



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:33 PM UTC

PDB ID : 8ICM / pdb_00008icm
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SEVEN BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF DATP (1 MILLIMOLAR), MNCL2 (5 MILLIMOLAR), AND AMMONIUM SULFATE (75 MILLIMOLAR)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-01-04
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

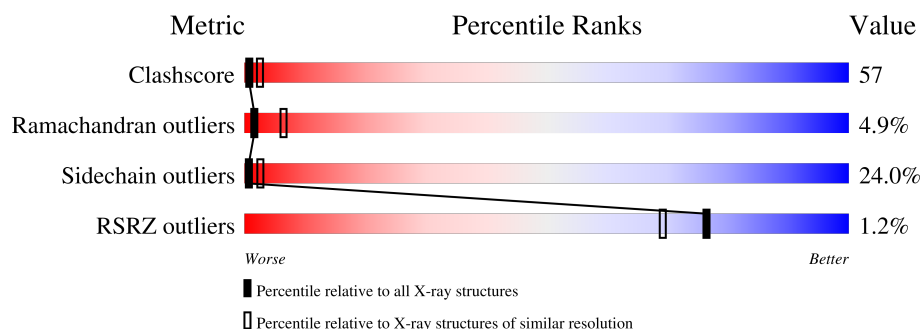
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 12% 88%
2	P	7	 14% 86%
3	A	335	 22% 44% 25% 7% •

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3057 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			

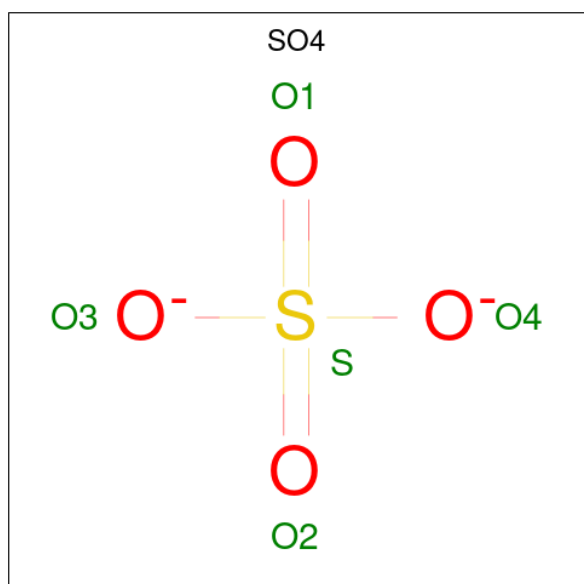
- Molecule 2 is a DNA chain called DNA (5'-D(*TP*CP*TP*AP*AP*TP*G)-3').

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 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	14	Total	O	0	0
			14	14		
6	P	19	Total	O	0	0
			19	19		
6	A	105	Total	O	0	0
			105	105		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

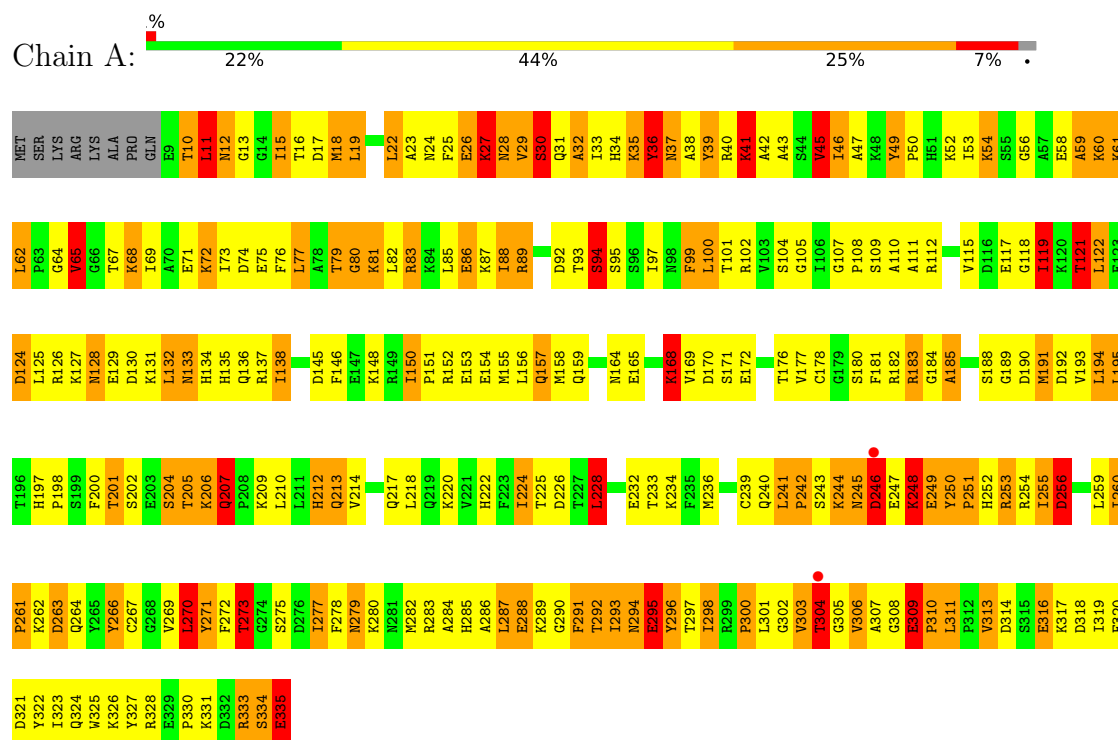
- Molecule 1: DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3')



