



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:33 AM UTC

PDB ID : 1ZQC / pdb_00001zqc
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SEVEN BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF CACL2 (15 MILLIMOLAR)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-04-12
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

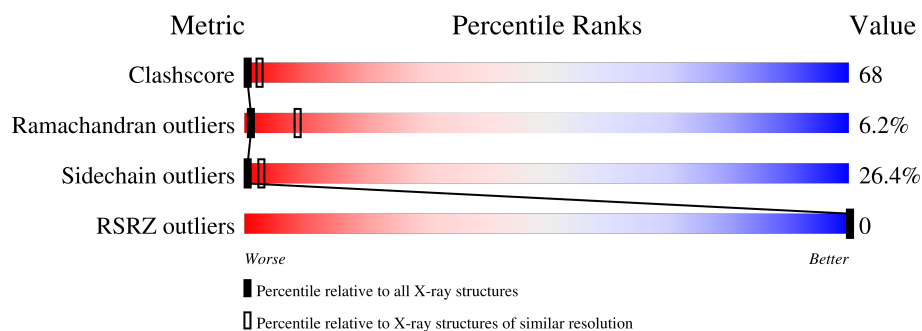
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

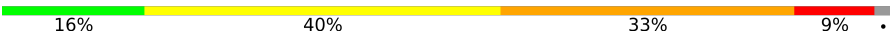
The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	8	
2	P	7	
3	A	335	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3061 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	18	0	0
			2623	1657	458	499	9			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	T	15	Total	O	0	0
			15	15		
5	P	23	Total	O	0	0
			23	23		
5	A	108	Total	O	0	0
			108	108		

3 Residue-property plots

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.

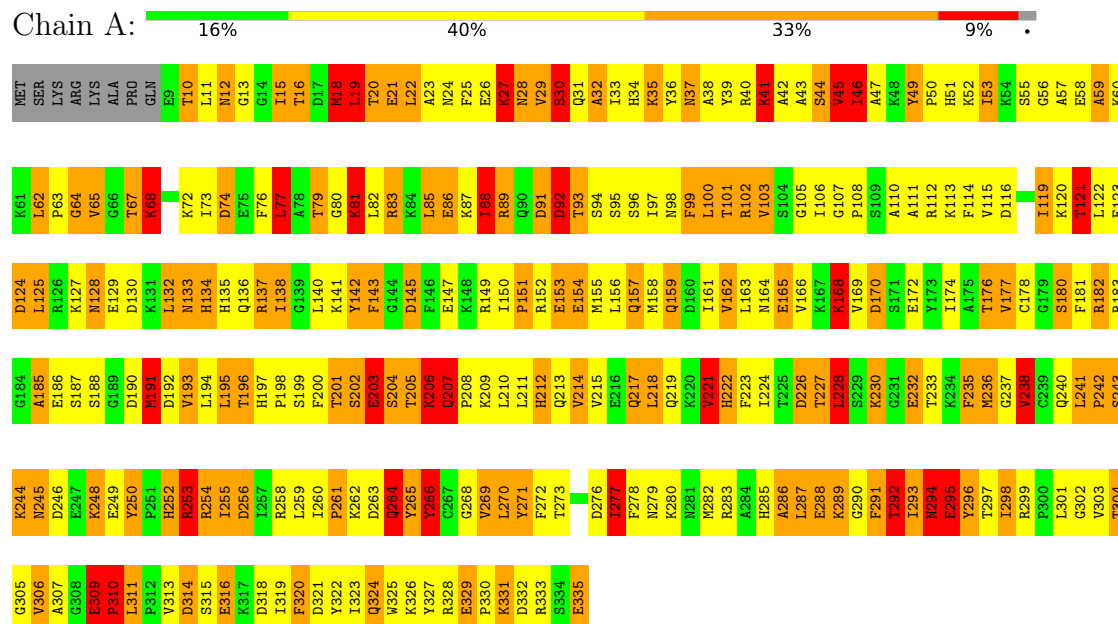
- Molecule 1: DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3')



- 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	178.06Å 57.64Å 48.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	89.0 (20.00-3.20) 88.4 (20.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.63Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.173 , (Not available) 0.151 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 309.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3061	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: CA

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	1.41	2/162 (1.2%)	2.90	8/249 (3.2%)
2	P	1.66	3/160 (1.9%)	3.71	12/243 (4.9%)
3	A	1.69	29/2672 (1.1%)	2.39	163/3590 (4.5%)
All	All	1.68	34/2994 (1.1%)	2.52	183/4082 (4.5%)

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 (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	203	GLU	C-N	13.15	1.52	1.33
3	A	196	THR	CA-C	-7.31	1.43	1.52
3	A	254	ARG	C-O	-7.03	1.15	1.23
2	P	1	DT	OP3-P	6.89	1.62	1.48
3	A	110	ALA	N-CA	-6.77	1.38	1.46
3	A	15	ILE	CA-C	-6.77	1.44	1.52
3	A	125	LEU	CA-C	-6.57	1.44	1.52
3	A	254	ARG	CA-C	-6.53	1.44	1.52
2	P	2	DC	C1'-N1	6.45	1.68	1.49
3	A	147	GLU	CA-C	-6.44	1.44	1.52
3	A	162	VAL	CA-C	-6.40	1.45	1.52
3	A	96	SER	CA-C	-6.40	1.44	1.52
3	A	296	TYR	C-N	-6.29	1.26	1.33
3	A	254	ARG	NE-CZ	6.28	1.40	1.33
3	A	103	VAL	C-N	-6.25	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	103	VAL	C-O	-6.18	1.17	1.24
1	T	6	DG	C3'-O3'	-5.98	1.24	1.42
3	A	162	VAL	N-CA	-5.96	1.39	1.46
3	A	30	SER	C-N	-5.77	1.26	1.33
3	A	269	VAL	N-CA	-5.75	1.39	1.46
3	A	81	LYS	CA-C	-5.63	1.46	1.53
3	A	226	ASP	CA-C	-5.61	1.45	1.52
3	A	65	VAL	N-CA	-5.60	1.39	1.46
3	A	242	PRO	CA-C	-5.58	1.44	1.52
3	A	165	GLU	N-CA	-5.50	1.39	1.46
3	A	124	ASP	CG-OD2	5.47	1.35	1.25
2	P	5	DA	O3'-P	-5.42	1.53	1.61
3	A	254	ARG	C-N	-5.42	1.26	1.33
1	T	1	DC	C3'-O3'	5.38	1.58	1.42
3	A	124	ASP	C-N	-5.30	1.27	1.33
3	A	27	LYS	CA-C	5.28	1.59	1.52
3	A	116	ASP	N-CA	-5.23	1.39	1.46
3	A	170	ASP	CA-C	-5.13	1.46	1.52
3	A	145	ASP	CG-OD2	5.01	1.34	1.25

