



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:39 PM UTC

PDB ID : 9ICY / pdb_00009icy
Title : DNA POLYMERASE BETA (E.C.2.7.7.7) COMPLEXED WITH SEVEN
BASE PAIRS OF DNA (NON GAPPED DNA ONLY)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-10-24
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

<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
Mogul : 2022.3.0, CSD as543be (2022)
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

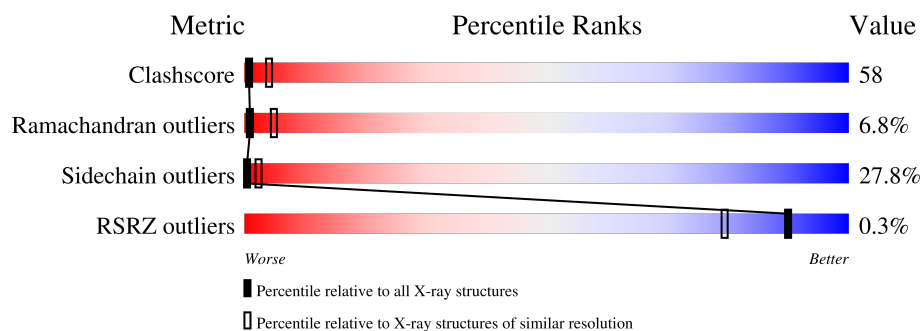
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	7	100%
2	P	7	29% 71%
3	A	335	19% 41% 30% 8% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3040 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*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	7	Total	C	N	O	P	0	0	0
			141	69	27	39	6			

- 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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is water.

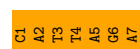
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	15	Total	O	0	0
			15	15		
6	P	16	Total	O	0	0
			16	16		
6	A	94	Total	O	0	0
			94	94		

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*A)-3')

Chain T: 

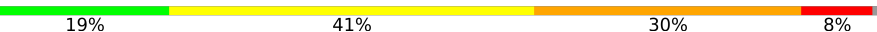


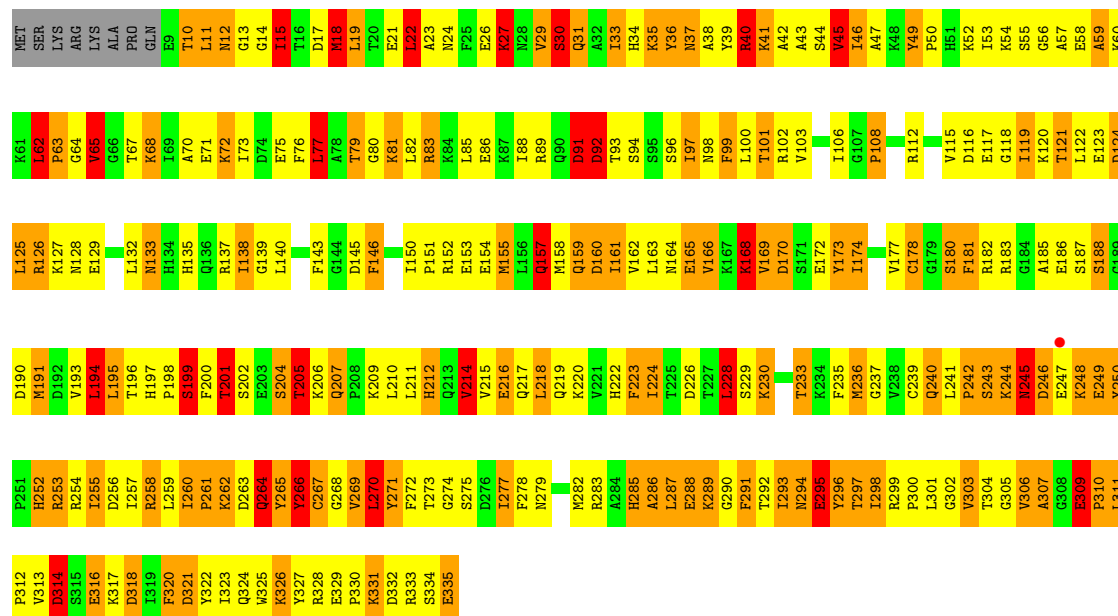
- Molecule 2: DNA (5'-D(*TP*CP*TP*AP*AP*TP*G)-3')

Chain P: 



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

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	180.83Å 57.65Å 48.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-3.00) 93.3 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.87Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.181 , (Not available) 0.176 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 275.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3040	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.81% 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: SO4, 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	0.92	0/158	2.88	13/242 (5.4%)
2	P	1.12	1/160 (0.6%)	3.43	15/243 (6.2%)
3	A	1.61	20/2672 (0.7%)	2.21	140/3590 (3.9%)
All	All	1.55	21/2990 (0.7%)	2.35	168/4075 (4.1%)

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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	15	ILE	CA-C	-6.42	1.44	1.52
3	A	63	PRO	C-O	6.38	1.29	1.23
3	A	63	PRO	N-CA	-6.00	1.40	1.47
3	A	178	CYS	CA-C	-5.99	1.46	1.53
2	P	1	DT	OP3-P	5.96	1.60	1.48
3	A	124	ASP	CA-C	-5.94	1.45	1.52
3	A	161	ILE	CA-CB	-5.88	1.47	1.54
3	A	246	ASP	CA-C	5.64	1.60	1.52
3	A	31	GLN	N-CA	-5.42	1.38	1.46
3	A	106	ILE	C-O	-5.29	1.18	1.24
3	A	30	SER	C-N	-5.28	1.26	1.33
3	A	75	GLU	C-N	-5.24	1.26	1.33
3	A	242	PRO	N-CA	-5.13	1.40	1.47
3	A	224	ILE	CA-C	-5.13	1.46	1.52
3	A	170	ASP	N-CA	-5.12	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	160	ASP	CG-OD2	5.11	1.35	1.25
3	A	94	SER	C-O	-5.09	1.18	1.24
3	A	269	VAL	N-CA	-5.05	1.40	1.46
3	A	62	LEU	C-N	-5.04	1.29	1.33
3	A	124	ASP	N-CA	-5.03	1.40	1.46
3	A	65	VAL	CA-C	-5.02	1.48	1.53