- 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	178.81Å 57.78Å 48.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-2.90) 93.9 (20.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.70Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.176 , (Not available) 0.167 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 161.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3057	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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, SO4

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	1.11	0/162	3.00	16/249 (6.4%)
2	P	1.42	1/160 (0.6%)	4.60	25/243 (10.3%)
3	A	1.58	25/2672 (0.9%)	2.24	127/3590 (3.5%)
All	All	1.55	26/2994 (0.9%)	2.49	168/4082 (4.1%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	30	SER	C-N	-7.41	1.23	1.33
3	A	224	ILE	CA-CB	-6.96	1.45	1.54
3	A	260	ILE	CA-C	-6.76	1.45	1.52
3	A	270	LEU	C-N	-6.55	1.25	1.33
3	A	195	LEU	CA-C	-6.39	1.44	1.52
3	A	35	LYS	C-N	-6.30	1.25	1.34
3	A	65	VAL	C-N	-6.29	1.26	1.33
2	P	1	DT	OP3-P	6.20	1.60	1.48
3	A	271	TYR	N-CA	-6.15	1.39	1.46
3	A	138	ILE	CA-CB	-6.14	1.46	1.54
3	A	193	VAL	CA-CB	-6.08	1.47	1.54
3	A	15	ILE	CA-C	-5.97	1.45	1.52
3	A	33	ILE	N-CA	-5.90	1.40	1.46
3	A	251	PRO	CA-C	-5.83	1.46	1.52
3	A	28	ASN	CA-C	-5.79	1.45	1.52
3	A	224	ILE	CA-C	-5.79	1.46	1.52
3	A	110	ALA	N-CA	-5.69	1.39	1.46
3	A	124	ASP	CA-C	-5.59	1.45	1.52
3	A	220	LYS	CA-C	-5.58	1.45	1.52
3	A	36	TYR	N-CA	-5.53	1.39	1.46
3	A	104	SER	CA-C	-5.30	1.46	1.52
3	A	273	THR	CA-C	-5.26	1.45	1.52
3	A	266	TYR	CA-C	-5.24	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	119	ILE	CA-CB	-5.15	1.48	1.54
3	A	242	PRO	N-CA	-5.11	1.40	1.47
3	A	177	VAL	N-CA	-5.04	1.40	1.46

