



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:38 am GMT

PDB ID : 9ICG
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SEVEN BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF DCTP (1 MILLIMOLAR) AND ZNCL2 (1 MILLIMOLAR)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1995-12-15
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

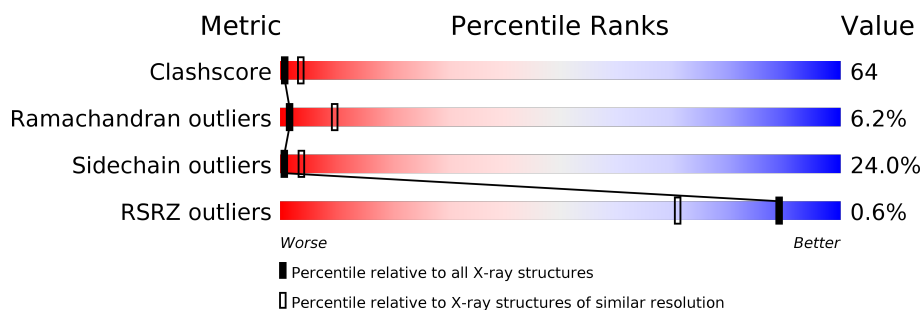
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	8	<div> <div>13%</div> <div>13% 38% 50%</div> </div>
2	P	7	<div> <div>29% 71%</div> </div>
3	A	335	<div> <div>20% 47% 27% . .</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3071 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	8	Total	C	N	O	P	0	0	0
			145	69	27	42	7			

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*CP*TP*AP*AP*TP*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	9	0	0
			2623	1657	458	499	9			

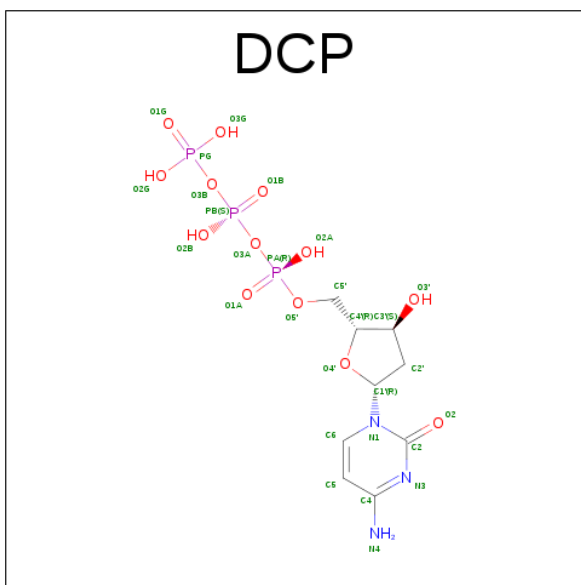
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Zn	0	0
			3	3		

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

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

- Molecule 6 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



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

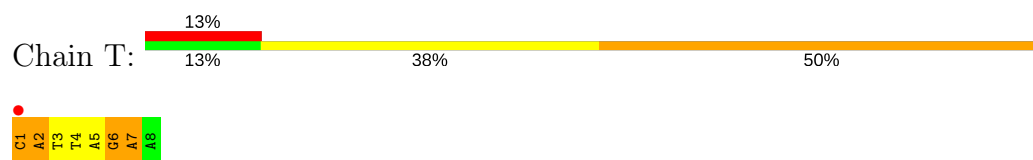
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	102	Total O 102 102	0	0
7	P	17	Total O 17 17	0	0
7	T	15	Total O 15 15	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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

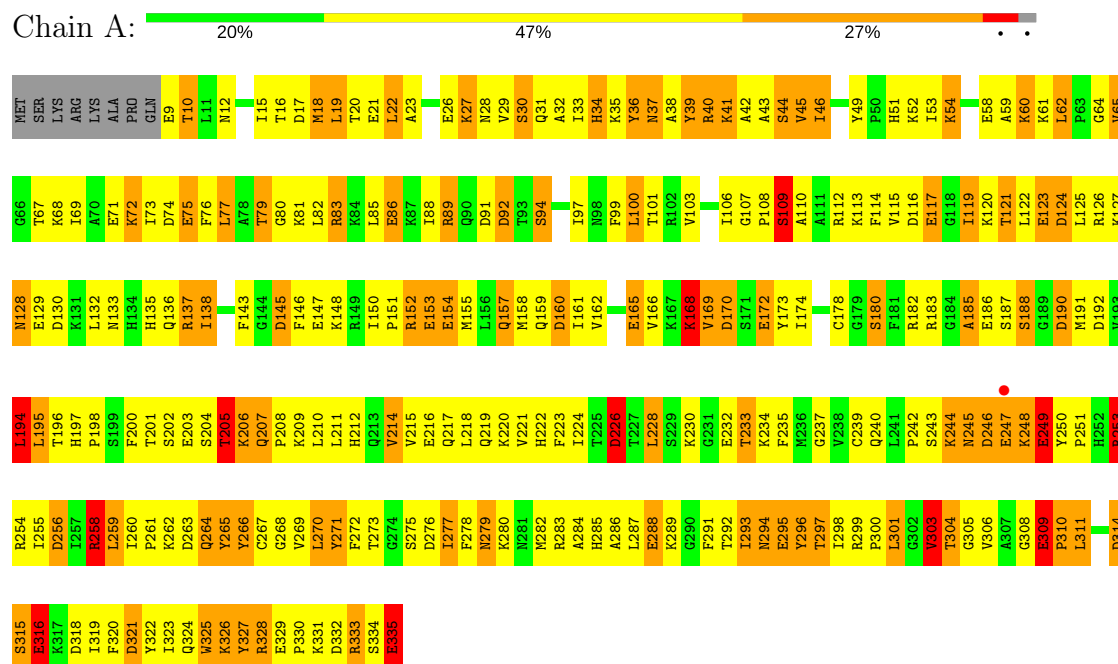
- Molecule 1: DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3')



- Molecule 2: DNA (5'-D(*TP*CP*TP*AP*AP*TP*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 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	179.89Å 57.60Å 48.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 11.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	87.0 (20.00-3.00) 81.5 (11.87-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	5.80	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.70Å)	Xtriage
Refinement program	TNT V. 5-D	Depositor
R, R_{free}	0.161 , (Not available) 0.155 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 110.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3071	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	2.70	11/162 (6.8%)	3.32	28/249 (11.2%)
2	P	2.91	12/160 (7.5%)	5.23	29/243 (11.9%)
3	A	1.30	30/2672 (1.1%)	1.79	63/3590 (1.8%)
All	All	1.53	53/2994 (1.8%)	2.26	120/4082 (2.9%)