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	6	DT	C2-N1-C1'	20.57	150.20	119.35
2	P	6	DT	C6-N1-C1'	-19.21	90.53	119.35
1	T	7	DA	C4-N9-C1'	-18.59	99.16	127.05
1	T	7	DA	C8-N9-C1'	17.14	152.76	127.05
2	P	1	DT	C6-N1-C1'	-15.62	95.92	119.35
2	P	1	DT	C2-N1-C1'	15.49	142.58	119.35
1	T	4	DT	C6-N1-C1'	-14.47	97.64	119.35
1	T	4	DT	C2-N1-C1'	13.82	140.08	119.35
2	P	3	DT	C2-N1-C1'	12.45	138.02	119.35
3	A	246	ASP	CA-CB-CG	-12.38	100.22	112.60
2	P	3	DT	C6-N1-C1'	-11.77	101.70	119.35
3	A	49	TYR	CA-C-N	11.27	133.93	119.84
3	A	49	TYR	C-N-CA	11.27	133.93	119.84
2	P	2	DC	C6-N1-C1'	-10.89	103.36	119.70
2	P	2	DC	C2-N1-C1'	10.77	135.85	119.70
2	P	7	DG	C4-N9-C1'	-10.26	111.61	127.00
2	P	7	DG	C8-N9-C1'	9.82	141.73	127.00
1	T	5	DA	C8-N9-C1'	9.24	140.91	127.05
3	A	161	ILE	N-CA-C	9.23	119.28	110.42
1	T	5	DA	C4-N9-C1'	-8.82	113.82	127.05
3	A	223	PHE	N-CA-C	-8.67	101.55	112.90
2	P	5	DA	C4-N9-C1'	8.49	139.78	127.05
3	A	27	LYS	CB-CA-C	8.47	124.01	110.96
3	A	291	PHE	N-CA-C	8.30	120.19	108.74
2	P	3	DT	P-O3'-C3'	8.26	132.59	120.20
3	A	157	GLN	N-CA-CB	8.20	122.29	110.16
3	A	65	VAL	N-CA-CB	8.08	120.87	111.66
3	A	98	ASN	CA-CB-CG	-7.94	104.66	112.60
3	A	124	ASP	N-CA-C	-7.87	102.70	111.28
3	A	271	TYR	N-CA-C	7.74	119.41	110.97
3	A	40	ARG	N-CA-C	7.73	119.71	111.28
1	T	2	DA	C4-N9-C1'	-7.70	115.50	127.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	12	ASN	N-CA-CB	7.57	121.81	110.53
2	P	5	DA	C8-N9-C1'	-7.55	115.72	127.05
3	A	252	HIS	CA-CB-CG	-7.55	106.25	113.80
1	T	2	DA	C8-N9-C1'	7.54	138.36	127.05
3	A	245	ASN	CA-C-N	7.45	135.76	121.54
3	A	245	ASN	C-N-CA	7.45	135.76	121.54
3	A	212	HIS	CA-CB-CG	-7.37	106.44	113.80
3	A	65	VAL	N-CA-C	7.29	118.30	107.15
1	T	1	DC	P-O3'-C3'	7.29	131.13	120.20
3	A	264	GLN	CB-CG-CD	-7.27	100.24	112.60
3	A	181	PHE	CA-CB-CG	-7.24	106.56	113.80
3	A	146	PHE	CA-CB-CG	-7.23	106.57	113.80
3	A	309	GLU	N-CA-C	7.10	125.50	109.81
3	A	309	GLU	CA-C-N	7.09	128.70	119.84
3	A	309	GLU	C-N-CA	7.09	128.70	119.84
3	A	250	TYR	N-CA-C	7.07	120.05	110.29
3	A	116	ASP	CB-CA-C	7.07	124.17	110.46
3	A	214	VAL	N-CA-CB	6.97	120.02	110.54
3	A	159	GLN	CB-CA-C	-6.93	99.72	110.81
3	A	155	MET	O-C-N	6.93	129.21	122.07
3	A	222	HIS	CA-CB-CG	-6.84	106.96	113.80
3	A	211	LEU	CA-C-N	6.77	130.26	120.38
3	A	211	LEU	C-N-CA	6.77	130.26	120.38
1	T	4	DT	P-O5'-C5'	6.70	130.05	120.00
3	A	270	LEU	CA-C-N	6.70	129.49	120.65
3	A	270	LEU	C-N-CA	6.70	129.49	120.65
3	A	321	ASP	CA-CB-CG	-6.70	105.90	112.60
3	A	195	LEU	N-CA-C	6.63	119.70	108.90
3	A	219	GLN	CB-CA-C	-6.59	99.65	110.85
3	A	91	ASP	N-CA-CB	6.58	121.61	110.49
3	A	57	ALA	CA-C-N	6.58	128.99	120.44
3	A	57	ALA	C-N-CA	6.58	128.99	120.44
3	A	240	GLN	N-CA-C	6.42	118.85	108.32
3	A	194	LEU	CA-C-N	-6.41	113.96	122.99
3	A	194	LEU	C-N-CA	-6.41	113.96	122.99
3	A	216	GLU	CB-CG-CD	-6.38	101.75	112.60
3	A	267	CYS	N-CA-C	-6.38	104.25	111.14
3	A	271	TYR	N-CA-CB	-6.38	100.60	109.91
3	A	88	ILE	CB-CA-C	-6.38	103.67	112.02
1	T	7	DA	N9-C1'-C2'	-6.37	103.94	113.50
3	A	62	LEU	N-CA-C	6.31	119.29	110.20
2	P	3	DT	O4'-C1'-N1	6.29	117.84	108.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	241	LEU	O-C-N	6.29	127.57	121.28
3	A	36	TYR	CA-CB-CG	-6.28	102.59	113.90
3	A	35	LYS	N-CA-C	-6.24	104.39	111.07
3	A	186	GLU	N-CA-C	6.21	118.85	111.71
3	A	45	VAL	N-CA-C	6.18	116.82	110.82
3	A	314	ASP	N-CA-CB	6.17	119.73	110.53
3	A	63	PRO	O-C-N	6.17	128.91	122.93
3	A	303	VAL	N-CA-C	6.16	120.58	112.76
3	A	18	MET	CA-C-N	6.14	128.84	120.54