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	1	DT	C6-N1-C1'	-23.30	84.41	119.35
2	P	1	DT	C2-N1-C1'	22.43	152.99	119.35
2	P	7	DG	C8-N9-C1'	19.80	156.69	127.00
2	P	7	DG	C4-N9-C1'	-19.75	97.38	127.00
1	T	7	DA	C4-N9-C1'	-18.77	98.90	127.05
1	T	7	DA	C8-N9-C1'	18.22	154.38	127.05
1	T	4	DT	C6-N1-C1'	-17.95	92.43	119.35
1	T	4	DT	C2-N1-C1'	17.42	145.48	119.35
1	T	6	DG	C8-N9-C1'	16.05	151.08	127.00
1	T	6	DG	C4-N9-C1'	-16.00	103.00	127.00
2	P	5	DA	C4-N9-C1'	15.85	150.83	127.05
2	P	5	DA	C8-N9-C1'	-15.71	103.48	127.05
2	P	6	DT	C6-N1-C1'	-14.75	97.22	119.35
2	P	2	DC	C2-N1-C1'	14.72	141.78	119.70
2	P	2	DC	C6-N1-C1'	-14.53	97.91	119.70
2	P	6	DT	C2-N1-C1'	14.31	140.81	119.35
3	A	206	LYS	O-C-N	12.60	139.35	122.59
3	A	256	ASP	CA-CB-CG	12.59	125.19	112.60
3	A	99	PHE	CA-CB-CG	-11.08	102.72	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	49	TYR	CA-C-N	10.45	132.90	119.84
3	A	49	TYR	C-N-CA	10.45	132.90	119.84
3	A	168	LYS	N-CA-CB	9.81	124.55	110.12
3	A	53	ILE	CB-CA-C	9.23	123.70	111.33
3	A	228	LEU	N-CA-C	-9.21	101.61	113.12
3	A	224	ILE	N-CA-CB	9.18	120.73	110.72
3	A	64	GLY	CA-C-N	-9.16	110.93	122.93
3	A	64	GLY	C-N-CA	-9.16	110.93	122.93
3	A	193	VAL	N-CA-C	9.07	121.97	108.54
3	A	18	MET	CA-C-N	9.00	132.34	120.28
3	A	18	MET	C-N-CA	9.00	132.34	120.28
3	A	164	ASN	CA-CB-CG	-8.75	103.85	112.60
3	A	64	GLY	N-CA-C	-8.63	103.42	115.32
3	A	20	THR	N-CA-CB	7.98	121.94	110.13
3	A	232	GLU	N-CA-C	7.96	122.43	112.87
3	A	57	ALA	N-CA-CB	-7.88	97.18	110.49
3	A	21	GLU	N-CA-C	-7.84	102.68	111.07
3	A	30	SER	CA-C-N	-7.73	110.54	122.60
3	A	30	SER	C-N-CA	-7.73	110.54	122.60
3	A	237	GLY	N-CA-C	7.73	121.94	111.20
3	A	264	GLN	N-CA-CB	7.71	122.06	110.95
3	A	157	GLN	N-CA-CB	7.63	121.33	110.12
3	A	222	HIS	CA-CB-CG	-7.60	106.20	113.80
3	A	270	LEU	O-C-N	7.59	129.99	122.09
3	A	28	ASN	CA-CB-CG	-7.55	105.05	112.60
3	A	190	ASP	CA-C-N	-7.44	111.56	122.65
3	A	190	ASP	C-N-CA	-7.44	111.56	122.65
3	A	35	LYS	N-CA-C	-7.21	103.42	111.28
3	A	41	LYS	N-CA-C	-7.20	103.37	111.14
3	A	212	HIS	CA-CB-CG	-6.88	106.92	113.80
3	A	192	ASP	N-CA-C	6.88	120.69	108.24
3	A	102	ARG	CD-NE-CZ	-6.86	114.79	124.40
3	A	83	ARG	N-CA-CB	6.83	119.88	109.91
3	A	277	ILE	N-CA-CB	6.77	120.74	110.58
3	A	35	LYS	CA-C-O	6.75	127.71	120.55
3	A	49	TYR	O-C-N	6.71	127.15	121.31
3	A	288	GLU	N-CA-C	-6.67	103.26	111.40
3	A	137	ARG	CA-C-O	6.67	127.82	120.82
3	A	88	ILE	CB-CA-C	-6.63	103.39	111.88
3	A	15	ILE	N-CA-CB	6.61	118.28	110.55
3	A	96	SER	N-CA-CB	6.60	119.77	109.94
3	A	121	THR	N-CA-C	6.59	119.83	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	77	LEU	N-CA-CB	6.59	119.53	109.98
3	A	227	THR	N-CA-CB	6.55	120.87	110.65
3	A	176	THR	CA-C-N	-6.53	113.95	123.10
3	A	176	THR	C-N-CA	-6.53	113.95	123.10
3	A	286	ALA	CA-C-N	6.50	129.53	120.29
3	A	286	ALA	C-N-CA	6.50	129.53	120.29
3	A	101	THR	CB-CA-C	6.49	121.57	110.79
3	A	151	PRO	N-CA-CB	6.49	109.07	103.36
3	A	134	HIS	CA-CB-CG	6.48	120.28	113.80
3	A	27	LYS	N-CA-CB	-6.41	100.72	110.01
3	A	255	ILE	CA-C-O	-6.39	115.30	121.63
3	A	95	SER	O-C-N	6.39	128.73	122.09
3	A	271	TYR	N-CA-C	6.37	118.79	111.02
3	A	24	ASN	CA-CB-CG	-6.35	106.25	112.60
3	A	45	VAL	O-C-N	6.32	128.11	121.91
3	A	224	ILE	CA-C-N	-6.28	112.37	122.23
3	A	224	ILE	C-N-CA	-6.28	112.37	122.23
3	A	266	TYR	CA-CB-CG	-6.26	102.64	113.90
3	A	315	SER	N-CA-C	6.24	118.02	108.42
3	A	195	LEU	N-CA-C	6.20	119.51	109.40
3	A	309	GLU	CA-C-N	6.20	127.59	119.84
3	A	309	GLU	C-N-CA	6.20	127.59	119.84
3	A	241	LEU	O-C-N	6.17	127.96	121.42
3	A	316	GLU	CA-C-N	6.14	128.79	120.44
3	A	316	GLU	C-N-CA	6.14	128.79	120.44
3	A	261	PRO	CB-CA-C	-6.12	103.93	111.64
3	A	15	ILE	O-C-N	6.08	127.87	121.91
3	A	16	THR	N-CA-CB	6.05	118.85	110.07
3	A	68	LYS	N-CA-CB	6.04	119.00	109.82
3	A	222	HIS	N-CA-CB	6.03	120.68	110.49