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	5	DA	N7-C5	-10.22	1.33	1.39
2	P	3	DT	N1-C2	9.97	1.46	1.38
2	P	3	DT	C1'-N1	9.86	1.62	1.49
2	P	2	DC	C1'-N1	9.52	1.61	1.49
2	P	7	DG	P-O5'	9.15	1.69	1.59
1	T	1	DC	C3'-O3'	8.93	1.55	1.44
3	A	75	GLU	CD-OE1	8.07	1.34	1.25
3	A	247	GLU	CD-OE1	7.92	1.34	1.25
1	T	5	DA	C6-N1	7.60	1.40	1.35
3	A	58	GLU	CD-OE1	7.59	1.33	1.25
1	T	5	DA	N9-C4	-7.55	1.33	1.37
2	P	3	DT	N3-C4	-7.38	1.32	1.38
2	P	7	DG	C5'-C4'	7.10	1.59	1.51
3	A	249	GLU	CD-OE2	7.04	1.33	1.25
2	P	2	DC	N1-C2	7.00	1.47	1.40
3	A	329	GLU	CD-OE2	6.93	1.33	1.25
3	A	71	GLU	CD-OE1	6.83	1.33	1.25
3	A	309	GLU	CD-OE1	6.61	1.32	1.25
2	P	7	DG	O5'-C5'	6.60	1.58	1.42
3	A	316	GLU	CD-OE2	6.47	1.32	1.25
3	A	295	GLU	CD-OE2	6.47	1.32	1.25
2	P	2	DC	C4-C5	6.39	1.48	1.43
1	T	3	DT	C5-C6	6.38	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	6	DT	C3'-O3'	-6.38	1.35	1.44
3	A	153	GLU	CD-OE2	6.22	1.32	1.25
3	A	86	GLU	CD-OE1	6.14	1.32	1.25
3	A	117	GLU	CD-OE2	6.10	1.32	1.25
3	A	147	GLU	CD-OE2	6.10	1.32	1.25
3	A	36	TYR	CB-CG	-6.06	1.42	1.51
3	A	165	GLU	CD-OE2	6.05	1.32	1.25
1	T	3	DT	C5-C7	6.01	1.53	1.50
3	A	335	GLU	CD-OE2	5.96	1.32	1.25
1	T	5	DA	C3'-O3'	-5.94	1.36	1.44
1	T	4	DT	C1'-N1	5.94	1.56	1.49
3	A	129	GLU	CD-OE1	5.94	1.32	1.25
2	P	6	DT	C4'-C3'	-5.81	1.46	1.52
3	A	203	GLU	CD-OE1	5.72	1.31	1.25
3	A	288	GLU	CD-OE2	5.71	1.31	1.25
1	T	6	DG	P-O5'	5.65	1.65	1.59
2	P	5	DA	C5-C6	-5.64	1.35	1.41
3	A	232	GLU	CD-OE2	5.56	1.31	1.25
3	A	154	GLU	CD-OE2	5.48	1.31	1.25
3	A	123	GLU	CD-OE1	5.42	1.31	1.25
3	A	172	GLU	CD-OE2	5.41	1.31	1.25
1	T	5	DA	C6-N6	5.38	1.38	1.33
3	A	186	GLU	CD-OE1	5.33	1.31	1.25
3	A	26	GLU	CD-OE1	5.33	1.31	1.25
3	A	326	LYS	CE-NZ	-5.30	1.35	1.49
3	A	9	GLU	CD-OE2	5.25	1.31	1.25
3	A	216	GLU	CD-OE1	5.20	1.31	1.25
3	A	271	TYR	CB-CG	-5.18	1.43	1.51
1	T	3	DT	N1-C2	5.14	1.42	1.38
3	A	39	TYR	CB-CG	-5.11	1.44	1.51

