0.41
3:A:174:ILE:HD13	3:A:174:ILE:HG21	1.79	0.41
2:P:5:DT:O5'	3:A:107:GLY:HA3	2.21	0.41
3:A:56:GLY:O	3:A:59:ALA:HB3	2.21	0.41
3:A:150:ILE:CG1	3:A:253:ARG:HG2	2.51	0.41
3:A:145:ASP:CB	3:A:252:HIS:H	2.34	0.40
3:A:62:LEU:CD1	3:A:63:PRO:HD2	2.33	0.40
3:A:215:VAL:HG12	3:A:215:VAL:O	2.21	0.40
3:A:100:LEU:C	3:A:106:ILE:HG21	2.42	0.40
3:A:330:PRO:HA	3:A:333:ARG:HD2	2.02	0.40
3:A:172:GLU:CG	3:A:198:PRO:HG3	2.51	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]	2.07	0.13

## 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%)	253 (78%)	53 (16%)	19 (6%)	2	12

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	32	ALA
3	A	185	ALA
3	A	202	SER
3	A	205	THR
3	A	206	LYS
3	A	244	LYS
3	A	247	GLU
3	A	309	GLU
3	A	13	GLY
3	A	204	SER
3	A	289	LYS
3	A	304	THR
3	A	80	GLY
3	A	246	ASP
3	A	30	SER
3	A	178	CYS
3	A	220	LYS
3	A	295	GLU
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%)	<b>2</b> <b>8</b>

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

Mol	Chain	Res	Type
3	A	11	LEU
3	A	16	THR
3	A	18	MET
3	A	19	LEU
3	A	22	LEU
3	A	30	SER
3	A	33	ILE
3	A	37	ASN
3	A	41	LYS
3	A	45	VAL
3	A	46	ILE
3	A	62	LEU
3	A	67	THR
3	A	79	THR
3	A	81	LYS
3	A	85	LEU
3	A	112	ARG
3	A	125	LEU
3	A	131	LYS
3	A	132	LEU
3	A	135	HIS
3	A	153	GLU
3	A	158	MET
3	A	168	LYS
3	A	171	SER
3	A	190	ASP
3	A	194	LEU
3	A	199	SER
3	A	205	THR
3	A	207	GLN
3	A	214	VAL
3	A	218	LEU
3	A	219	GLN
3	A	221	VAL
3	A	226	ASP
3	A	233	THR
3	A	235	PHE
3	A	245	ASN

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Mol	Chain	Res	Type
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE
3	A	258	ARG
3	A	264	GLN
3	A	270	LEU
3	A	277	ILE
3	A	287	LEU
3	A	288	GLU
3	A	293	ILE
3	A	294	ASN
3	A	298	ILE
3	A	301	LEU
3	A	311	LEU
3	A	325	TRP
3	A	331	LYS
3	A	335	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	28	ASN
3	A	31	GLN
3	A	37	ASN
3	A	90	GLN
3	A	136	GLN
3	A	157	GLN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	222	HIS
3	A	245	ASN
3	A	294	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	T	7/7 (100%)	-0.82	0 100 100	16, 23, 54, 98	0
2	P	6/6 (100%)	-1.11	0 100 100	12, 20, 30, 31	0
3	A	324/335 (96%)	-0.81	0 100 100	3, 32, 83, 100	0
All	All	337/348 (96%)	-0.82	0 100 100	3, 32, 84, 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NA	A	342	1/1	0.69	0.20	1.92	34,34,34,34	0
4	NA	A	341	1/1	0.94	0.15	0.65	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.