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	1	DT	C6-N1-C1'	-26.44	79.70	119.35
2	P	1	DT	C2-N1-C1'	25.63	157.79	119.35
2	P	6	DT	C2-N1-C1'	22.99	153.83	119.35
2	P	6	DT	C6-N1-C1'	-22.70	85.30	119.35
2	P	3	DT	C2-N1-C1'	19.62	148.79	119.35
2	P	3	DT	C6-N1-C1'	-19.57	89.99	119.35
1	T	6	DG	C8-N9-C1'	17.63	153.45	127.00
1	T	6	DG	C4-N9-C1'	-16.80	101.80	127.00
1	T	4	DT	C6-N1-C1'	-16.56	94.51	119.35
1	T	4	DT	C2-N1-C1'	16.18	143.62	119.35
2	P	7	DG	C8-N9-C1'	14.76	149.15	127.00
2	P	7	DG	C4-N9-C1'	-14.44	105.34	127.00
2	P	4	DA	C8-N9-C1'	-12.66	108.06	127.05
3	A	303	VAL	N-CA-C	10.93	121.77	110.62
2	P	4	DA	C4-N9-C1'	10.88	143.38	127.05
3	A	28	ASN	CA-CB-CG	-10.48	102.12	112.60
3	A	49	TYR	CA-C-N	9.76	130.96	120.12
3	A	49	TYR	C-N-CA	9.76	130.96	120.12
3	A	49	TYR	O-C-N	9.59	129.24	121.38
2	P	5	DA	C4-N9-C1'	9.36	141.08	127.05
3	A	192	ASP	CB-CA-C	-9.27	95.81	110.74
3	A	157	GLN	N-CA-CB	9.21	123.36	110.01
3	A	24	ASN	CA-CB-CG	-9.14	103.46	112.60
1	T	3	DT	C2-N1-C1'	9.06	132.94	119.35
2	P	2	DC	C2-N1-C1'	8.94	133.10	119.70
3	A	99	PHE	CA-CB-CG	-8.84	104.96	113.80
3	A	333	ARG	N-CA-C	-8.74	102.75	112.72
2	P	5	DA	C8-N9-C1'	-8.58	114.18	127.05
3	A	121	THR	N-CA-C	8.42	121.40	110.53
3	A	83	ARG	N-CA-CB	8.20	121.86	109.98
3	A	250	TYR	CA-C-N	-8.20	112.41	120.52
3	A	250	TYR	C-N-CA	-8.20	112.41	120.52
1	T	3	DT	C6-N1-C1'	-8.15	107.13	119.35
3	A	34	HIS	CA-CB-CG	-8.03	105.77	113.80
1	T	2	DA	C4-N9-C1'	-7.96	115.12	127.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	309	GLU	CA-C-N	7.71	129.48	119.84
3	A	309	GLU	C-N-CA	7.71	129.48	119.84
3	A	88	ILE	CB-CA-C	-7.60	102.15	111.88
3	A	266	TYR	N-CA-C	7.58	120.50	111.33
3	A	29	VAL	N-CA-C	7.55	118.09	110.23
3	A	105	GLY	CA-C-N	-7.52	113.07	122.93
3	A	105	GLY	C-N-CA	-7.52	113.07	122.93
3	A	94	SER	CA-CB-OG	-7.51	96.09	111.10
3	A	17	ASP	CB-CA-C	7.44	123.15	110.79
3	A	176	THR	CA-C-N	-7.31	113.23	122.37
3	A	176	THR	C-N-CA	-7.31	113.23	122.37
3	A	335	GLU	N-CA-CB	7.27	122.86	110.50
3	A	33	ILE	CB-CA-C	7.11	120.80	111.70
1	T	2	DA	C8-N9-C1'	7.04	137.61	127.05
3	A	224	ILE	CA-CB-CG1	-7.00	98.49	110.40
3	A	74	ASP	CA-CB-CG	6.96	119.56	112.60
2	P	3	DT	C5'-C4'-O4'	6.88	119.72	109.40
3	A	313	VAL	N-CA-C	6.87	117.75	107.80
3	A	15	ILE	N-CA-CB	6.84	119.33	110.57
3	A	164	ASN	CA-CB-CG	-6.79	105.81	112.60