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	1	DT	C6-N1-C1'	-34.29	68.96	120.40
2	P	1	DT	C2-N1-C1'	31.66	168.85	118.20
2	P	7	DG	C8-N9-C1'	25.53	160.19	127.00
2	P	7	DG	C4-N9-C1'	-25.12	93.84	126.50
2	P	6	DT	C6-N1-C1'	-18.61	92.48	120.40
2	P	6	DT	C2-N1-C1'	16.58	144.72	118.20
1	T	4	DT	C6-N1-C1'	-16.50	95.66	120.40
1	T	4	DT	C2-N1-C1'	15.80	143.48	118.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	3	DT	C2-N1-C1'	13.77	140.23	118.20
2	P	2	DC	C2-N1-C1'	13.61	133.77	118.80
2	P	3	DT	O4'-C1'-N1	13.40	117.38	108.00
2	P	3	DT	C6-N1-C1'	-12.77	101.24	120.40
2	P	3	DT	N3-C2-O2	-12.37	114.88	122.30
2	P	1	DT	O4'-C1'-N1	12.18	116.53	108.00
1	T	5	DA	N1-C6-N6	11.91	125.75	118.60
1	T	6	DG	C8-N9-C1'	10.69	140.89	127.00
2	P	2	DC	C6-N1-C1'	-10.68	107.98	120.80
3	A	258	ARG	NE-CZ-NH1	10.47	125.54	120.30
1	T	6	DG	C4-N9-C1'	-10.37	113.02	126.50
1	T	1	DC	P-O3'-C3'	10.18	131.92	119.70
3	A	137	ARG	NE-CZ-NH1	9.82	125.21	120.30
3	A	253	ARG	NE-CZ-NH1	9.49	125.05	120.30
2	P	5	DA	O4'-C1'-N9	-8.63	101.96	108.00
3	A	124	ASP	CB-CG-OD2	-8.62	110.54	118.30
1	T	1	DC	C6-N1-C1'	-8.18	110.99	120.80
3	A	271	TYR	CB-CG-CD1	-8.14	116.12	121.00
1	T	5	DA	C5-N7-C8	-7.91	99.94	103.90
3	A	116	ASP	CB-CG-OD1	-7.90	111.19	118.30
3	A	74	ASP	CB-CG-OD1	7.83	125.35	118.30
3	A	39	TYR	CB-CG-CD1	-7.80	116.32	121.00
2	P	6	DT	P-O5'-C5'	-7.79	108.44	120.90
2	P	2	DC	O4'-C1'-N1	7.77	113.44	108.00
3	A	124	ASP	CB-CG-OD1	7.64	125.18	118.30
3	A	192	ASP	CB-CG-OD2	-7.60	111.46	118.30
3	A	256	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	T	5	DA	C6-C5-N7	-7.55	127.02	132.30
1	T	1	DC	C2-N1-C1'	7.54	127.10	118.80
2	P	3	DT	O4'-C1'-C2'	-7.50	99.90	105.90
3	A	256	ASP	CB-CG-OD1	7.44	125.00	118.30
3	A	20	THR	N-CA-CB	7.44	124.43	110.30
3	A	258	ARG	NE-CZ-NH2	-7.42	116.59	120.30
2	P	1	DT	C1'-O4'-C4'	-7.35	102.75	110.10
3	A	74	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	T	5	DA	C4-C5-N7	7.28	114.34	110.70
3	A	332	ASP	CB-CG-OD1	-7.28	111.75	118.30
3	A	333	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	T	2	DA	O4'-C1'-N9	7.15	113.01	108.00
1	T	7	DA	C4-N9-C1'	-7.12	113.49	126.30
2	P	3	DT	N1-C2-O2	6.91	128.63	123.10
2	P	4	DA	C8-N9-C1'	-6.89	115.30	127.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	3	DT	C6-N1-C2	-6.83	117.89	121.30
3	A	160	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	T	5	DA	C5-C6-N1	-6.71	114.34	117.70
3	A	314	ASP	CB-CG-OD1	-6.67	112.30	118.30
1	T	2	DA	C8-N9-C1'	-6.63	115.76	127.70
2	P	5	DA	P-O5'-C5'	-6.61	110.33	120.90
2	P	2	DC	N3-C2-O2	-6.59	117.29	121.90
3	A	152	ARG	NE-CZ-NH2	-6.55	117.02	120.30
2	P	4	DA	C4-N9-C1'	6.53	138.05	126.30
3	A	246	ASP	CB-CG-OD1	-6.46	112.48	118.30
3	A	190	ASP	CB-CG-OD1	6.44	124.10	118.30
3	A	137	ARG	NE-CZ-NH2	-6.42	117.09	120.30
3	A	326	LYS	CD-CE-NZ	6.36	126.33	111.70
1	T	6	DG	P-O3'-C3'	6.33	127.30	119.70
1	T	4	DT	C6-C5-C7	-6.28	119.14	122.90
1	T	7	DA	C8-N9-C1'	6.27	138.99	127.70
3	A	332	ASP	CB-CG-OD2	6.26	123.94	118.30
3	A	190	ASP	CB-CG-OD2	-6.25	112.68	118.30
3	A	17	ASP	CB-CG-OD1	-6.22	112.70	118.30
3	A	246	ASP	CB-CG-OD2	6.22	123.90	118.30
3	A	22	LEU	CB-CG-CD1	-6.21	100.45	111.00
3	A	222	HIS	CA-CB-CG	-6.12	103.19	113.60
1	T	5	DA	N7-C8-N9	6.08	116.84	113.80
1	T	2	DA	C4-N9-C1'	6.08	137.25	126.30
3	A	263	ASP	CB-CG-OD2	-5.99	112.91	118.30
3	A	271	TYR	CA-CB-CG	-5.99	102.03	113.40
3	A	34	HIS	CA-CB-CG	-5.95	103.49	113.60
3	A	276	ASP	CB-CG-OD2	-5.94	112.95	118.30
3	A	224	ILE	CA-CB-CG1	-5.86	99.86	111.00
3	A	61	LYS	CB-CA-C	-5.83	98.73	110.40
3	A	146	PHE	N-CA-CB	5.81	121.05	110.60
3	A	297	THR	N-CA-CB	-5.80	99.27	110.30
3	A	194	LEU	CB-CG-CD1	-5.79	101.15	111.00
2	P	3	DT	C5-C4-O4	5.79	128.95	124.90
3	A	83	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	T	3	DT	N3-C2-O2	-5.68	118.89	122.30
3	A	195	LEU	CA-CB-CG	-5.60	102.43	115.30
2	P	3	DT	C6-N1-C2	-5.55	118.52	121.30
1	T	4	DT	C4-C5-C7	5.54	122.32	119.00
3	A	145	ASP	CB-CG-OD2	-5.52	113.33	118.30
3	A	60	LYS	CA-CB-CG	-5.51	101.28	113.40
3	A	314	ASP	CB-CG-OD2	5.48	123.23	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	130	ASP	CB-CG-OD1	5.47	123.22	118.30
3	A	321	ASP	CB-CG-OD2	-5.44	113.40	118.30
3	A	168	LYS	N-CA-CB	5.44	120.39	110.60
3	A	165	GLU	CA-CB-CG	-5.43	101.44	113.40
1	T	5	DA	P-O3'-C3'	-5.42	113.20	119.70
1	T	4	DT	N1-C1'-C2'	5.41	122.88	112.60
3	A	170	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	T	6	DG	O4'-C1'-N9	5.31	111.72	108.00
2	P	2	DC	N1-C2-N3	5.30	122.91	119.20
3	A	194	LEU	CA-CB-CG	-5.30	103.11	115.30
3	A	192	ASP	CB-CG-OD1	5.29	123.06	118.30
2	P	6	DT	P-O3'-C3'	-5.24	113.42	119.70
3	A	192	ASP	N-CA-CB	5.21	119.99	110.60
3	A	116	ASP	CB-CG-OD2	5.19	122.97	118.30
3	A	130	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	T	5	DA	C6-N1-C2	5.16	121.69	118.60
2	P	2	DC	C6-N1-C2	-5.15	118.24	120.30
3	A	314	ASP	N-CA-CB	5.13	119.83	110.60
3	A	226	ASP	CB-CG-OD2	-5.12	113.69	118.30
3	A	297	THR	CB-CA-C	-5.10	97.84	111.60
2	P	3	DT	N3-C4-O4	-5.08	116.85	119.90
3	A	39	TYR	CA-CB-CG	-5.07	103.76	113.40
3	A	303	VAL	CB-CA-C	5.07	121.03	111.40
3	A	30	SER	C-N-CA	-5.05	109.07	121.70
1	T	3	DT	N1-C2-N3	5.05	117.63	114.60
3	A	109	SER	CB-CA-C	-5.04	100.53	110.10
3	A	92	ASP	N-CA-CB	5.03	119.66	110.60
3	A	92	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

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	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	144	0	80	17	0
3	A	2623	0	2641	345	0
4	A	3	0	0	0	0
5	A	2	0	0	0	0
6	A	20	0	7	3	0
7	A	102	0	0	23	0
7	P	17	0	0	8	0
7	T	15	0	0	1	0
All	All	3071	0	2808	363	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 64.