3	A	65	VAL	CB-CA-C	6.03	119.75	111.31
3	A	147	GLU	CA-CB-CG	-6.02	102.06	114.10
3	A	320	PHE	CA-CB-CG	-6.00	107.81	113.80
3	A	318	ASP	CA-CB-CG	-5.98	106.62	112.60
3	A	12	ASN	CB-CA-C	5.96	121.16	109.72
3	A	74	ASP	CA-CB-CG	5.94	118.54	112.60
3	A	72	LYS	CB-CA-C	5.93	120.27	110.90
3	A	67	THR	CA-CB-OG1	5.92	118.49	109.60
1	T	2	DA	C4-N9-C1'	-5.92	118.18	127.05
2	P	3	DT	C6-N1-C1'	-5.91	110.48	119.35
3	A	253	ARG	NE-CZ-NH1	5.90	127.40	121.50
3	A	12	ASN	N-CA-C	5.90	120.48	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	68	LYS	N-CA-C	5.87	118.18	111.02
3	A	238	VAL	CA-CB-CG2	5.86	120.35	110.40
3	A	235	PHE	CA-CB-CG	-5.85	107.95	113.80
3	A	154	GLU	CA-C-N	5.84	128.11	120.28
3	A	154	GLU	C-N-CA	5.84	128.11	120.28
3	A	256	ASP	CB-CA-C	-5.84	101.72	110.24
3	A	92	ASP	CB-CA-C	5.80	120.55	110.68
3	A	223	PHE	N-CA-C	-5.79	104.57	111.69
3	A	125	LEU	O-C-N	5.79	128.25	122.12
3	A	101	THR	CA-CB-OG1	-5.77	100.95	109.60
3	A	105	GLY	CA-C-N	5.76	129.80	122.37
3	A	105	GLY	C-N-CA	5.76	129.80	122.37
3	A	221	VAL	N-CA-CB	-5.76	103.32	112.07
3	A	196	THR	N-CA-CB	5.75	120.65	111.56
3	A	321	ASP	CB-CA-C	-5.75	101.19	110.74
3	A	296	TYR	CA-C-N	-5.75	110.68	121.95
3	A	296	TYR	C-N-CA	-5.75	110.68	121.95
3	A	243	SER	CB-CA-C	5.75	119.41	110.67
3	A	18	MET	O-C-N	5.73	127.98	122.07
3	A	96	SER	O-C-N	5.71	128.02	122.09
3	A	236	MET	CA-C-N	-5.67	112.32	123.04
3	A	236	MET	C-N-CA	-5.67	112.32	123.04
3	A	309	GLU	N-CA-C	5.62	122.23	109.81
3	A	21	GLU	CB-CA-C	-5.60	102.08	110.88
3	A	45	VAL	N-CA-CB	5.60	117.10	110.55
1	T	2	DA	C8-N9-C1'	5.59	135.43	127.05
3	A	153	GLU	N-CA-CB	5.59	118.97	110.14
3	A	306	VAL	CB-CA-C	-5.59	101.75	110.52
3	A	68	LYS	CB-CA-C	5.58	119.79	110.92
3	A	142	TYR	N-CA-C	5.54	118.83	112.57
3	A	91	ASP	N-CA-C	5.52	122.56	110.80
3	A	238	VAL	N-CA-CB	5.52	120.49	111.44
3	A	164	ASN	CA-C-N	-5.50	112.47	120.29
3	A	164	ASN	C-N-CA	-5.50	112.47	120.29
3	A	18	MET	CG-SD-CE	-5.49	88.83	100.90
3	A	59	ALA	O-C-N	5.46	127.70	122.03
3	A	53	ILE	CA-C-N	-5.44	113.61	122.26
3	A	53	ILE	C-N-CA	-5.44	113.61	122.26
3	A	143	PHE	CB-CA-C	5.38	119.77	110.84
2	P	3	DT	C2-N1-C1'	5.38	127.41	119.35
3	A	29	VAL	N-CA-C	5.37	118.57	111.17
3	A	292	THR	CB-CA-C	5.37	118.40	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	314	ASP	CA-CB-CG	-5.36	107.24	112.60
3	A	254	ARG	CD-NE-CZ	5.35	131.89	124.40
3	A	46	ILE	N-CA-CB	5.34	121.36	110.78
3	A	101	THR	CA-CB-CG2	5.34	119.58	110.50
3	A	258	ARG	N-CA-C	5.33	118.12	108.69
3	A	19	LEU	O-C-N	5.31	127.75	122.12
3	A	116	ASP	CB-CA-C	5.30	120.44	110.63
3	A	294	ASN	N-CA-CB	5.29	119.54	110.77
3	A	222	HIS	N-CA-C	5.25	121.97	110.80
3	A	125	LEU	N-CA-C	5.24	117.00	111.28
3	A	297	THR	N-CA-CB	-5.24	103.07	110.51
3	A	30	SER	O-C-N	-5.23	115.46	122.94
3	A	191	MET	N-CA-C	5.23	118.33	109.76
3	A	164	ASN	N-CA-C	5.22	116.66	111.07
3	A	177	VAL	CB-CA-C	5.22	118.32	111.53
3	A	212	HIS	CA-C-N	5.21	128.64	120.82
3	A	212	HIS	C-N-CA	5.21	128.64	120.82
3	A	238	VAL	CG1-CB-CG2	-5.19	99.38	110.80
3	A	132	LEU	N-CA-C	5.18	117.93	109.59
3	A	313	VAL	N-CA-C	5.18	115.44	107.77
3	A	176	THR	CA-CB-CG2	-5.18	101.70	110.50
3	A	310	PRO	CA-C-N	-5.16	113.75	120.67
3	A	310	PRO	C-N-CA	-5.16	113.75	120.67
3	A	186	GLU	N-CA-CB	5.16	118.29	110.14
3	A	165	GLU	O-C-N	5.15	128.02	122.15
3	A	291	PHE	N-CA-C	5.14	116.80	109.14
3	A	162	VAL	N-CA-CB	5.12	116.19	110.51
3	A	207	GLN	CA-C-N	5.11	126.23	119.84
3	A	207	GLN	C-N-CA	5.11	126.23	119.84
3	A	212	HIS	N-CA-C	5.11	117.25	111.02
3	A	86	GLU	N-CA-CB	5.07	117.57	110.12
3	A	98	ASN	N-CA-C	5.06	118.22	111.75
3	A	238	VAL	N-CA-C	-5.04	100.96	108.46
3	A	235	PHE	CA-C-O	-5.02	115.22	120.80
3	A	170	ASP	O-C-N	5.02	129.41	123.33
3	A	250	TYR	N-CA-C	5.02	117.22	110.29
3	A	85	LEU	N-CA-C	-5.01	105.73	111.14
3	A	252	HIS	CA-CB-CG	-5.00	108.80	113.80