2	P	3	DT	O4'-C1'-N1	6.79	118.58	108.40
3	A	266	TYR	CA-CB-CG	-6.75	101.75	113.90
3	A	183	ARG	CB-CA-C	-6.73	102.88	111.22
2	P	3	DT	C1'-O4'-C4'	-6.70	99.64	109.70
3	A	134	HIS	CA-CB-CG	6.68	120.48	113.80
3	A	318	ASP	CA-CB-CG	-6.67	105.93	112.60
3	A	252	HIS	CA-CB-CG	-6.63	107.17	113.80
3	A	249	GLU	CB-CA-C	6.50	120.48	109.50
2	P	2	DC	C6-N1-C1'	-6.45	110.03	119.70
2	P	7	DG	O5'-C5'-C4'	6.41	120.41	110.80
3	A	212	HIS	CA-CB-CG	-6.41	107.39	113.80
2	P	3	DT	C4'-C3'-O3'	-6.40	100.41	110.00
3	A	59	ALA	O-C-N	6.36	128.62	122.07
3	A	177	VAL	N-CA-CB	6.35	118.24	111.00
3	A	41	LYS	N-CA-C	-6.34	104.47	111.82
3	A	12	ASN	CB-CA-C	6.33	121.41	110.72
3	A	271	TYR	N-CA-CB	-6.32	100.52	109.94
3	A	224	ILE	CB-CA-C	-6.29	102.98	111.15
3	A	86	GLU	N-CA-CB	6.25	119.40	110.16
3	A	288	GLU	N-CA-C	-6.23	104.41	111.14
3	A	271	TYR	CA-CB-CG	-6.22	102.70	113.90
3	A	117	GLU	N-CA-C	-6.16	105.92	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	291	PHE	CA-CB-CG	-6.14	107.66	113.80
3	A	17	ASP	N-CA-CB	6.12	119.12	110.12
3	A	35	LYS	CA-C-O	6.11	127.03	120.55
3	A	45	VAL	N-CA-C	6.08	116.86	110.72
2	P	3	DT	N1-C1'-C2'	6.07	122.60	113.50
3	A	157	GLN	CB-CA-C	6.06	120.40	110.88
3	A	292	THR	CB-CA-C	6.05	120.09	109.80
3	A	168	LYS	N-CA-CB	6.05	119.01	110.12
2	P	4	DA	C1'-O4'-C4'	-6.03	100.65	109.70
3	A	65	VAL	N-CA-CB	6.03	117.70	110.95
3	A	109	SER	N-CA-CB	6.03	118.75	110.01
3	A	151	PRO	N-CA-CB	5.98	108.64	103.31
1	T	5	DA	C4-N9-C1'	-5.96	118.11	127.05
3	A	30	SER	CA-C-N	-5.94	110.20	121.54
3	A	30	SER	C-N-CA	-5.94	110.20	121.54
3	A	68	LYS	CB-CA-C	5.94	122.24	110.42
2	P	2	DC	P-O3'-C3'	5.93	129.10	120.20
3	A	300	PRO	N-CA-CB	5.92	108.58	103.31
3	A	32	ALA	N-CA-C	5.90	118.35	107.73
1	T	7	DA	C4-N9-C1'	-5.90	118.20	127.05
3	A	205	THR	N-CA-C	5.85	123.27	110.80
3	A	146	PHE	CA-CB-CG	-5.83	107.97	113.80
3	A	60	LYS	CA-CB-CG	-5.81	102.48	114.10
3	A	272	PHE	N-CA-C	5.81	118.56	111.82
3	A	29	VAL	N-CA-CB	5.79	116.70	110.62
1	T	1	DC	P-O3'-C3'	5.76	128.85	120.20
3	A	222	HIS	N-CA-C	5.73	121.82	113.40
2	P	3	DT	P-O5'-C5'	5.72	128.58	120.00
3	A	222	HIS	CA-CB-CG	-5.71	108.09	113.80
1	T	6	DG	C4'-C3'-O3'	-5.71	101.43	110.00
3	A	272	PHE	O-C-N	5.70	129.28	122.27
3	A	246	ASP	N-CA-C	5.69	122.92	110.80
3	A	228	LEU	N-CA-C	-5.69	103.85	112.04
3	A	109	SER	CA-CB-OG	-5.66	99.78	111.10
3	A	261	PRO	CB-CA-C	-5.64	104.38	111.71