All (363) 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:245:ASN:H	3:A:245:ASN:ND2	1.54	1.04
3:A:151:PRO:HG2	3:A:154:GLU:HG3	1.42	1.01
2:P:5:DA:H2''	2:P:6:DT:H5'	1.40	0.99
3:A:245:ASN:N	3:A:245:ASN:HD22	1.61	0.97
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.50	0.90
3:A:60:LYS:HA	3:A:65:VAL:HG23	1.53	0.89
3:A:41:LYS:HD3	3:A:42:ALA:H	1.40	0.86
3:A:52:LYS:HD3	3:A:54:LYS:HE3	1.56	0.86
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.06	0.85
3:A:41:LYS:HD3	3:A:42:ALA:N	1.92	0.84
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.10	0.81
3:A:12:ASN:HB3	3:A:46:ILE:CD1	2.11	0.81
3:A:244:LYS:HB3	3:A:245:ASN:ND2	1.95	0.80
3:A:172:GLU:CG	3:A:198:PRO:HG2	2.12	0.79
3:A:29:VAL:HG21	3:A:94:SER:HB2	1.63	0.79
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.64	0.78
3:A:330:PRO:HA	3:A:333:ARG:CG	2.13	0.78
3:A:27:LYS:HB3	3:A:36:TYR:CD1	2.17	0.78
3:A:272:PHE:HD1	6:A:338:DCP:H4'	1.49	0.78
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.20	0.77
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.13	0.77
3:A:271:TYR:HB2	7:A:592:HOH:O	1.84	0.76
3:A:277:ILE:HG12	3:A:335:GLU:CB	2.15	0.76
3:A:272:PHE:CD1	6:A:338:DCP:H4'	2.21	0.76
3:A:207:GLN:O	3:A:210:LEU:HB2	1.86	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:108:PRO:O	3:A:112:ARG:HG3	1.86	0.75
3:A:18:MET:CE	3:A:82:LEU:HD22	2.17	0.74
3:A:172:GLU:HG2	3:A:198:PRO:HG2	1.70	0.74
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.52	0.74
3:A:277:ILE:HG12	3:A:335:GLU:HB2	1.70	0.73
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.18	0.73
3:A:41:LYS:HE2	3:A:64:GLY:HA3	1.68	0.73
3:A:33:ILE:HG23	3:A:34:HIS:H	1.54	0.73
2:P:5:DA:H2''	2:P:6:DT:C5'	2.18	0.72
2:P:6:DT:H2''	2:P:7:DG:H5''	1.71	0.72
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.04	0.72
3:A:210:LEU:HB3	3:A:259:LEU:HD21	1.72	0.72
3:A:158:MET:HB3	3:A:191:MET:CE	2.20	0.71
3:A:18:MET:HE2	3:A:82:LEU:HD22	1.72	0.71
1:T:6:DG:H2''	1:T:7:DA:C8	2.26	0.71
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.20	0.70
3:A:12:ASN:HA	7:A:553:HOH:O	1.89	0.70
3:A:286:ALA:HA	3:A:323:ILE:HG21	1.73	0.70
3:A:30:SER:HA	7:A:558:HOH:O	1.90	0.70
3:A:286:ALA:HA	3:A:323:ILE:CG2	2.22	0.70
3:A:60:LYS:HA	3:A:65:VAL:CG2	2.20	0.70
2:P:6:DT:H2'	7:P:567:HOH:O	1.92	0.70
3:A:29:VAL:HG22	3:A:97:ILE:HD12	1.73	0.70
3:A:323:ILE:O	3:A:324:GLN:HG2	1.92	0.69
3:A:282:MET:HG3	3:A:282:MET:O	1.92	0.69
3:A:299:ARG:HG2	3:A:310:PRO:HA	1.75	0.68
3:A:162:VAL:O	3:A:166:VAL:HG23	1.94	0.68
3:A:133:ASN:ND2	3:A:135:HIS:H	1.91	0.68
3:A:172:GLU:HB3	3:A:197:HIS:NE2	2.08	0.68
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.58	0.68
3:A:278:PHE:HE1	3:A:328:ARG:HD3	1.59	0.68
3:A:172:GLU:HG3	3:A:198:PRO:HG2	1.76	0.67
3:A:291:PHE:O	3:A:301:LEU:HD22	1.94	0.67
3:A:19:LEU:HB3	3:A:43:ALA:HB2	1.76	0.67
3:A:278:PHE:CZ	3:A:328:ARG:HG3	2.30	0.67
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.76	0.67
3:A:211:LEU:O	3:A:211:LEU:HD12	1.94	0.67
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.28	0.67
3:A:260:ILE:HG22	3:A:261:PRO:HD2	1.77	0.67
2:P:5:DA:OP2	3:A:109:SER:HB3	1.95	0.67
3:A:35:LYS:O	3:A:38:ALA:HB3	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:277:ILE:HG12	3:A:335:GLU:HA	1.76	0.66
3:A:180:SER:HB3	3:A:183:ARG:HH21	1.60	0.66
7:P:568:HOH:O	3:A:110:ALA:HB2	1.94	0.66
3:A:245:ASN:H	3:A:245:ASN:HD22	0.77	0.66
3:A:75:GLU:O	3:A:79:THR:HG23	1.95	0.66
3:A:151:PRO:HB2	3:A:153:GLU:HG2	1.77	0.66
3:A:68:LYS:O	3:A:72:LYS:HE3	1.96	0.65
3:A:333:ARG:NH1	7:A:584:HOH:O	2.29	0.65
3:A:253:ARG:HG2	3:A:253:ARG:HH11	1.61	0.65
3:A:240:GLN:NE2	3:A:250:TYR:O	2.30	0.65
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.31	0.65
1:T:6:DG:N7	7:T:652:HOH:O	2.29	0.65
3:A:33:ILE:HG23	3:A:34:HIS:N	2.11	0.64
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.45	0.64
3:A:286:ALA:CA	3:A:323:ILE:HG21	2.28	0.63
3:A:172:GLU:HB3	3:A:197:HIS:HE2	1.63	0.63
3:A:278:PHE:O	3:A:282:MET:N	2.30	0.63
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.78	0.63
3:A:152:ARG:HA	3:A:155:MET:HB2	1.80	0.63
3:A:264:GLN:NE2	3:A:296:TYR:HB3	2.14	0.62
3:A:88:ILE:HG22	3:A:89:ARG:N	2.15	0.62
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.81	0.62
3:A:243:SER:CB	3:A:249:GLU:HA	2.30	0.62
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.34	0.62
3:A:270:LEU:HD23	3:A:319:ILE:HD13	1.82	0.61
3:A:245:ASN:N	3:A:245:ASN:ND2	2.28	0.61
3:A:30:SER:HB2	7:A:641:HOH:O	2.00	0.61
3:A:133:ASN:O	3:A:137:ARG:HG3	2.01	0.61
3:A:285:HIS:CE1	3:A:289:LYS:HG2	2.36	0.61
3:A:270:LEU:HD13	3:A:316:GLU:OE2	2.00	0.61
3:A:23:ALA:HB2	3:A:39:TYR:HB2	1.82	0.61
3:A:253:ARG:HH11	3:A:253:ARG:CG	2.13	0.61
3:A:267:CYS:SG	3:A:297:THR:HA	2.40	0.61
3:A:286:ALA:HB2	3:A:293:ILE:HD11	1.82	0.60
3:A:79:THR:O	3:A:81:LYS:N	2.33	0.60
3:A:188:SER:HB3	7:A:522:HOH:O	2.00	0.60
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.36	0.60
3:A:81:LYS:NZ	3:A:86:GLU:HB3	2.16	0.60
3:A:119:ILE:HG22	3:A:124:ASP:HB2	1.84	0.60
3:A:299:ARG:HG2	3:A:310:PRO:CA	2.31	0.60
3:A:243:SER:OG	3:A:249:GLU:HA	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:121:THR:O	3:A:124:ASP:HB2	2.02	0.60
3:A:292:THR:O	3:A:298:ILE:HA	2.01	0.59
3:A:309:GLU:H	3:A:310:PRO:HD3	1.66	0.59
3:A:69:ILE:O	3:A:73:ILE:HG13	2.02	0.59
3:A:158:MET:HB3	3:A:191:MET:HE3	1.85	0.59
3:A:278:PHE:CE1	3:A:328:ARG:HD3	2.36	0.59
3:A:15:ILE:HD13	3:A:73:ILE:HG23	1.84	0.59
3:A:18:MET:CE	3:A:76:PHE:HB2	2.33	0.59