All (2) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
3	A	12	ASN	CA
3	A	264	GLN	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	145	0	80	9	0
2	P	144	0	80	30	0
3	A	2623	0	2641	352	0
4	A	3	0	0	0	0
5	A	108	0	0	17	0
5	P	23	0	0	6	0
5	T	15	0	0	2	0
All	All	3061	0	2801	386	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 68.

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)
2:P:2:DC:C1'	2:P:2:DC:N1	1.68	1.52
2:P:2:DC:C1'	2:P:2:DC:C6	2.31	1.12
3:A:201:THR:HA	3:A:261:PRO:HB3	1.31	1.08
2:P:6:DT:H2''	2:P:7:DG:H5''	1.39	1.05
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.56	1.03
3:A:243:SER:HB3	3:A:249:GLU:HA	1.41	1.02
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.44	0.98
2:P:5:DA:H2''	2:P:6:DT:C5'	1.97	0.94
3:A:245:ASN:H	3:A:245:ASN:ND2	1.56	0.94
3:A:245:ASN:HD22	3:A:245:ASN:N	1.53	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.34	0.93
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.08	0.92
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.51	0.92
3:A:82:LEU:HD23	3:A:85:LEU:HB2	1.50	0.91
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.02	0.90
3:A:41:LYS:HE2	3:A:64:GLY:HA3	1.52	0.90
1:T:6:DG:H2''	1:T:7:DA:C8	2.06	0.89
3:A:201:THR:HA	3:A:261:PRO:CB	2.04	0.87
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.09	0.87
2:P:5:DA:H2''	2:P:6:DT:H5'	1.57	0.87
3:A:330:PRO:HA	3:A:333:ARG:CG	2.08	0.83
3:A:243:SER:CB	3:A:249:GLU:HA	2.10	0.81
3:A:15:ILE:HB	3:A:46:ILE:HD11	1.62	0.80
3:A:97:ILE:HG23	3:A:111:ALA:HB1	1.63	0.80
3:A:270:LEU:HD21	3:A:282:MET:HE1	1.62	0.79
3:A:155:MET:HE2	3:A:188:SER:HB2	1.64	0.79
3:A:19:LEU:HD23	3:A:43:ALA:HA	1.64	0.78
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.66	0.77
3:A:29:VAL:HG22	3:A:97:ILE:HD12	1.67	0.76
3:A:299:ARG:HG2	3:A:310:PRO:HD3	1.67	0.76
3:A:11:LEU:HD23	3:A:11:LEU:H	1.50	0.76
3:A:197:HIS:CE1	3:A:199:SER:HB3	2.21	0.76
3:A:73:ILE:O	3:A:77:LEU:HD13	1.85	0.76
2:P:5:DA:H2''	2:P:6:DT:H5''	1.66	0.75
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.17	0.75
3:A:62:LEU:HD12	3:A:63:PRO:HD2	1.67	0.75
3:A:289:LYS:HD3	3:A:289:LYS:N	2.01	0.74
1:T:1:DC:H2''	1:T:2:DA:OP2	1.85	0.74
3:A:209:LYS:HA	3:A:212:HIS:HB2	1.70	0.73
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.86	0.72
3:A:180:SER:HB3	3:A:183:ARG:HH21	1.54	0.72
3:A:159:GLN:O	3:A:163:LEU:HG	1.88	0.72
3:A:41:LYS:HD3	3:A:42:ALA:H	1.54	0.72
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.72	0.72
3:A:259:LEU:O	3:A:260:ILE:HD13	1.89	0.72
2:P:4:DA:H5'	5:P:569:HOH:O	1.90	0.71
3:A:157:GLN:HE22	3:A:244:LYS:NZ	1.88	0.71
3:A:129:GLU:HG2	3:A:137:ARG:HD3	1.73	0.70
3:A:162:VAL:O	3:A:166:VAL:HG23	1.91	0.70
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.26	0.70
3:A:19:LEU:HD23	3:A:43:ALA:CA	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:26:GLU:HB3	3:A:32:ALA:HB3	1.73	0.70
3:A:97:ILE:HG23	3:A:111:ALA:CB	2.21	0.70
3:A:207:GLN:HB3	3:A:210:LEU:HG	1.74	0.69
3:A:150:ILE:HG12	3:A:253:ARG:HG2	1.72	0.69
3:A:201:THR:CA	3:A:261:PRO:HB3	2.16	0.69
3:A:108:PRO:O	3:A:112:ARG:HG3	1.92	0.69
3:A:294:ASN:O	3:A:296:TYR:N	2.25	0.69
3:A:306:VAL:HG22	5:A:650:HOH:O	1.91	0.69
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.74	0.69
3:A:138:ILE:HD12	3:A:228:LEU:CD1	2.23	0.69
3:A:330:PRO:HA	3:A:333:ARG:HG2	1.73	0.69
3:A:18:MET:O	3:A:21:GLU:HB2	1.92	0.68
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.74	0.68
3:A:328:ARG:O	3:A:333:ARG:NE	2.23	0.68
3:A:138:ILE:HD12	3:A:228:LEU:HD12	1.75	0.68
3:A:197:HIS:ND1	3:A:199:SER:HB3	2.08	0.67
3:A:211:LEU:HD12	3:A:211:LEU:O	1.94	0.67
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.30	0.67
3:A:180:SER:HB2	3:A:185:ALA:HB2	1.75	0.67
3:A:299:ARG:CG	3:A:310:PRO:HD3	2.24	0.67
1:T:6:DG:N7	5:T:652:HOH:O	2.27	0.66
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.76	0.66
3:A:327:TYR:HD1	3:A:328:ARG:N	1.93	0.66
3:A:88:ILE:HG22	3:A:89:ARG:N	2.10	0.66
3:A:18:MET:HG2	3:A:19:LEU:N	2.05	0.66
2:P:5:DA:H1'	5:P:565:HOH:O	1.96	0.66
3:A:299:ARG:CD	3:A:310:PRO:HD3	2.25	0.66
3:A:152:ARG:HA	3:A:155:MET:HB2	1.78	0.66
3:A:157:GLN:HE22	3:A:244:LYS:HZ1	1.43	0.65
3:A:299:ARG:HG2	3:A:310:PRO:CD	2.26	0.65
3:A:243:SER:OG	3:A:249:GLU:HG3	1.97	0.65
3:A:128:ASN:N	3:A:128:ASN:HD22	1.94	0.65
3:A:285:HIS:NE2	5:A:583:HOH:O	2.29	0.65
3:A:277:ILE:HD11	3:A:335:GLU:HB3	1.77	0.65
3:A:15:ILE:O	3:A:19:LEU:HB2	1.97	0.65
3:A:200:PHE:O	3:A:262:LYS:N	2.28	0.65