3	A	18	MET	C-N-CA	6.14	128.84	120.54
3	A	40	ARG	N-CA-CB	6.12	119.12	110.12
3	A	24	ASN	CA-CB-CG	-6.11	106.49	112.60
3	A	116	ASP	N-CA-CB	6.10	119.78	110.14
3	A	214	VAL	CB-CA-C	-6.09	103.92	112.14
3	A	92	ASP	N-CA-CB	5.92	118.91	110.16
3	A	267	CYS	O-C-N	5.90	128.47	122.09
3	A	49	TYR	O-C-N	5.90	128.10	121.32
3	A	59	ALA	O-C-N	5.87	128.14	122.03
3	A	170	ASP	N-CA-C	-5.85	99.11	109.06
3	A	257	ILE	CB-CA-C	-5.85	102.53	110.42
3	A	168	LYS	N-CA-CB	5.84	118.82	110.06
2	P	4	DA	P-O3'-C3'	5.83	128.95	120.20
3	A	205	THR	N-CA-CB	5.83	120.34	110.49
1	T	3	DT	P-O5'-C5'	5.79	128.68	120.00
3	A	29	VAL	N-CA-C	5.78	115.97	110.53
3	A	17	ASP	CB-CA-C	5.77	120.37	110.79
3	A	286	ALA	CA-C-N	5.77	128.48	120.29
3	A	286	ALA	C-N-CA	5.77	128.48	120.29
3	A	260	ILE	N-CA-C	5.76	113.91	109.19
3	A	125	LEU	N-CA-CB	5.75	118.51	109.94
3	A	91	ASP	CA-CB-CG	-5.73	106.87	112.60
3	A	267	CYS	CA-C-N	5.73	126.30	119.94
3	A	267	CYS	C-N-CA	5.73	126.30	119.94
3	A	77	LEU	N-CA-CB	5.72	118.63	110.16
3	A	30	SER	CA-C-N	-5.70	114.66	122.87
3	A	30	SER	C-N-CA	-5.70	114.66	122.87
3	A	173	TYR	CB-CA-C	-5.70	101.29	109.84
3	A	243	SER	CA-C-N	5.68	132.38	121.54
3	A	243	SER	C-N-CA	5.68	132.38	121.54
3	A	266	TYR	CA-CB-CG	-5.66	103.72	113.90
3	A	161	ILE	N-CA-CB	5.63	117.14	110.55
3	A	34	HIS	CA-CB-CG	-5.60	108.20	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	99	PHE	N-CA-C	5.56	118.18	111.40
3	A	70	ALA	CA-C-N	5.50	127.59	120.44
3	A	70	ALA	C-N-CA	5.50	127.59	120.44
3	A	97	ILE	CB-CA-C	-5.49	104.94	111.97
3	A	58	GLU	O-C-N	5.49	127.72	122.07
3	A	62	LEU	CA-C-O	5.48	126.89	120.87
3	A	173	TYR	N-CA-C	5.45	118.25	110.24
3	A	313	VAL	N-CA-C	5.44	115.69	107.80
3	A	155	MET	CA-C-N	5.43	127.82	120.38
3	A	155	MET	C-N-CA	5.43	127.82	120.38
3	A	88	ILE	N-CA-C	5.43	115.63	110.53
3	A	181	PHE	O-C-N	5.43	127.73	122.09
3	A	261	PRO	N-CA-CB	5.42	106.86	103.23
3	A	15	ILE	N-CA-CB	5.42	117.24	110.47
3	A	318	ASP	CA-CB-CG	-5.40	107.20	112.60
3	A	117	GLU	N-CA-C	-5.38	106.56	113.23
3	A	296	TYR	CB-CA-C	-5.35	102.26	109.16
3	A	181	PHE	CA-C-N	5.33	128.42	120.31
3	A	181	PHE	C-N-CA	5.33	128.42	120.31
3	A	72	LYS	N-CA-C	-5.31	105.58	111.36
3	A	11	LEU	N-CA-CB	5.30	118.47	110.30
3	A	285	HIS	CA-CB-CG	-5.29	108.50	113.80
3	A	17	ASP	N-CA-C	5.29	117.04	111.28
3	A	313	VAL	N-CA-CB	-5.29	104.80	111.46
3	A	320	PHE	O-C-N	5.29	127.53	122.03
3	A	129	GLU	CB-CG-CD	-5.27	103.64	112.60
3	A	125	LEU	CB-CA-C	5.27	119.24	110.81
3	A	230	LYS	CA-C-N	5.26	127.15	122.47
3	A	230	LYS	C-N-CA	5.26	127.15	122.47
3	A	295	GLU	CB-CG-CD	5.26	121.54	112.60
3	A	97	ILE	N-CA-CB	5.25	116.69	110.55
3	A	102	ARG	CD-NE-CZ	-5.25	117.06	124.40
3	A	83	ARG	N-CA-CB	5.23	117.65	110.07
3	A	63	PRO	N-CA-CB	5.22	106.73	103.23
3	A	12	ASN	CB-CA-C	5.22	118.73	109.65
3	A	288	GLU	N-CA-C	-5.22	105.50	111.14
3	A	116	ASP	CA-CB-CG	-5.20	107.40	112.60
3	A	309	GLU	CB-CA-C	5.20	120.40	110.17
3	A	205	THR	N-CA-C	5.18	121.84	110.80
3	A	165	GLU	O-C-N	5.18	127.69	122.09
3	A	216	GLU	CA-C-N	-5.17	113.59	120.63
3	A	216	GLU	C-N-CA	-5.17	113.59	120.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	250	TYR	CA-C-O	5.14	125.23	120.60
3	A	139	GLY	CA-C-N	5.14	127.42	120.44
3	A	139	GLY	C-N-CA	5.14	127.42	120.44
3	A	228	LEU	N-CA-C	-5.12	105.15	111.40
3	A	297	THR	N-CA-C	5.11	114.98	108.24
3	A	108	PRO	N-CA-CB	5.07	108.90	103.33
3	A	201	THR	N-CA-CB	-5.04	103.75	111.56
1	T	6	DG	O4'-C1'-N9	5.03	115.95	108.40
3	A	160	ASP	CB-CA-C	-5.02	102.78	110.81
3	A	22	LEU	N-CA-CB	-5.01	102.75	110.01