3:A:100:LEU:HD21	3:A:119:ILE:O	2.02	0.59
3:A:282:MET:SD	3:A:323:ILE:HD11	2.43	0.58
3:A:294:ASN:ND2	3:A:297:THR:H	2.01	0.58
3:A:150:ILE:O	3:A:187:SER:HA	2.03	0.58
3:A:285:HIS:CE1	3:A:289:LYS:HE3	2.39	0.58
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.85	0.58
3:A:158:MET:HB3	3:A:191:MET:HE1	1.86	0.58
3:A:327:TYR:HD1	3:A:328:ARG:N	2.02	0.58
3:A:165:GLU:O	3:A:169:VAL:HG12	2.03	0.57
3:A:243:SER:HB3	3:A:249:GLU:HA	1.86	0.57
3:A:151:PRO:HG2	3:A:154:GLU:CG	2.25	0.57
3:A:316:GLU:HA	3:A:319:ILE:HD12	1.87	0.57
2:P:1:DT:H72	7:P:571:HOH:O	2.04	0.57
3:A:59:ALA:O	3:A:62:LEU:N	2.30	0.57
3:A:182:ARG:NH2	3:A:316:GLU:OE1	2.32	0.57
2:P:6:DT:H71	7:P:567:HOH:O	2.05	0.57
3:A:46:ILE:O	3:A:46:ILE:HD12	2.05	0.57
3:A:157:GLN:O	3:A:161:ILE:HG13	2.04	0.56
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.40	0.56
3:A:183:ARG:HD3	3:A:273:THR:O	2.05	0.56
3:A:195:LEU:O	3:A:260:ILE:N	2.30	0.56
3:A:270:LEU:HD21	3:A:282:MET:CE	2.35	0.56
3:A:293:ILE:HD13	3:A:298:ILE:CG1	2.31	0.56
3:A:319:ILE:O	3:A:322:TYR:HB2	2.05	0.56
3:A:303:VAL:C	3:A:305:GLY:H	2.08	0.56
3:A:286:ALA:HB2	3:A:323:ILE:HG21	1.85	0.56
3:A:16:THR:HG23	3:A:46:ILE:HG13	1.88	0.56
3:A:285:HIS:HE1	3:A:289:LYS:HE3	1.71	0.56
3:A:308:GLY:O	3:A:309:GLU:HB2	2.06	0.55
3:A:207:GLN:HB2	7:A:625:HOH:O	2.07	0.55
3:A:296:TYR:HD1	7:A:629:HOH:O	1.89	0.55
3:A:334:SER:O	3:A:335:GLU:HB3	2.06	0.55
3:A:328:ARG:HB2	3:A:333:ARG:HD3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:133:ASN:HD22	3:A:135:HIS:H	1.53	0.55
3:A:16:THR:HG23	3:A:46:ILE:CG1	2.37	0.55
3:A:309:GLU:OE1	3:A:309:GLU:HA	2.05	0.55
3:A:85:LEU:O	3:A:89:ARG:HB2	2.07	0.54
3:A:180:SER:HB2	3:A:185:ALA:CB	2.37	0.54
3:A:275:SER:OG	3:A:277:ILE:HD13	2.06	0.54
3:A:306:VAL:HG22	7:A:650:HOH:O	2.06	0.54
3:A:266:TYR:HA	3:A:269:VAL:HB	1.90	0.54
3:A:83:ARG:HA	3:A:86:GLU:HG2	1.90	0.54
3:A:279:ASN:O	3:A:282:MET:N	2.41	0.54
3:A:41:LYS:O	3:A:45:VAL:HG13	2.07	0.54
3:A:278:PHE:HB2	3:A:333:ARG:O	2.07	0.54
3:A:101:THR:HA	3:A:106:ILE:HG22	1.90	0.53
3:A:60:LYS:HG2	3:A:60:LYS:O	2.05	0.53
3:A:278:PHE:HZ	3:A:320:PHE:CZ	2.27	0.53
3:A:217:GLN:O	3:A:220:LYS:HB3	2.08	0.53
3:A:282:MET:HG2	7:A:555:HOH:O	2.07	0.53
3:A:97:ILE:O	3:A:101:THR:HG23	2.08	0.53
3:A:195:LEU:O	3:A:259:LEU:HD12	2.07	0.53
3:A:272:PHE:O	6:A:338:DCP:O3'	2.27	0.53
3:A:59:ALA:O	3:A:62:LEU:HB2	2.09	0.53
3:A:291:PHE:HD1	3:A:300:PRO:HA	1.74	0.53
3:A:49:TYR:CE2	3:A:53:ILE:HG12	2.44	0.53
3:A:174:ILE:O	3:A:195:LEU:HD12	2.09	0.52
3:A:270:LEU:HD12	3:A:270:LEU:O	2.09	0.52
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.40	0.52
3:A:52:LYS:HG2	7:A:642:HOH:O	2.10	0.52
3:A:165:GLU:OE1	3:A:217:GLN:OE1	2.27	0.52
2:P:6:DT:H5'	7:P:567:HOH:O	2.08	0.52
3:A:244:LYS:CB	3:A:245:ASN:HD22	2.22	0.52
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.89	0.52
3:A:212:HIS:CD2	3:A:212:HIS:N	2.76	0.52
3:A:250:TYR:HB3	7:A:577:HOH:O	2.10	0.52
3:A:31:GLN:N	7:A:641:HOH:O	2.29	0.52
3:A:200:PHE:O	3:A:262:LYS:N	2.37	0.51
3:A:264:GLN:HE22	3:A:296:TYR:CB	2.24	0.51
2:P:5:DA:P	3:A:107:GLY:HA3	2.50	0.51
3:A:223:PHE:O	3:A:239:CYS:HA	2.10	0.51
3:A:242:PRO:HB2	7:A:589:HOH:O	2.10	0.51
3:A:214:VAL:O	3:A:218:LEU:HD13	2.10	0.51
3:A:323:ILE:C	3:A:324:GLN:HG2	2.29	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:15:ILE:HD13	3:A:73:ILE:CG2	2.40	0.51
3:A:122:LEU:HD23	3:A:126:ARG:NH1	2.25	0.51
3:A:280:LYS:O	3:A:284:ALA:N	2.38	0.51
3:A:180:SER:HB2	3:A:185:ALA:HB2	1.92	0.51
3:A:19:LEU:HD23	3:A:43:ALA:HB2	1.93	0.51
2:P:5:DA:C2'	2:P:6:DT:H5'	2.28	0.50
3:A:114:PHE:HB3	3:A:119:ILE:HB	1.94	0.50
3:A:157:GLN:O	3:A:160:ASP:HB3	2.10	0.50
3:A:234:LYS:NZ	7:A:617:HOH:O	2.29	0.50
3:A:81:LYS:HZ3	3:A:86:GLU:HB3	1.76	0.50
3:A:233:THR:HB	7:A:538:HOH:O	2.11	0.50
3:A:265:TYR:O	3:A:268:GLY:N	2.44	0.50
3:A:40:ARG:O	3:A:44:SER:N	2.43	0.50
3:A:282:MET:HB3	7:A:555:HOH:O	2.11	0.50
1:T:6:DG:C6	2:P:2:DC:N3	2.80	0.50
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.41	0.49
3:A:122:LEU:HA	3:A:125:LEU:HB2	1.94	0.49
3:A:215:VAL:O	3:A:219:GLN:HB2	2.12	0.49
3:A:326:LYS:O	3:A:326:LYS:HG3	2.12	0.49
3:A:125:LEU:HD22	3:A:132:LEU:HD11	1.94	0.49
3:A:291:PHE:HD2	3:A:323:ILE:CG2	2.22	0.49
3:A:277:ILE:HG12	3:A:335:GLU:CA	2.41	0.49
3:A:33:ILE:O	3:A:37:ASN:HB2	2.12	0.49
3:A:296:TYR:HB2	3:A:297:THR:HG23	1.94	0.49
3:A:119:ILE:HG22	3:A:124:ASP:CB	2.42	0.49
3:A:218:LEU:HD12	3:A:218:LEU:N	2.27	0.49
3:A:29:VAL:HA	3:A:97:ILE:HD13	1.93	0.49
3:A:254:ARG:HA	3:A:254:ARG:HH11	1.78	0.49
3:A:127:LYS:HB2	3:A:128:ASN:ND2	2.28	0.48
3:A:248:LYS:HG2	3:A:248:LYS:O	2.12	0.48
3:A:268:GLY:O	3:A:271:TYR:HB3	2.14	0.48
3:A:29:VAL:HA	3:A:97:ILE:CD1	2.43	0.48
3:A:12:ASN:HB3	3:A:46:ILE:HD11	1.93	0.48
3:A:254:ARG:NH2	3:A:256:ASP:OD1	2.39	0.48
3:A:18:MET:HE3	3:A:76:PHE:HB2	1.94	0.48
3:A:16:THR:CG2	3:A:46:ILE:HG13	2.43	0.48
3:A:237:GLY:O	3:A:254:ARG:NH1	2.47	0.48
3:A:260:ILE:HG22	3:A:261:PRO:CD	2.44	0.48
3:A:115:VAL:C	3:A:117:GLU:H	2.17	0.47
3:A:120:LYS:N	3:A:124:ASP:OD2	2.47	0.47
3:A:27:LYS:HB3	3:A:36:TYR:CG	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:330:PRO:HA	3:A:333:ARG:HG2	1.91	0.47
3:A:12:ASN:HD21	3:A:53:ILE:H	1.61	0.47
3:A:278:PHE:HZ	3:A:320:PHE:CE1	2.33	0.47
3:A:170:ASP:HB3	3:A:173:TYR:CE2	2.49	0.47
3:A:270:LEU:HD12	3:A:270:LEU:C	2.34	0.47
3:A:122:LEU:O	3:A:126:ARG:HG3	2.14	0.47
3:A:23:ALA:O	3:A:36:TYR:HD1	1.98	0.47
3:A:170:ASP:HB3	3:A:173:TYR:CD2	2.49	0.47
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.96	0.47
3:A:138:ILE:HD11	3:A:226:ASP:HB3	1.96	0.47