3:A:12:ASN:ND2	5:A:642:HOH:O	2.30	0.64
3:A:277:ILE:CG1	3:A:335:GLU:HB2	2.27	0.64
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.32	0.64
2:P:2:DC:H1'	5:P:635:HOH:O	1.96	0.64
3:A:34:HIS:O	3:A:38:ALA:N	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:73:ILE:HG22	3:A:77:LEU:HD22	1.79	0.64
3:A:253:ARG:NH1	5:A:503:HOH:O	2.30	0.64
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.30	0.64
3:A:15:ILE:CB	3:A:46:ILE:HD11	2.28	0.64
3:A:127:LYS:HB2	3:A:128:ASN:ND2	2.13	0.64
3:A:121:THR:HG23	3:A:124:ASP:CG	2.24	0.63
2:P:2:DC:C6	2:P:2:DC:C2'	2.81	0.63
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.28	0.63
1:T:6:DG:O6	2:P:2:DC:N3	2.31	0.63
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.62	0.63
3:A:180:SER:HA	3:A:183:ARG:HE	1.64	0.63
3:A:276:ASP:O	3:A:280:LYS:HG3	1.98	0.63
3:A:265:TYR:O	3:A:268:GLY:N	2.32	0.62
3:A:286:ALA:O	3:A:291:PHE:N	2.31	0.62
3:A:99:PHE:HD2	3:A:100:LEU:HD13	1.62	0.62
3:A:248:LYS:O	3:A:248:LYS:HG2	1.98	0.62
3:A:180:SER:CB	3:A:183:ARG:HH21	2.12	0.62
3:A:270:LEU:HD21	3:A:282:MET:CE	2.29	0.62
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.34	0.62
3:A:26:GLU:HA	3:A:30:SER:OG	1.99	0.61
3:A:180:SER:CA	3:A:183:ARG:HH21	2.12	0.61
3:A:282:MET:HE3	5:A:555:HOH:O	2.00	0.61
3:A:254:ARG:CZ	3:A:254:ARG:HB3	2.31	0.61
3:A:180:SER:HA	3:A:183:ARG:HH21	1.66	0.60
2:P:5:DA:H2'	2:P:6:DT:H71	1.83	0.60
3:A:18:MET:CE	3:A:76:PHE:HB2	2.31	0.60
3:A:278:PHE:HB2	3:A:333:ARG:O	2.01	0.60
3:A:182:ARG:HG2	3:A:182:ARG:NH1	2.08	0.60
3:A:242:PRO:HB2	5:A:589:HOH:O	2.02	0.60
3:A:331:LYS:HG2	3:A:332:ASP:N	2.06	0.60
3:A:309:GLU:N	3:A:309:GLU:OE1	2.34	0.60
3:A:181:PHE:HD1	5:A:530:HOH:O	1.85	0.60
3:A:16:THR:O	3:A:20:THR:HG23	2.02	0.59
3:A:29:VAL:HA	3:A:97:ILE:HD12	1.83	0.59
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.31	0.59
3:A:328:ARG:HB2	3:A:333:ARG:HD3	1.84	0.59
3:A:73:ILE:HG22	3:A:77:LEU:CD2	2.31	0.59
3:A:83:ARG:O	3:A:86:GLU:N	2.35	0.59
3:A:125:LEU:HD22	3:A:132:LEU:HD21	1.84	0.59
3:A:92:ASP:HB3	5:A:647:HOH:O	2.02	0.59
3:A:123:GLU:O	3:A:127:LYS:HG2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:56:GLY:O	3:A:59:ALA:HB3	2.03	0.58
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.84	0.58
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.19	0.58
3:A:277:ILE:HG13	3:A:335:GLU:HB2	1.86	0.58
3:A:245:ASN:H	3:A:245:ASN:HD22	0.73	0.58
3:A:323:ILE:O	3:A:324:GLN:HG2	2.04	0.58
2:P:1:DT:H2''	2:P:2:DC:C5'	2.34	0.58
3:A:82:LEU:CD2	3:A:85:LEU:HB2	2.31	0.58
3:A:264:GLN:NE2	3:A:296:TYR:HB3	2.19	0.58
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.34	0.58
3:A:29:VAL:HG21	3:A:94:SER:CB	2.33	0.58
3:A:180:SER:HB3	3:A:183:ARG:NH2	2.18	0.58
3:A:150:ILE:CG1	3:A:253:ARG:HG2	2.34	0.58
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.39	0.57
3:A:60:LYS:HA	3:A:65:VAL:HG12	1.87	0.57
3:A:59:ALA:O	3:A:62:LEU:HB2	2.05	0.57
3:A:201:THR:HA	3:A:261:PRO:CA	2.33	0.57
3:A:326:LYS:HG3	3:A:326:LYS:O	2.04	0.57
3:A:141:LYS:HE2	3:A:142:TYR:CZ	2.39	0.57
3:A:180:SER:HB2	3:A:185:ALA:CB	2.35	0.57
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.20	0.57
3:A:203:GLU:O	3:A:205:THR:N	2.37	0.57
3:A:255:ILE:HG12	3:A:256:ASP:N	2.20	0.57
3:A:169:VAL:HG13	3:A:170:ASP:H	1.70	0.56
2:P:6:DT:H5'	5:P:567:HOH:O	2.04	0.56
3:A:226:ASP:HB2	3:A:238:VAL:HG23	1.88	0.56
3:A:93:THR:HG22	3:A:94:SER:N	2.20	0.56
3:A:82:LEU:HD23	3:A:85:LEU:CB	2.31	0.56
3:A:128:ASN:N	3:A:128:ASN:ND2	2.53	0.56
3:A:111:ALA:O	3:A:115:VAL:HG23	2.06	0.56
3:A:323:ILE:C	3:A:324:GLN:HG2	2.31	0.56
3:A:129:GLU:O	3:A:137:ARG:NE	2.34	0.56
3:A:134:HIS:O	3:A:137:ARG:HB2	2.06	0.56
3:A:205:THR:HA	5:A:624:HOH:O	2.06	0.56
3:A:207:GLN:HB2	5:A:625:HOH:O	2.06	0.55
3:A:254:ARG:HB3	3:A:254:ARG:NH1	2.21	0.55
3:A:217:GLN:O	3:A:221:VAL:HG13	2.06	0.55
3:A:11:LEU:H	3:A:11:LEU:CD2	2.18	0.55
3:A:155:MET:HA	3:A:158:MET:HE3	1.88	0.55
3:A:142:TYR:CE2	3:A:238:VAL:HG11	2.41	0.55
3:A:253:ARG:HG3	3:A:253:ARG:HH11	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:27:LYS:HG3	3:A:28:ASN:ND2	2.22	0.55
3:A:210:LEU:HB3	3:A:259:LEU:HD21	1.88	0.54
3:A:243:SER:HB3	3:A:249:GLU:CA	2.28	0.54
3:A:316:GLU:O	3:A:320:PHE:HD1	1.89	0.54
2:P:1:DT:H2'	2:P:2:DC:C6	2.42	0.54
3:A:15:ILE:CG2	3:A:46:ILE:HD11	2.37	0.54
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.37	0.54
3:A:176:THR:HG22	3:A:177:VAL:N	2.23	0.54
2:P:1:DT:H2''	2:P:2:DC:O4'	2.08	0.54
3:A:133:ASN:H	3:A:136:GLN:HE21	1.55	0.54
3:A:295:GLU:HA	5:A:592:HOH:O	2.05	0.54