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	12	ASN	CA
3	A	309	GLU	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	141	0	81	7	0
2	P	144	0	81	7	0
3	A	2623	0	2641	316	0
4	A	5	0	0	0	0
5	A	2	0	0	0	0
6	A	94	0	0	15	0
6	P	16	0	0	0	0
6	T	15	0	0	2	0
All	All	3040	0	2803	329	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 58.

All (329) 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:180:SER:HB3	3:A:183:ARG:HH21	1.15	1.09
3:A:151:PRO:HG2	3:A:154:GLU:HG3	1.33	1.09
3:A:270:LEU:HD21	3:A:282:MET:HE1	1.35	1.08
2:P:1:DT:H2''	2:P:2:DC:H5'	1.32	1.07
3:A:245:ASN:N	3:A:245:ASN:HD22	1.55	1.02
3:A:243:SER:HB3	3:A:249:GLU:HA	1.38	1.01
3:A:41:LYS:HE2	3:A:64:GLY:HA3	1.43	0.98
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.09	0.94
3:A:245:ASN:H	3:A:245:ASN:ND2	1.64	0.94
3:A:155:MET:HA	3:A:158:MET:HE3	1.50	0.94
3:A:60:LYS:HA	3:A:65:VAL:HG23	1.49	0.93
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.51	0.93
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.51	0.92
3:A:155:MET:HE2	3:A:188:SER:HB2	1.50	0.91
3:A:191:MET:HG2	3:A:255:ILE:HG13	1.50	0.90
3:A:41:LYS:HD3	3:A:42:ALA:N	1.85	0.90
3:A:245:ASN:HD22	3:A:245:ASN:H	0.90	0.89
3:A:210:LEU:HB3	3:A:259:LEU:HD21	1.54	0.89
3:A:172:GLU:HB3	3:A:197:HIS:NE2	1.85	0.88
2:P:1:DT:H2''	2:P:2:DC:C5'	2.07	0.84
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.60	0.84
3:A:11:LEU:HD23	3:A:11:LEU:H	1.42	0.83
3:A:121:THR:HG23	3:A:124:ASP:CG	2.03	0.83
3:A:264:GLN:NE2	3:A:296:TYR:HB3	1.95	0.81
3:A:243:SER:CB	3:A:249:GLU:HA	2.11	0.81
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.10	0.80
3:A:253:ARG:HG3	3:A:253:ARG:HH11	1.46	0.79
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.12	0.79
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.64	0.79
3:A:277:ILE:HG12	3:A:335:GLU:HA	1.63	0.79
3:A:180:SER:CB	3:A:183:ARG:HH21	1.93	0.78
3:A:180:SER:HB3	3:A:183:ARG:NH2	1.95	0.78
3:A:12:ASN:HD21	3:A:53:ILE:H	1.29	0.78
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.65	0.77
3:A:151:PRO:HG2	3:A:154:GLU:CG	2.12	0.77
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.14	0.77
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.20	0.77
3:A:108:PRO:O	3:A:112:ARG:HG3	1.85	0.76
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.66	0.75
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.82	0.75
3:A:18:MET:O	3:A:21:GLU:HB2	1.87	0.75
3:A:123:GLU:HG3	6:A:623:HOH:O	1.86	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:41:LYS:O	3:A:45:VAL:HG13	1.87	0.74
3:A:323:ILE:O	3:A:324:GLN:HG2	1.87	0.74
3:A:270:LEU:CD2	3:A:282:MET:HE1	2.16	0.74
3:A:60:LYS:HA	3:A:65:VAL:CG2	2.18	0.73
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.18	0.73
3:A:155:MET:HE2	3:A:188:SER:CB	2.19	0.73
2:P:5:DA:H2''	2:P:6:DT:H5'	1.71	0.72
3:A:162:VAL:HG13	3:A:218:LEU:HD21	1.71	0.72
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.72	0.71
3:A:123:GLU:O	3:A:127:LYS:HG2	1.89	0.71
3:A:41:LYS:HD3	3:A:42:ALA:H	1.54	0.71
3:A:248:LYS:HD2	3:A:248:LYS:N	2.03	0.71
3:A:299:ARG:CD	3:A:310:PRO:HD3	2.21	0.71
3:A:155:MET:HA	3:A:158:MET:CE	2.20	0.70
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.89	0.70
3:A:15:ILE:HB	3:A:46:ILE:CD1	2.22	0.70
3:A:207:GLN:O	3:A:210:LEU:HB2	1.92	0.70
3:A:200:PHE:HB2	6:A:625:HOH:O	1.92	0.69
3:A:330:PRO:HA	3:A:333:ARG:CG	2.22	0.69
3:A:245:ASN:N	3:A:245:ASN:ND2	2.29	0.69
3:A:165:GLU:HB3	3:A:217:GLN:HG2	1.74	0.68
3:A:180:SER:HA	3:A:183:ARG:HE	1.57	0.68
3:A:299:ARG:HG2	3:A:310:PRO:HD3	1.74	0.68
3:A:73:ILE:HG22	3:A:77:LEU:HD22	1.76	0.67
3:A:194:LEU:HD21	3:A:272:PHE:HD2	1.58	0.67
3:A:229:SER:OG	3:A:236:MET:HE2	1.93	0.67
1:T:6:DG:H2''	1:T:7:DA:C8	2.30	0.67
3:A:248:LYS:HD2	3:A:248:LYS:H	1.58	0.67
3:A:133:ASN:ND2	3:A:135:HIS:H	1.92	0.66
3:A:266:TYR:HA	3:A:269:VAL:HB	1.76	0.66