2:P:5:DA:P	3:A:109:SER:HB3	2.55	0.47
3:A:264:GLN:NE2	3:A:296:TYR:CB	2.77	0.47
3:A:270:LEU:HD21	3:A:282:MET:HE3	1.96	0.47
3:A:264:GLN:HE22	3:A:296:TYR:HB3	1.79	0.47
3:A:30:SER:HB3	7:A:561:HOH:O	2.15	0.47
3:A:197:HIS:O	3:A:262:LYS:HB2	2.15	0.46
3:A:165:GLU:HB3	3:A:217:GLN:CG	2.45	0.46
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.98	0.46
3:A:41:LYS:NZ	3:A:64:GLY:O	2.44	0.46
3:A:221:VAL:O	3:A:221:VAL:HG23	2.15	0.46
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.61	0.46
3:A:73:ILE:HG22	3:A:77:LEU:HD22	1.97	0.46
3:A:159:GLN:N	3:A:191:MET:HE1	2.30	0.46
3:A:178:CYS:SG	3:A:194:LEU:HD23	2.55	0.46
3:A:165:GLU:O	3:A:168:LYS:HG2	2.16	0.46
3:A:194:LEU:HA	3:A:194:LEU:HD12	1.03	0.46
3:A:19:LEU:CB	3:A:43:ALA:HB2	2.46	0.46
3:A:279:ASN:O	3:A:283:ARG:N	2.42	0.45
3:A:197:HIS:CG	3:A:198:PRO:CD	3.00	0.45
3:A:205:THR:O	3:A:206:LYS:O	2.34	0.45
3:A:218:LEU:H	3:A:218:LEU:HD12	1.82	0.45
3:A:267:CYS:O	3:A:271:TYR:HB2	2.16	0.45
2:P:6:DT:H6	7:P:567:HOH:O	1.99	0.45
3:A:285:HIS:NE2	7:A:583:HOH:O	2.36	0.45
3:A:264:GLN:NE2	3:A:297:THR:CG2	2.80	0.45
3:A:18:MET:O	3:A:21:GLU:HB2	2.17	0.45
3:A:33:ILE:CG2	3:A:34:HIS:H	2.24	0.45
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.97	0.45
3:A:32:ALA:O	3:A:36:TYR:HB3	2.17	0.45
3:A:195:LEU:HA	3:A:195:LEU:HD12	1.34	0.45
3:A:275:SER:O	3:A:278:PHE:N	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:27:LYS:HE3	3:A:28:ASN:HD21	1.82	0.45
3:A:315:SER:OG	3:A:316:GLU:N	2.49	0.45
3:A:145:ASP:HA	3:A:148:LYS:HG3	1.97	0.45
3:A:170:ASP:OD2	3:A:197:HIS:NE2	2.50	0.45
3:A:301:LEU:HD12	3:A:301:LEU:HA	1.52	0.45
3:A:270:LEU:HA	3:A:316:GLU:OE2	2.17	0.45
3:A:309:GLU:N	3:A:310:PRO:HD3	2.32	0.44
3:A:138:ILE:HG23	3:A:138:ILE:HD13	1.63	0.44
3:A:254:ARG:NH1	3:A:255:ILE:H	2.15	0.44
3:A:267:CYS:HB2	3:A:296:TYR:O	2.17	0.44
3:A:151:PRO:O	3:A:154:GLU:N	2.45	0.44
3:A:195:LEU:HB3	3:A:258:ARG:O	2.17	0.44
3:A:81:LYS:NZ	3:A:86:GLU:CB	2.81	0.44
3:A:300:PRO:HD3	3:A:311:LEU:HD22	1.99	0.44
3:A:31:GLN:NE2	3:A:112:ARG:HH12	2.14	0.44
3:A:253:ARG:NH1	3:A:253:ARG:CG	2.79	0.44
3:A:285:HIS:NE2	3:A:289:LYS:CG	2.79	0.44
3:A:82:LEU:HD23	3:A:85:LEU:HB2	2.00	0.44
3:A:209:LYS:HA	3:A:209:LYS:HD3	1.70	0.44
3:A:266:TYR:O	3:A:270:LEU:HB2	2.18	0.44
3:A:23:ALA:CB	3:A:39:TYR:HB2	2.46	0.44
3:A:251:PRO:HG2	3:A:253:ARG:NH2	2.33	0.44
3:A:33:ILE:CG2	3:A:34:HIS:N	2.78	0.44
3:A:79:THR:O	3:A:79:THR:OG1	2.29	0.43
3:A:12:ASN:ND2	7:A:642:HOH:O	2.50	0.43
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.33	0.43
3:A:330:PRO:O	3:A:333:ARG:HG2	2.18	0.43
3:A:277:ILE:CG1	3:A:335:GLU:HB2	2.46	0.43
3:A:119:ILE:CG2	3:A:124:ASP:CB	2.96	0.43
3:A:260:ILE:HD12	3:A:260:ILE:HG23	1.74	0.43
3:A:327:TYR:C	3:A:327:TYR:CD1	2.92	0.43
3:A:77:LEU:HA	3:A:77:LEU:HD12	1.55	0.43
3:A:99:PHE:HD1	3:A:100:LEU:HD13	1.82	0.43
3:A:34:HIS:O	3:A:38:ALA:N	2.45	0.43
3:A:62:LEU:N	3:A:62:LEU:HD13	2.33	0.43
3:A:81:LYS:HZ2	3:A:86:GLU:HB3	1.84	0.43
3:A:81:LYS:HZ2	3:A:86:GLU:CB	2.32	0.43
3:A:99:PHE:CD1	3:A:99:PHE:C	2.92	0.43
3:A:315:SER:O	3:A:318:ASP:HB2	2.19	0.43
3:A:41:LYS:HE2	3:A:64:GLY:HA2	1.94	0.43
3:A:278:PHE:HZ	3:A:328:ARG:HG3	1.79	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:148:LYS:HB3	7:A:620:HOH:O	2.18	0.43
1:T:1:DC:H2''	1:T:2:DA:OP2	2.19	0.43
3:A:178:CYS:SG	3:A:194:LEU:CD2	3.07	0.42
3:A:125:LEU:HD23	3:A:125:LEU:HA	1.42	0.42
3:A:122:LEU:HD21	3:A:126:ARG:NH2	2.34	0.42
3:A:286:ALA:O	3:A:291:PHE:N	2.48	0.42
3:A:230:LYS:HB3	3:A:230:LYS:HE2	1.68	0.42
3:A:196:THR:OG1	3:A:262:LYS:HA	2.18	0.42
3:A:126:ARG:HH11	3:A:126:ARG:HD2	1.67	0.42
3:A:228:LEU:HA	3:A:228:LEU:HD12	1.70	0.42
3:A:197:HIS:CD2	3:A:198:PRO:CD	2.99	0.42
2:P:5:DA:H3'	7:P:648:HOH:O	2.19	0.42
2:P:5:DA:H4'	7:P:565:HOH:O	2.18	0.42
3:A:172:GLU:HB3	3:A:197:HIS:CD2	2.54	0.42
3:A:182:ARG:NH1	3:A:273:THR:CG2	2.82	0.42
3:A:299:ARG:HG2	3:A:310:PRO:N	2.35	0.42
1:T:2:DA:H2'	1:T:2:DA:H8	1.55	0.42
3:A:128:ASN:ND2	3:A:128:ASN:N	2.67	0.42
3:A:158:MET:CB	3:A:191:MET:HE3	2.49	0.42
3:A:318:ASP:O	3:A:321:ASP:HB2	2.20	0.42
3:A:79:THR:C	3:A:81:LYS:H	2.23	0.42
3:A:169:VAL:HG22	3:A:173:TYR:HE2	1.85	0.41
3:A:255:ILE:HG12	3:A:256:ASP:N	2.35	0.41
3:A:298:ILE:HG23	3:A:298:ILE:O	2.20	0.41
3:A:49:TYR:CE2	3:A:51:HIS:HB2	2.55	0.41
3:A:73:ILE:O	3:A:77:LEU:HD22	2.19	0.41
3:A:31:GLN:HE21	3:A:112:ARG:HH22	1.67	0.41
3:A:154:GLU:O	3:A:158:MET:HE2	2.20	0.41
3:A:200:PHE:CE2	3:A:261:PRO:N	2.88	0.41
3:A:205:THR:O	3:A:205:THR:HG23	2.21	0.41
3:A:211:LEU:C	3:A:211:LEU:HD12	2.37	0.41
3:A:278:PHE:CE1	3:A:325:TRP:HZ3	2.39	0.41
3:A:31:GLN:HE21	3:A:112:ARG:NH1	2.15	0.41
3:A:103:VAL:HG22	3:A:143:PHE:CE2	2.56	0.41
3:A:122:LEU:CD2	3:A:126:ARG:CZ	2.98	0.41
3:A:200:PHE:HB2	7:A:625:HOH:O	2.20	0.41
3:A:289:LYS:HG3	3:A:324:GLN:OE1	2.20	0.41
3:A:315:SER:O	3:A:318:ASP:N	2.54	0.41
3:A:321:ASP:O	3:A:324:GLN:HA	2.21	0.41
1:T:2:DA:H2	2:P:6:DT:O2	2.04	0.41
3:A:172:GLU:HG3	3:A:198:PRO:CG	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:194:LEU:HD11	3:A:258:ARG:HG3	2.02	0.41
3:A:267:CYS:N	7:A:508:HOH:O	2.30	0.41
1:T:6:DG:N1	2:P:2:DC:O2	2.53	0.41
3:A:296:TYR:CD1	3:A:296:TYR:N	2.88	0.40
3:A:124:ASP:O	3:A:128:ASN:ND2	2.53	0.40
3:A:45:VAL:CG2	3:A:46:ILE:N	2.84	0.40
3:A:77:LEU:N	3:A:77:LEU:HD13	2.36	0.40
3:A:85:LEU:HA	3:A:85:LEU:HD12	1.85	0.40
3:A:123:GLU:O	3:A:126:ARG:N	2.54	0.40
3:A:311:LEU:HB3	3:A:322:TYR:HE2	1.85	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%)	262 (81%)	43 (13%)	20 (6%)	2 10