3:A:326:LYS:O	3:A:328:ARG:HG2	2.07	0.54
3:A:81:LYS:HZ2	3:A:86:GLU:CB	2.21	0.54
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.90	0.54
3:A:155:MET:CE	3:A:188:SER:HB2	2.36	0.54
2:P:2:DC:C6	2:P:2:DC:H2'	2.43	0.54
3:A:286:ALA:HB2	3:A:323:ILE:HG21	1.90	0.54
3:A:287:LEU:HD13	3:A:291:PHE:O	2.08	0.54
3:A:288:GLU:C	3:A:290:GLY:H	2.16	0.54
3:A:49:TYR:CE2	3:A:51:HIS:HB2	2.44	0.53
2:P:5:DA:C2'	2:P:6:DT:H5''	2.37	0.53
3:A:292:THR:O	3:A:298:ILE:HA	2.08	0.53
3:A:82:LEU:HD22	3:A:85:LEU:HD22	1.91	0.53
3:A:196:THR:OG1	3:A:262:LYS:HA	2.08	0.53
3:A:295:GLU:N	3:A:295:GLU:OE1	2.35	0.53
2:P:6:DT:H5'	2:P:6:DT:H6	1.74	0.53
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.90	0.53
3:A:169:VAL:HG13	3:A:170:ASP:N	2.23	0.53
3:A:200:PHE:C	3:A:201:THR:HG22	2.33	0.53
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.73	0.53
3:A:299:ARG:HG2	3:A:310:PRO:N	2.24	0.53
3:A:103:VAL:CB	3:A:106:ILE:HD12	2.37	0.52
3:A:11:LEU:HD23	3:A:11:LEU:N	2.21	0.52
3:A:212:HIS:N	3:A:212:HIS:CD2	2.74	0.52
3:A:40:ARG:O	3:A:44:SER:HB3	2.09	0.52
3:A:292:THR:HG23	5:A:580:HOH:O	2.09	0.52
3:A:294:ASN:HB2	3:A:295:GLU:OE1	2.09	0.52
3:A:303:VAL:C	3:A:305:GLY:H	2.17	0.52
3:A:330:PRO:CA	3:A:333:ARG:HG2	2.37	0.52
3:A:207:GLN:O	3:A:210:LEU:N	2.41	0.52
3:A:217:GLN:NE2	3:A:217:GLN:HA	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:6:DT:H2''	2:P:7:DG:C8	2.44	0.52
3:A:36:TYR:CD2	3:A:37:ASN:N	2.78	0.52
3:A:152:ARG:O	3:A:155:MET:HB2	2.10	0.51
3:A:182:ARG:HH11	3:A:273:THR:CG2	2.23	0.51
3:A:183:ARG:HD3	3:A:273:THR:O	2.10	0.51
3:A:215:VAL:HG12	3:A:219:GLN:OE1	2.10	0.51
3:A:100:LEU:HD21	3:A:120:LYS:HA	1.91	0.51
3:A:182:ARG:O	3:A:182:ARG:HG3	2.10	0.51
3:A:271:TYR:CE1	3:A:283:ARG:NH2	2.78	0.51
3:A:81:LYS:HZ2	3:A:86:GLU:HB2	1.76	0.51
3:A:31:GLN:N	5:A:641:HOH:O	2.27	0.51
3:A:320:PHE:CE2	3:A:328:ARG:HG3	2.46	0.51
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.59	0.51
3:A:81:LYS:NZ	3:A:86:GLU:HB2	2.25	0.50
3:A:277:ILE:HD11	3:A:335:GLU:CB	2.41	0.50
3:A:240:GLN:NE2	3:A:252:HIS:CE1	2.80	0.50
3:A:149:ARG:NH2	3:A:188:SER:HA	2.27	0.50
3:A:151:PRO:HD2	3:A:154:GLU:CD	2.36	0.50
3:A:253:ARG:HD3	5:A:521:HOH:O	2.11	0.50
3:A:254:ARG:NH1	3:A:255:ILE:O	2.45	0.50
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.94	0.50
3:A:182:ARG:HH11	3:A:273:THR:HG21	1.73	0.50
3:A:202:SER:H	3:A:261:PRO:HB3	1.77	0.50
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.46	0.50
3:A:129:GLU:CG	3:A:137:ARG:HD3	2.40	0.49
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.42	0.49
3:A:210:LEU:CB	3:A:259:LEU:HD21	2.41	0.49
3:A:270:LEU:CD2	3:A:282:MET:HE1	2.37	0.49
3:A:29:VAL:HG21	3:A:94:SER:HA	1.95	0.49
3:A:41:LYS:HD3	3:A:42:ALA:N	2.24	0.49
3:A:283:ARG:HG2	3:A:293:ILE:HB	1.95	0.49
2:P:5:DA:C2'	2:P:6:DT:H71	2.41	0.49
3:A:15:ILE:HG21	3:A:46:ILE:CD1	2.43	0.49
3:A:59:ALA:O	3:A:62:LEU:N	2.41	0.49
3:A:243:SER:O	3:A:244:LYS:O	2.31	0.49
3:A:240:GLN:NE2	3:A:250:TYR:O	2.41	0.48
3:A:68:LYS:HB2	3:A:68:LYS:NZ	2.28	0.48
3:A:195:LEU:HA	3:A:195:LEU:HD12	1.32	0.48
3:A:103:VAL:HG22	3:A:143:PHE:CD2	2.48	0.48
2:P:7:DG:H4'	5:P:665:HOH:O	2.13	0.48
3:A:35:LYS:O	3:A:38:ALA:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:182:ARG:HH11	3:A:182:ARG:CG	2.16	0.48
3:A:200:PHE:O	3:A:261:PRO:HA	2.13	0.48
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.31	0.48
3:A:77:LEU:N	3:A:77:LEU:CD1	2.76	0.48
3:A:119:ILE:HA	3:A:124:ASP:HB3	1.95	0.48
3:A:149:ARG:HH21	3:A:187:SER:C	2.22	0.48
3:A:271:TYR:CD1	3:A:283:ARG:NH2	2.81	0.48
3:A:211:LEU:HD12	3:A:211:LEU:C	2.39	0.48
3:A:133:ASN:HD21	3:A:135:HIS:HB3	1.79	0.48
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.54	0.48
3:A:278:PHE:CE1	3:A:328:ARG:HD3	2.49	0.48
3:A:45:VAL:HG21	3:A:63:PRO:O	2.14	0.48
3:A:114:PHE:CZ	3:A:132:LEU:HD23	2.48	0.48
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.42	0.47
3:A:33:ILE:O	3:A:37:ASN:HB2	2.13	0.47
3:A:218:LEU:HD13	3:A:218:LEU:H	1.78	0.47
3:A:259:LEU:HD12	3:A:259:LEU:HA	1.36	0.47
3:A:18:MET:HE1	3:A:76:PHE:CB	2.42	0.47
3:A:22:LEU:HD21	3:A:82:LEU:HD21	1.97	0.47
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.30	0.47
1:T:6:DG:H2''	1:T:7:DA:H8	1.74	0.47
3:A:32:ALA:HB1	3:A:35:LYS:HB2	1.97	0.47
3:A:83:ARG:O	3:A:87:LYS:N	2.44	0.47
3:A:156:LEU:HD23	3:A:156:LEU:HA	1.69	0.47
3:A:44:SER:O	3:A:47:ALA:HB3	2.15	0.46
3:A:76:PHE:HD2	3:A:77:LEU:HD12	1.80	0.46
3:A:129:GLU:HG2	3:A:137:ARG:CD	2.43	0.46