3:A:37:ASN:HB3	6:A:556:HOH:O	1.96	0.65
3:A:79:THR:O	3:A:81:LYS:N	2.27	0.65
3:A:15:ILE:HD13	3:A:73:ILE:HG23	1.79	0.65
3:A:240:GLN:NE2	3:A:250:TYR:O	2.27	0.65
3:A:299:ARG:HG2	3:A:310:PRO:CD	2.26	0.64
2:P:5:DA:H2''	2:P:6:DT:C5'	2.28	0.64
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.78	0.64
3:A:294:ASN:O	3:A:296:TYR:N	2.29	0.64
3:A:163:LEU:HD23	3:A:163:LEU:N	2.11	0.64
3:A:326:LYS:HG3	3:A:326:LYS:O	1.98	0.64
3:A:121:THR:O	3:A:124:ASP:HB2	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:327:TYR:HD1	3:A:328:ARG:N	1.96	0.64
3:A:121:THR:HG23	3:A:124:ASP:OD1	1.97	0.64
3:A:212:HIS:HB3	6:A:541:HOH:O	1.98	0.64
3:A:41:LYS:NZ	3:A:64:GLY:O	2.29	0.63
3:A:306:VAL:HG23	3:A:307:ALA:N	2.12	0.63
3:A:286:ALA:O	3:A:291:PHE:N	2.31	0.63
3:A:195:LEU:O	3:A:260:ILE:N	2.31	0.63
3:A:30:SER:HB3	6:A:561:HOH:O	1.98	0.63
3:A:249:GLU:HG3	3:A:250:TYR:N	2.13	0.63
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.28	0.63
3:A:103:VAL:HA	6:A:600:HOH:O	1.97	0.62
3:A:172:GLU:HB3	3:A:197:HIS:CD2	2.33	0.62
3:A:323:ILE:C	3:A:324:GLN:HG2	2.23	0.62
3:A:18:MET:HE3	3:A:82:LEU:HD13	1.81	0.62
3:A:306:VAL:HG22	6:A:650:HOH:O	1.99	0.62
3:A:194:LEU:HD21	3:A:272:PHE:CD2	2.34	0.62
1:T:3:DT:H1'	6:T:617:HOH:O	1.99	0.62
3:A:133:ASN:HD22	3:A:135:HIS:H	1.47	0.62
3:A:191:MET:CG	3:A:255:ILE:HG13	2.25	0.62
3:A:18:MET:CE	3:A:82:LEU:HD13	2.29	0.62
3:A:331:LYS:HG2	3:A:332:ASP:N	2.11	0.61
3:A:127:LYS:HB2	3:A:128:ASN:ND2	2.16	0.61
3:A:270:LEU:HD12	3:A:270:LEU:O	2.01	0.60
3:A:286:ALA:HB1	3:A:291:PHE:HB2	1.82	0.60
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.82	0.60
3:A:92:ASP:HB3	6:A:647:HOH:O	2.01	0.60
3:A:253:ARG:HH11	3:A:253:ARG:CG	2.14	0.60
3:A:150:ILE:O	3:A:187:SER:HA	2.02	0.60
3:A:286:ALA:HB2	3:A:323:ILE:HG21	1.82	0.60
3:A:210:LEU:CB	3:A:259:LEU:HD21	2.28	0.60
3:A:302:GLY:H	3:A:307:ALA:HB3	1.65	0.60
3:A:73:ILE:HG22	3:A:77:LEU:CD2	2.32	0.59
3:A:164:ASN:O	3:A:168:LYS:HG2	2.02	0.59
3:A:299:ARG:CG	3:A:310:PRO:HD3	2.32	0.59
3:A:150:ILE:HD11	3:A:253:ARG:HG2	1.84	0.59
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.66	0.59
3:A:15:ILE:HB	3:A:46:ILE:HD13	1.84	0.59
3:A:277:ILE:HD13	3:A:277:ILE:H	1.67	0.59
3:A:292:THR:O	3:A:298:ILE:HA	2.03	0.59
3:A:228:LEU:HB2	3:A:236:MET:O	2.02	0.58
3:A:11:LEU:H	3:A:11:LEU:CD2	2.15	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:270:LEU:HA	3:A:316:GLU:OE2	2.03	0.58
3:A:210:LEU:HB3	3:A:259:LEU:CD2	2.30	0.58
1:T:5:DA:H2''	1:T:6:DG:O5'	2.03	0.58
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.39	0.58
3:A:286:ALA:HB2	3:A:293:ILE:HD11	1.86	0.58
3:A:122:LEU:HD23	3:A:122:LEU:O	2.05	0.57
3:A:299:ARG:HG2	3:A:310:PRO:HA	1.86	0.57
3:A:120:LYS:N	3:A:124:ASP:OD2	2.34	0.57
3:A:217:GLN:O	3:A:220:LYS:N	2.37	0.57
3:A:299:ARG:HD2	3:A:310:PRO:HD3	1.85	0.57
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.87	0.57
3:A:82:LEU:HB3	3:A:85:LEU:CB	2.32	0.57
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.36	0.57
3:A:299:ARG:HG2	3:A:310:PRO:N	2.21	0.56
3:A:121:THR:HG23	3:A:124:ASP:OD2	2.03	0.56
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.20	0.56
3:A:194:LEU:HD12	3:A:258:ARG:HG3	1.87	0.56
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.40	0.56
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.35	0.56
3:A:122:LEU:O	3:A:126:ARG:HG3	2.05	0.56
3:A:196:THR:OG1	3:A:197:HIS:N	2.38	0.56
3:A:198:PRO:C	3:A:200:PHE:H	2.14	0.56
3:A:270:LEU:HD12	3:A:270:LEU:C	2.32	0.55
3:A:165:GLU:HA	3:A:168:LYS:CG	2.36	0.55
3:A:18:MET:HG2	3:A:22:LEU:HD23	1.88	0.55
3:A:21:GLU:OE1	3:A:85:LEU:HD11	2.07	0.55
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.87	0.55
3:A:122:LEU:HD23	3:A:122:LEU:C	2.32	0.55
3:A:277:ILE:HD11	3:A:334:SER:O	2.07	0.55
3:A:237:GLY:O	3:A:254:ARG:NH1	2.40	0.54
3:A:115:VAL:O	3:A:118:GLY:N	2.39	0.54