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	185	ALA
3	A	206	LYS
3	A	244	LYS
3	A	265	TYR
3	A	309	GLU
3	A	80	GLY
3	A	202	SER
3	A	246	ASP
3	A	247	GLU
3	A	266	TYR
3	A	304	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	316	GLU
3	A	10	THR
3	A	91	ASP
3	A	204	SER
3	A	205	THR
3	A	279	ASN
3	A	310	PRO
3	A	315	SER
3	A	207	GLN

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	288/295 (98%)	219 (76%)	69 (24%)	1 4

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	THR
3	A	18	MET
3	A	19	LEU
3	A	22	LEU
3	A	27	LYS
3	A	37	ASN
3	A	40	ARG
3	A	41	LYS
3	A	44	SER
3	A	45	VAL
3	A	46	ILE
3	A	54	LYS
3	A	62	LEU
3	A	65	VAL
3	A	67	THR
3	A	72	LYS
3	A	77	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	79	THR
3	A	89	ARG
3	A	92	ASP
3	A	94	SER
3	A	100	LEU
3	A	109	SER
3	A	113	LYS
3	A	119	ILE
3	A	121	THR
3	A	128	ASN
3	A	136	GLN
3	A	138	ILE
3	A	157	GLN
3	A	168	LYS
3	A	169	VAL
3	A	180	SER
3	A	188	SER
3	A	190	ASP
3	A	194	LEU
3	A	201	THR
3	A	205	THR
3	A	208	PRO
3	A	214	VAL
3	A	226	ASP
3	A	228	LEU
3	A	233	THR
3	A	245	ASN
3	A	248	LYS
3	A	249	GLU
3	A	253	ARG
3	A	258	ARG
3	A	259	LEU
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	295	GLU
3	A	296	TYR
3	A	301	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	303	VAL
3	A	304	THR
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	325	TRP
3	A	327	TYR
3	A	328	ARG
3	A	331	LYS
3	A	335	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	28	ASN
3	A	31	GLN
3	A	37	ASN
3	A	90	GLN
3	A	128	ASN
3	A	133	ASN
3	A	136	GLN
3	A	157	GLN
3	A	213	GLN
3	A	217	GLN
3	A	245	ASN
3	A	264	GLN
3	A	279	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 ⓘ