3:A:254:ARG:NH2	5:A:657:HOH:O	2.48	0.46
3:A:81:LYS:NZ	3:A:86:GLU:CB	2.79	0.46
3:A:29:VAL:HG21	3:A:94:SER:OG	2.16	0.46
3:A:202:SER:N	3:A:261:PRO:HB3	2.30	0.46
3:A:266:TYR:HA	3:A:269:VAL:HB	1.96	0.46
3:A:33:ILE:O	3:A:36:TYR:HD2	1.98	0.46
3:A:130:ASP:HA	3:A:137:ARG:HH21	1.81	0.46
3:A:174:ILE:O	3:A:195:LEU:HD12	2.16	0.46
3:A:177:VAL:HG22	3:A:193:VAL:HG22	1.97	0.46
3:A:140:LEU:HD12	3:A:140:LEU:O	2.16	0.46
3:A:38:ALA:O	3:A:41:LYS:HD3	2.16	0.45
3:A:15:ILE:CG2	3:A:46:ILE:CD1	2.94	0.45
3:A:18:MET:HE2	3:A:82:LEU:HD13	1.97	0.45
2:P:6:DT:C2'	2:P:7:DG:C8	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:19:LEU:HB3	3:A:43:ALA:HB2	1.98	0.45
3:A:22:LEU:HD13	3:A:22:LEU:HA	1.43	0.45
2:P:5:DA:O5'	3:A:107:GLY:HA3	2.16	0.45
3:A:133:ASN:ND2	3:A:135:HIS:H	2.13	0.45
3:A:244:LYS:C	3:A:246:ASP:H	2.23	0.45
3:A:208:PRO:HB3	3:A:232:GLU:HB2	1.97	0.45
3:A:79:THR:C	3:A:81:LYS:H	2.25	0.45
3:A:135:HIS:C	3:A:135:HIS:CD2	2.95	0.45
3:A:270:LEU:HA	3:A:316:GLU:OE2	2.16	0.45
3:A:245:ASN:ND2	3:A:245:ASN:N	2.28	0.45
1:T:7:DA:H61	2:P:1:DT:H3	1.64	0.45
3:A:218:LEU:N	3:A:218:LEU:CD1	2.79	0.45
3:A:182:ARG:NH1	3:A:182:ARG:CG	2.78	0.45
3:A:138:ILE:HG21	3:A:228:LEU:HD11	1.99	0.45
3:A:303:VAL:O	3:A:305:GLY:N	2.50	0.45
3:A:302:GLY:N	3:A:307:ALA:CB	2.79	0.44
3:A:293:ILE:HD12	3:A:293:ILE:HG23	1.47	0.44
3:A:214:VAL:O	3:A:218:LEU:HD13	2.17	0.44
3:A:205:THR:HG23	3:A:205:THR:O	2.18	0.44
3:A:260:ILE:HG22	3:A:261:PRO:N	2.32	0.44
3:A:29:VAL:HG21	3:A:94:SER:CA	2.48	0.44
3:A:60:LYS:C	3:A:62:LEU:H	2.26	0.44
2:P:7:DG:C4'	5:P:665:HOH:O	2.64	0.44
3:A:27:LYS:HB2	3:A:36:TYR:CD1	2.53	0.44
3:A:250:TYR:HB3	5:A:577:HOH:O	2.16	0.44
3:A:259:LEU:HD12	3:A:260:ILE:H	1.82	0.44
3:A:265:TYR:HB3	3:A:266:TYR:H	1.55	0.44
3:A:329:GLU:O	3:A:333:ARG:HG2	2.18	0.44
3:A:85:LEU:HD12	3:A:85:LEU:HA	1.96	0.44
3:A:197:HIS:HD1	3:A:199:SER:HB3	1.81	0.44
2:P:1:DT:H2''	2:P:2:DC:H5'	1.99	0.43
3:A:235:PHE:CD2	3:A:235:PHE:C	2.95	0.43
3:A:172:GLU:HG2	3:A:198:PRO:HG2	2.00	0.43
3:A:103:VAL:CG1	3:A:106:ILE:HD12	2.49	0.43
3:A:23:ALA:HB2	3:A:39:TYR:HB2	2.00	0.43
3:A:100:LEU:HA	3:A:100:LEU:HD12	1.60	0.43
3:A:100:LEU:O	3:A:106:ILE:HG21	2.17	0.43
3:A:12:ASN:HD21	3:A:53:ILE:H	1.67	0.43
3:A:260:ILE:CG2	3:A:261:PRO:CD	2.97	0.43
3:A:302:GLY:H	3:A:307:ALA:CB	2.32	0.43
3:A:303:VAL:C	3:A:305:GLY:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:319:ILE:O	3:A:322:TYR:HB2	2.19	0.43
3:A:138:ILE:HD11	3:A:226:ASP:HB3	2.01	0.43
3:A:204:SER:O	3:A:206:LYS:N	2.52	0.43
3:A:302:GLY:N	3:A:307:ALA:HB2	2.34	0.43
3:A:22:LEU:HD22	3:A:85:LEU:HD13	2.01	0.42
3:A:79:THR:O	3:A:81:LYS:N	2.51	0.42
3:A:188:SER:HB3	5:A:522:HOH:O	2.19	0.42
3:A:227:THR:HG21	3:A:230:LYS:HB2	2.01	0.42
3:A:266:TYR:O	3:A:270:LEU:HB2	2.19	0.42
3:A:299:ARG:HE	3:A:299:ARG:HB2	1.66	0.42
3:A:19:LEU:HD23	3:A:43:ALA:N	2.33	0.42
3:A:55:SER:O	3:A:58:GLU:HB3	2.19	0.42
3:A:99:PHE:CD2	3:A:99:PHE:C	2.97	0.42
3:A:309:GLU:HA	3:A:310:PRO:HD2	1.61	0.42
3:A:28:ASN:ND2	3:A:28:ASN:N	2.59	0.42
3:A:32:ALA:O	3:A:36:TYR:HB3	2.19	0.42
3:A:82:LEU:CD2	3:A:85:LEU:HD22	2.50	0.42
3:A:327:TYR:HD1	3:A:327:TYR:C	2.27	0.42
3:A:195:LEU:O	3:A:260:ILE:N	2.53	0.42
3:A:41:LYS:HE2	3:A:64:GLY:HA2	1.95	0.42
3:A:197:HIS:CD2	3:A:198:PRO:CD	3.00	0.42
3:A:270:LEU:CD2	3:A:319:ILE:HG21	2.50	0.42
3:A:288:GLU:O	3:A:290:GLY:N	2.53	0.42
3:A:327:TYR:C	3:A:327:TYR:CD1	2.98	0.41
3:A:26:GLU:HA	3:A:30:SER:HG	1.84	0.41
3:A:56:GLY:O	3:A:59:ALA:N	2.54	0.41
3:A:328:ARG:HB2	3:A:333:ARG:CD	2.50	0.41
3:A:60:LYS:C	3:A:62:LEU:N	2.76	0.41
3:A:97:ILE:HD13	3:A:112:ARG:HG2	2.01	0.41
3:A:149:ARG:NH2	3:A:188:SER:CA	2.84	0.41
3:A:207:GLN:O	3:A:210:LEU:HB2	2.20	0.41
2:P:2:DC:C6	2:P:2:DC:O4'	2.71	0.41
3:A:191:MET:CG	3:A:255:ILE:HG13	2.50	0.41
1:T:6:DG:C6	2:P:2:DC:N3	2.89	0.41
3:A:25:PHE:CE1	3:A:88:ILE:HG12	2.55	0.41
1:T:6:DG:N1	2:P:2:DC:O2	2.41	0.41
3:A:286:ALA:O	3:A:291:PHE:HB2	2.19	0.41
3:A:56:GLY:H	3:A:74:ASP:CG	2.28	0.41
3:A:241:LEU:HB2	3:A:250:TYR:CG	2.56	0.41
3:A:309:GLU:O	3:A:311:LEU:HD13	2.21	0.41
3:A:180:SER:HA	3:A:183:ARG:NH2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:277:ILE:CG1	3:A:335:GLU:CB	2.97	0.40
1:T:4:DT:H1'	5:T:527:HOH:O	2.21	0.40
3:A:210:LEU:HB2	3:A:259:LEU:CD2	2.51	0.40
3:A:12:ASN:HD22	3:A:12:ASN:HA	1.75	0.40
3:A:194:LEU:N	3:A:194:LEU:HD12	2.35	0.40
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.56	0.40
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	325/335 (97%)	272 (84%)	33 (10%)	20 (6%)	1 9