3	A	273	THR	CA-CB-OG1	-5.63	101.15	109.60
1	T	6	DG	O3'-P-O5'	-5.63	95.55	104.00
3	A	241	LEU	O-C-N	5.63	126.91	121.28
1	T	6	DG	P-O3'-C3'	5.62	128.63	120.20
3	A	270	LEU	O-C-N	5.59	127.85	122.03
3	A	296	TYR	N-CA-C	5.58	120.95	114.04
3	A	27	LYS	N-CA-CB	-5.57	101.64	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	192	ASP	CA-C-N	-5.55	116.31	123.19
3	A	192	ASP	C-N-CA	-5.55	116.31	123.19
3	A	250	TYR	N-CA-C	5.54	117.78	110.36
3	A	256	ASP	CA-CB-CG	5.54	118.14	112.60
3	A	26	GLU	N-CA-CB	5.53	118.03	110.01
3	A	49	TYR	CA-C-O	5.50	124.33	119.71
2	P	4	DA	O5'-C5'-C4'	-5.49	102.57	110.80
3	A	102	ARG	CD-NE-CZ	-5.48	116.73	124.40
3	A	303	VAL	N-CA-CB	5.47	117.98	110.54
3	A	15	ILE	CA-C-N	-5.46	112.01	120.31
3	A	15	ILE	C-N-CA	-5.46	112.01	120.31
3	A	104	SER	N-CA-CB	5.46	117.94	109.48
3	A	150	ILE	N-CA-C	5.45	113.88	107.77
3	A	207	GLN	CA-C-N	5.44	125.27	119.28
3	A	207	GLN	C-N-CA	5.44	125.27	119.28
3	A	65	VAL	CA-C-N	-5.44	117.03	122.69
3	A	65	VAL	C-N-CA	-5.44	117.03	122.69
3	A	260	ILE	O-C-N	5.43	127.29	121.10
3	A	151	PRO	CB-CA-C	-5.42	104.46	111.46
3	A	192	ASP	N-CA-CB	5.40	119.18	110.65
3	A	246	ASP	CA-C-N	5.39	131.83	121.54
3	A	246	ASP	C-N-CA	5.39	131.83	121.54
3	A	248	LYS	N-CA-C	5.38	116.98	107.61
3	A	261	PRO	CA-C-O	-5.35	115.65	121.27
1	T	5	DA	C8-N9-C1'	5.33	135.04	127.05
3	A	270	LEU	CA-C-O	5.32	126.59	121.00
3	A	145	ASP	CB-CA-C	-5.31	100.16	110.46
3	A	334	SER	N-CA-C	5.29	118.52	111.75
3	A	41	LYS	N-CA-CB	5.29	118.47	110.28
3	A	87	LYS	CB-CA-C	5.28	119.14	110.95
3	A	295	GLU	CB-CG-CD	5.22	121.47	112.60
3	A	40	ARG	N-CA-C	5.21	118.10	111.69
3	A	118	GLY	CA-C-N	-5.21	115.85	122.37
3	A	118	GLY	C-N-CA	-5.21	115.85	122.37
2	P	3	DT	N3-C4-O4	-5.19	114.82	122.60
3	A	316	GLU	CA-C-N	5.18	127.49	120.65
3	A	316	GLU	C-N-CA	5.18	127.49	120.65
3	A	68	LYS	N-CA-CB	5.13	119.16	110.49
3	A	72	LYS	CB-CA-C	5.12	118.99	110.90
3	A	119	ILE	CB-CA-C	-5.12	104.77	110.96
3	A	11	LEU	CA-C-N	-5.10	114.64	122.60
3	A	11	LEU	C-N-CA	-5.10	114.64	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	11	LEU	N-CA-C	-5.09	105.82	112.23
3	A	213	GLN	CB-CA-C	-5.06	102.71	110.81
3	A	266	TYR	CA-C-O	-5.06	115.17	120.63
3	A	300	PRO	N-CA-C	-5.05	103.26	111.14
3	A	39	TYR	CA-CB-CG	-5.04	104.83	113.90
3	A	74	ASP	N-CA-CB	5.03	117.26	109.91
1	T	3	DT	P-O5'-C5'	5.02	127.53	120.00