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 5 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	DCP	A	338	4	17,20,29	0.77	0	16,31,45	1.27	2 (12%)

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	DCP	A	338	4	-	0/18/28/34	0/1/1/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	338	DCP	O3'-C3'-C2'	-3.79	102.90	111.60
6	A	338	DCP	O2G-PG-O1G	2.10	118.71	110.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	338	DCP	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	T	8/8 (100%)	-0.51	1 (12%) 4 2	18, 36, 99, 100	0
2	P	7/7 (100%)	-1.02	0 100 100	16, 21, 37, 99	0
3	A	326/335 (97%)	-1.21	1 (0%) 93 82	1, 27, 83, 100	0
All	All	341/350 (97%)	-1.19	2 (0%) 89 71	1, 27, 86, 100	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	1	DC	2.7
3	A	247	GLU	2.4

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
6	DCP	A	338	20/28	0.87	0.23	1.98	9,79,100,100	20
5	NA	A	342	1/1	0.96	0.12	1.16	46,46,46,46	0
5	NA	A	341	1/1	0.96	0.10	0.80	7,7,7,7	0
4	ZN	A	339	1/1	0.87	0.09	-	30,30,30,30	1
4	ZN	A	343	1/1	0.98	0.04	-	30,30,30,30	1
4	ZN	A	340	1/1	0.93	0.17	-	30,30,30,30	1

6.5 Other polymers [i](#)

There are no such residues in this entry.