3:A:59:ALA:O	3:A:62:LEU:HB2	2.08	0.54
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.55	0.54
3:A:56:GLY:O	3:A:59:ALA:HB3	2.07	0.54
3:A:268:GLY:O	3:A:271:TYR:HB3	2.08	0.54
3:A:201:THR:HA	3:A:261:PRO:HB3	1.89	0.54
3:A:279:ASN:O	3:A:283:ARG:HG3	2.07	0.54
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.43	0.53
3:A:233:THR:HB	6:A:538:HOH:O	2.09	0.53
3:A:41:LYS:HD3	3:A:41:LYS:C	2.29	0.53
3:A:165:GLU:HB3	3:A:217:GLN:CG	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.24	0.53
3:A:248:LYS:O	3:A:248:LYS:HG2	2.09	0.53
3:A:11:LEU:HD23	3:A:11:LEU:N	2.10	0.53
3:A:150:ILE:HD13	3:A:253:ARG:HG2	1.90	0.53
3:A:174:ILE:O	3:A:195:LEU:HD12	2.09	0.53
3:A:266:TYR:O	3:A:270:LEU:HB2	2.08	0.53
3:A:145:ASP:OD2	3:A:252:HIS:HB2	2.08	0.52
3:A:223:PHE:O	3:A:239:CYS:HA	2.09	0.52
3:A:264:GLN:HE22	3:A:296:TYR:HB3	1.72	0.52
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.37	0.52
3:A:15:ILE:HB	3:A:46:ILE:HD11	1.91	0.52
1:T:2:DA:H2"	1:T:3:DT:OP2	2.09	0.52
3:A:45:VAL:HG21	3:A:63:PRO:O	2.08	0.52
3:A:277:ILE:HG13	3:A:335:GLU:CB	2.39	0.52
3:A:172:GLU:HG3	3:A:198:PRO:HG2	1.91	0.51
3:A:33:ILE:O	3:A:37:ASN:N	2.44	0.51
3:A:182:ARG:HH12	3:A:273:THR:HG21	1.76	0.51
3:A:199:SER:O	3:A:199:SER:OG	2.30	0.51
3:A:300:PRO:HD3	3:A:311:LEU:HD13	1.92	0.50
3:A:152:ARG:NH2	3:A:181:PHE:O	2.40	0.50
3:A:299:ARG:HG2	3:A:310:PRO:CA	2.41	0.50
3:A:316:GLU:O	3:A:320:PHE:HD2	1.95	0.50
3:A:288:GLU:C	3:A:290:GLY:H	2.19	0.50
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.46	0.50
3:A:14:GLY:O	3:A:18:MET:N	2.38	0.50
3:A:15:ILE:O	3:A:19:LEU:HD22	2.12	0.50
3:A:26:GLU:HA	3:A:30:SER:OG	2.11	0.50
3:A:197:HIS:O	3:A:262:LYS:HB2	2.12	0.50
3:A:119:ILE:HG23	3:A:124:ASP:CB	2.40	0.49
3:A:277:ILE:HG13	3:A:335:GLU:HB3	1.94	0.49
3:A:194:LEU:CD1	3:A:258:ARG:HG3	2.42	0.49
3:A:23:ALA:HB2	3:A:39:TYR:HB2	1.93	0.49
3:A:294:ASN:N	3:A:294:ASN:HD22	2.09	0.49
3:A:303:VAL:C	3:A:305:GLY:H	2.20	0.49
3:A:267:CYS:SG	3:A:297:THR:HA	2.53	0.49
3:A:274:GLY:O	3:A:278:PHE:HD2	1.96	0.49
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.35	0.49
3:A:302:GLY:N	3:A:307:ALA:HB3	2.26	0.49
3:A:79:THR:C	3:A:81:LYS:H	2.18	0.49
3:A:145:ASP:HB3	3:A:252:HIS:O	2.12	0.48
3:A:291:PHE:CD1	3:A:300:PRO:HA	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:295:GLU:HA	6:A:592:HOH:O	2.12	0.48
3:A:212:HIS:N	3:A:212:HIS:CD2	2.80	0.48
3:A:302:GLY:H	3:A:307:ALA:CB	2.25	0.48
3:A:310:PRO:HB3	6:A:626:HOH:O	2.13	0.48
3:A:150:ILE:N	3:A:188:SER:O	2.40	0.48
3:A:40:ARG:HE	3:A:40:ARG:HB2	1.47	0.48
3:A:172:GLU:CG	3:A:198:PRO:HG2	2.43	0.48
3:A:218:LEU:CB	3:A:224:ILE:HD12	2.43	0.48
3:A:76:PHE:HD1	3:A:77:LEU:CD1	2.27	0.47
3:A:166:VAL:HG13	3:A:173:TYR:HB3	1.96	0.47
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.49	0.47
3:A:259:LEU:HD12	3:A:260:ILE:H	1.78	0.47
3:A:286:ALA:HA	3:A:323:ILE:CG2	2.44	0.47
3:A:322:TYR:C	3:A:324:GLN:H	2.21	0.47
3:A:44:SER:O	3:A:47:ALA:HB3	2.14	0.47
3:A:287:LEU:HD22	3:A:291:PHE:O	2.13	0.47
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.50	0.47
3:A:218:LEU:HB2	3:A:224:ILE:HD12	1.97	0.47
3:A:327:TYR:CD1	3:A:328:ARG:N	2.82	0.47
3:A:22:LEU:HD13	3:A:22:LEU:HA	1.36	0.46
3:A:265:TYR:O	3:A:268:GLY:N	2.48	0.46
3:A:294:ASN:HB2	3:A:295:GLU:OE1	2.15	0.46
3:A:306:VAL:O	3:A:307:ALA:HB2	2.15	0.46
3:A:218:LEU:N	3:A:218:LEU:CD1	2.78	0.46
1:T:5:DA:C2	2:P:4:DA:C2	3.02	0.46
3:A:170:ASP:HB3	3:A:173:TYR:CE2	2.51	0.46
3:A:27:LYS:HB2	3:A:36:TYR:CG	2.51	0.46
3:A:77:LEU:HD12	3:A:77:LEU:HA	1.72	0.46
3:A:275:SER:OG	3:A:277:ILE:HD13	2.16	0.46
3:A:302:GLY:N	3:A:307:ALA:CB	2.79	0.46
3:A:152:ARG:HA	3:A:155:MET:HB2	1.98	0.45
3:A:329:GLU:O	3:A:333:ARG:HG2	2.17	0.45
3:A:209:LYS:HA	3:A:212:HIS:HB2	1.97	0.45
3:A:138:ILE:O	3:A:138:ILE:HG22	2.16	0.45
3:A:190:ASP:HB3	3:A:254:ARG:HB2	1.99	0.45
3:A:209:LYS:HA	3:A:209:LYS:HD3	1.73	0.45