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	32	ALA
3	A	185	ALA
3	A	202	SER
3	A	204	SER
3	A	205	THR
3	A	244	LYS
3	A	265	TYR
3	A	295	GLU
3	A	266	TYR
3	A	289	LYS
3	A	304	THR
3	A	222	HIS
3	A	10	THR
3	A	91	ASP

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Mol	Chain	Res	Type
3	A	207	GLN
3	A	13	GLY
3	A	206	LYS
3	A	309	GLU
3	A	80	GLY
3	A	310	PRO

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%)	212 (74%)	76 (26%)	0 3

All (76) 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	30	SER
3	A	37	ASN
3	A	41	LYS
3	A	44	SER
3	A	45	VAL
3	A	46	ILE
3	A	52	LYS
3	A	62	LEU
3	A	67	THR
3	A	68	LYS
3	A	77	LEU
3	A	79	THR
3	A	81	LYS
3	A	88	ILE
3	A	89	ARG

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Mol	Chain	Res	Type
3	A	92	ASP
3	A	93	THR
3	A	100	LEU
3	A	101	THR
3	A	102	ARG
3	A	113	LYS
3	A	119	ILE
3	A	121	THR
3	A	122	LEU
3	A	128	ASN
3	A	133	ASN
3	A	138	ILE
3	A	145	ASP
3	A	153	GLU
3	A	159	GLN
3	A	161	ILE
3	A	168	LYS
3	A	180	SER
3	A	182	ARG
3	A	191	MET
3	A	201	THR
3	A	203	GLU
3	A	213	GLN
3	A	214	VAL
3	A	217	GLN
3	A	218	LEU
3	A	221	VAL
3	A	228	LEU
3	A	230	LYS
3	A	233	THR
3	A	236	MET
3	A	238	VAL
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	263	ASP
3	A	264	GLN
3	A	272	PHE
3	A	277	ILE
3	A	279	ASN
3	A	287	LEU
3	A	292	THR

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Mol	Chain	Res	Type
3	A	293	ILE
3	A	294	ASN
3	A	295	GLU
3	A	298	ILE
3	A	301	LEU
3	A	304	THR
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	324	GLN
3	A	325	TRP
3	A	329	GLU
3	A	331	LYS
3	A	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) 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	98	ASN
3	A	128	ASN
3	A	133	ASN
3	A	136	GLN
3	A	157	GLN
3	A	217	GLN
3	A	245	ASN
3	A	252	HIS
3	A	264	GLN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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, 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%)	-0.66	0 100 100	25, 38, 88, 98	0
2	P	7/7 (100%)	-0.84	0 100 100	14, 23, 49, 70	0
3	A	325/335 (97%)	-0.94	0 100 100	1, 31, 84, 100	0
All	All	340/350 (97%)	-0.93	0 100 100	1, 32, 86, 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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CA	A	342	1/1	0.93	0.08	92,92,92,92	0
4	CA	A	340	1/1	0.97	0.04	93,93,93,93	0
4	CA	A	341	1/1	0.99	0.04	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.