3:A:260:ILE:HG22	3:A:261:PRO:N	2.31	0.45
3:A:214:VAL:CG2	3:A:215:VAL:N	2.76	0.45
3:A:253:ARG:NH2	6:A:620:HOH:O	2.27	0.45
3:A:258:ARG:H	3:A:258:ARG:HG2	1.50	0.45
3:A:292:THR:O	3:A:298:ILE:HG13	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:99:PHE:CD1	3:A:99:PHE:C	2.95	0.45
3:A:46:ILE:HB	3:A:53:ILE:CD1	2.47	0.45
3:A:76:PHE:CD1	3:A:76:PHE:C	2.95	0.45
3:A:254:ARG:NH2	3:A:256:ASP:OD1	2.34	0.44
3:A:54:LYS:HD2	3:A:54:LYS:HA	1.65	0.44
3:A:143:PHE:CD1	3:A:143:PHE:C	2.95	0.44
3:A:317:LYS:HG3	3:A:321:ASP:OD2	2.17	0.44
3:A:68:LYS:O	3:A:71:GLU:HB3	2.17	0.44
3:A:196:THR:HB	3:A:265:TYR:CD1	2.53	0.44
3:A:204:SER:O	3:A:206:LYS:N	2.50	0.44
3:A:133:ASN:ND2	3:A:135:HIS:N	2.65	0.44
3:A:312:PRO:O	3:A:322:TYR:OH	2.28	0.44
3:A:260:ILE:CG2	3:A:261:PRO:N	2.80	0.44
3:A:18:MET:HE3	3:A:76:PHE:HB2	1.99	0.43
3:A:115:VAL:C	3:A:118:GLY:H	2.25	0.43
3:A:265:TYR:O	3:A:267:CYS:N	2.51	0.43
3:A:302:GLY:HA3	3:A:307:ALA:HB2	2.00	0.43
3:A:198:PRO:O	3:A:200:PHE:N	2.51	0.43
3:A:285:HIS:NE2	6:A:583:HOH:O	2.36	0.43
3:A:295:GLU:OE1	3:A:295:GLU:N	2.48	0.43
3:A:304:THR:H	3:A:304:THR:HG23	1.56	0.43
3:A:326:LYS:O	3:A:328:ARG:HG2	2.18	0.43
2:P:6:DT:H5'	2:P:6:DT:H2'	1.78	0.43
3:A:119:ILE:CG2	3:A:124:ASP:CB	2.96	0.43
3:A:159:GLN:HG2	3:A:160:ASP:N	2.33	0.43
3:A:195:LEU:O	3:A:259:LEU:HD12	2.18	0.43
3:A:332:ASP:C	3:A:334:SER:H	2.26	0.43
3:A:19:LEU:HD23	3:A:43:ALA:HA	2.01	0.43
3:A:35:LYS:O	3:A:38:ALA:N	2.52	0.43
3:A:198:PRO:C	3:A:200:PHE:N	2.77	0.43
3:A:217:GLN:O	3:A:220:LYS:HB3	2.19	0.43
3:A:177:VAL:HG22	3:A:193:VAL:HG22	2.01	0.43
3:A:96:SER:OG	3:A:120:LYS:HB3	2.19	0.42
3:A:191:MET:HE2	3:A:191:MET:HB2	1.69	0.42
3:A:287:LEU:HD13	3:A:287:LEU:HA	1.62	0.42
3:A:311:LEU:HB3	3:A:322:TYR:HE2	1.83	0.42
3:A:132:LEU:HB2	3:A:137:ARG:HG2	2.02	0.42
3:A:157:GLN:O	3:A:160:ASP:HB3	2.20	0.42
3:A:201:THR:HA	3:A:261:PRO:CB	2.49	0.42
3:A:296:TYR:C	3:A:297:THR:HG23	2.44	0.42
3:A:316:GLU:OE1	3:A:333:ARG:NH2	2.46	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:91:ASP:OD1	3:A:92:ASP:N	2.51	0.42
3:A:122:LEU:CD2	3:A:126:ARG:CZ	2.97	0.42
3:A:146:PHE:HD1	3:A:146:PHE:HA	1.53	0.42
3:A:183:ARG:HE	3:A:183:ARG:HB2	1.55	0.42
3:A:229:SER:O	3:A:236:MET:N	2.38	0.42
1:T:4:DT:H1'	6:T:527:HOH:O	2.19	0.42
3:A:85:LEU:HA	3:A:85:LEU:HD12	1.50	0.42
3:A:228:LEU:HD12	3:A:228:LEU:HA	1.73	0.42
3:A:177:VAL:O	3:A:182:ARG:HD2	2.19	0.42
3:A:303:VAL:C	3:A:305:GLY:N	2.78	0.42
3:A:178:CYS:SG	3:A:194:LEU:CD2	3.07	0.42
3:A:303:VAL:O	3:A:303:VAL:HG22	2.20	0.42
2:P:6:DT:H2'	2:P:6:DT:H6	1.06	0.42
3:A:29:VAL:HG22	3:A:97:ILE:HD12	2.02	0.42
3:A:182:ARG:NH1	3:A:273:THR:CG2	2.83	0.42
3:A:216:GLU:O	3:A:220:LYS:HB2	2.19	0.41
3:A:44:SER:HB2	6:A:608:HOH:O	2.19	0.41
3:A:122:LEU:HD22	3:A:126:ARG:NH1	2.36	0.41
3:A:166:VAL:O	3:A:169:VAL:HG13	2.18	0.41
3:A:200:PHE:CE2	3:A:260:ILE:C	2.99	0.41
3:A:275:SER:N	3:A:278:PHE:HB3	2.35	0.41
3:A:267:CYS:N	6:A:508:HOH:O	2.36	0.41
3:A:314:ASP:N	3:A:318:ASP:OD2	2.42	0.41
1:T:1:DC:H2''	1:T:2:DA:OP2	2.20	0.41
3:A:177:VAL:HG12	3:A:181:PHE:CD2	2.56	0.41
3:A:322:TYR:C	3:A:324:GLN:N	2.78	0.41
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.61	0.41
3:A:194:LEU:HD12	3:A:258:ARG:CG	2.51	0.41
3:A:83:ARG:HA	3:A:86:GLU:HG2	2.02	0.41
3:A:125:LEU:HD23	3:A:125:LEU:HA	1.61	0.41
3:A:154:GLU:O	3:A:158:MET:HG3	2.21	0.41
3:A:260:ILE:CG2	3:A:261:PRO:CD	2.99	0.41
3:A:271:TYR:CD2	3:A:272:PHE:N	2.89	0.41
3:A:289:LYS:N	3:A:289:LYS:HD3	2.32	0.41
3:A:27:LYS:HB3	3:A:36:TYR:CD1	2.56	0.40
3:A:205:THR:O	3:A:206:LYS:HB2	2.21	0.40
3:A:200:PHE:HE2	3:A:260:ILE:C	2.29	0.40
3:A:200:PHE:HE2	3:A:261:PRO:N	2.20	0.40
3:A:201:THR:HG1	3:A:263:ASP:CG	2.21	0.40
3:A:15:ILE:CD1	3:A:77:LEU:HD11	2.48	0.40
3:A:327:TYR:CD1	3:A:327:TYR:C	2.98	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%)	266 (82%)	37 (11%)	22 (7%)	1 5

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	202	SER
3	A	204	SER
3	A	205	THR
3	A	244	LYS
3	A	246	ASP
3	A	265	TYR
3	A	295	GLU
3	A	80	GLY
3	A	185	ALA
3	A	199	SER
3	A	247	GLU
3	A	266	TYR
3	A	310	PRO
3	A	316	GLU
3	A	10	THR
3	A	207	GLN
3	A	289	LYS
3	A	309	GLU
3	A	13	GLY
3	A	91	ASP
3	A	101	THR
3	A	307	ALA

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%)	208 (72%)	80 (28%)	0 2

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	THR
3	A	15	ILE
3	A	18	MET
3	A	19	LEU
3	A	22	LEU
3	A	27	LYS
3	A	30	SER
3	A	33	ILE
3	A	37	ASN
3	A	40	ARG
3	A	41	LYS
3	A	45	VAL
3	A	46	ILE
3	A	52	LYS
3	A	55	SER
3	A	62	LEU
3	A	65	VAL
3	A	67	THR
3	A	68	LYS
3	A	72	LYS
3	A	77	LEU
3	A	79	THR
3	A	81	LYS
3	A	89	ARG
3	A	92	ASP
3	A	93	THR
3	A	100	LEU
3	A	101	THR
3	A	119	ILE
3	A	121	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	126	ARG
3	A	133	ASN
3	A	138	ILE
3	A	140	LEU
3	A	153	GLU
3	A	157	GLN
3	A	161	ILE
3	A	166	VAL
3	A	168	LYS
3	A	169	VAL
3	A	174	ILE
3	A	180	SER
3	A	188	SER
3	A	191	MET
3	A	194	LEU
3	A	199	SER
3	A	201	THR
3	A	205	THR
3	A	214	VAL
3	A	218	LEU
3	A	226	ASP
3	A	228	LEU
3	A	230	LYS
3	A	233	THR
3	A	236	MET
3	A	242	PRO
3	A	245	ASN
3	A	248	LYS
3	A	249	GLU
3	A	253	ARG
3	A	255	ILE
3	A	258	ARG
3	A	262	LYS
3	A	264	GLN
3	A	270	LEU
3	A	277	ILE
3	A	287	LEU
3	A	293	ILE
3	A	294	ASN
3	A	295	GLU
3	A	298	ILE
3	A	301	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	306	VAL
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	325	TRP
3	A	326	LYS
3	A	331	LYS
3	A	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) 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	133	ASN
3	A	134	HIS
3	A	136	GLN
3	A	159	GLN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	222	HIS
3	A	245	ASN
3	A	264	GLN
3	A	279	ASN
3	A	294	ASN
3	A	324	GLN

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, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	338	-	4,4,4	1.21	0	6,6,6	0.78	0

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	7/7 (100%)	-0.16	0	100 100	18, 34, 57, 94	0
2	P	7/7 (100%)	-0.63	0	100 100	17, 25, 37, 61	0
3	A	326/335 (97%)	-0.47	1 (0%)	90 79	2, 31, 83, 100	0
All	All	340/349 (97%)	-0.47	1 (0%)	90 79	2, 31, 84, 100	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	247	GLU	3.3

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	SO4	A	338	5/5	0.66	0.16	57,61,66,67	5
5	NA	A	342	1/1	0.82	0.17	60,60,60,60	0
5	NA	A	341	1/1	1.00	0.04	1,1,1,1	0

6.5 Other polymers [i](#)

There are no such residues in this entry.