There are no chirality outliers.

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	145	0	80	7	0
2	P	144	0	80	16	0
3	A	2623	0	2641	299	0
4	A	5	0	0	1	0
5	A	2	0	0	0	0
6	A	105	0	0	17	0
6	P	19	0	0	2	0
6	T	14	0	0	1	0
All	All	3057	0	2801	319	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 57.

All (319) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.32	1.10
3:A:29:VAL:HG21	3:A:94:SER:HB2	1.38	1.04
3:A:245:ASN:H	3:A:245:ASN:ND2	1.56	1.00
3:A:245:ASN:HD22	3:A:245:ASN:N	1.55	0.99
3:A:285:HIS:HD2	3:A:323:ILE:HD12	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:180:SER:HB3	3:A:183:ARG:HH21	1.37	0.90
2:P:5:DA:H2''	2:P:6:DT:H5''	1.56	0.88
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.55	0.88
3:A:29:VAL:HG22	3:A:97:ILE:HD12	1.55	0.87
3:A:11:LEU:HD23	3:A:11:LEU:H	1.42	0.84
3:A:60:LYS:HA	3:A:65:VAL:HG23	1.56	0.84
2:P:6:DT:H2''	2:P:7:DG:H5''	1.58	0.83
3:A:18:MET:HE2	3:A:82:LEU:HD13	1.60	0.82
3:A:330:PRO:HA	3:A:333:ARG:CG	2.11	0.81
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.28	0.81
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.79	0.80
3:A:286:ALA:HB2	3:A:323:ILE:HG21	1.60	0.80
3:A:254:ARG:NH1	3:A:255:ILE:H	1.79	0.80
2:P:5:DA:H2''	2:P:6:DT:C5'	2.13	0.79
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.12	0.79
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.47	0.78
3:A:285:HIS:CD2	3:A:323:ILE:HD12	2.17	0.78
3:A:37:ASN:HB3	6:A:556:HOH:O	1.84	0.77
3:A:271:TYR:HB2	6:A:592:HOH:O	1.84	0.77
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.14	0.77
3:A:18:MET:CE	3:A:82:LEU:HD13	2.16	0.75
3:A:183:ARG:HH11	3:A:275:SER:HA	1.51	0.75
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.16	0.75
2:P:3:DT:H1'	6:P:511:HOH:O	1.87	0.75
3:A:59:ALA:O	3:A:62:LEU:HB2	1.87	0.75
3:A:73:ILE:HG22	3:A:77:LEU:HD22	1.68	0.74
2:P:1:DT:H2''	2:P:2:DC:H5'	1.69	0.74
3:A:60:LYS:HA	3:A:65:VAL:CG2	2.17	0.74
3:A:259:LEU:O	3:A:260:ILE:HD13	1.88	0.73
3:A:183:ARG:NH1	3:A:275:SER:HA	2.04	0.73
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.24	0.73
3:A:234:LYS:HD3	6:A:617:HOH:O	1.89	0.72
3:A:172:GLU:HB3	3:A:197:HIS:NE2	2.05	0.72
3:A:212:HIS:HB3	6:A:541:HOH:O	1.88	0.72
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.88	0.71
3:A:330:PRO:HA	3:A:333:ARG:HG2	1.73	0.71
3:A:150:ILE:CG2	3:A:158:MET:HE1	2.21	0.71
3:A:323:ILE:O	3:A:324:GLN:HG2	1.91	0.70
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.16	0.70
3:A:270:LEU:HD21	3:A:282:MET:HE1	1.73	0.70
3:A:217:GLN:NE2	3:A:217:GLN:HA	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:254:ARG:NH1	3:A:255:ILE:N	2.39	0.69
3:A:35:LYS:O	3:A:38:ALA:HB3	1.93	0.68
3:A:58:GLU:O	3:A:61:LYS:HG3	1.94	0.68
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.76	0.68
3:A:19:LEU:HB3	3:A:43:ALA:HB2	1.74	0.68
3:A:295:GLU:HA	6:A:592:HOH:O	1.93	0.67
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.29	0.67
3:A:16:THR:HG21	3:A:47:ALA:HB2	1.75	0.67
3:A:155:MET:HE2	3:A:188:SER:CB	2.25	0.67
3:A:207:GLN:O	3:A:210:LEU:HB2	1.95	0.67
3:A:72:LYS:HG2	3:A:82:LEU:HD11	1.76	0.66
3:A:155:MET:HA	3:A:158:MET:HE3	1.77	0.66
1:T:6:DG:H2'	1:T:7:DA:C8	2.31	0.66
3:A:292:THR:O	3:A:298:ILE:HA	1.95	0.66
3:A:181:PHE:HA	6:A:530:HOH:O	1.93	0.66
3:A:180:SER:HB2	3:A:185:ALA:HB2	1.76	0.66
3:A:326:LYS:O	3:A:328:ARG:HG2	1.96	0.66
3:A:27:LYS:HG3	3:A:28:ASN:ND2	2.12	0.65
3:A:254:ARG:HH11	3:A:255:ILE:H	1.42	0.65
2:P:5:DA:C2'	2:P:6:DT:H5''	2.27	0.65
3:A:29:VAL:HG21	3:A:94:SER:CB	2.23	0.65
3:A:92:ASP:HB2	6:A:647:HOH:O	1.97	0.65
3:A:319:ILE:O	3:A:322:TYR:HB2	1.96	0.65
3:A:79:THR:O	3:A:81:LYS:N	2.30	0.65
2:P:6:DT:C2'	2:P:7:DG:H5''	2.27	0.64
3:A:279:ASN:O	3:A:283:ARG:HG3	1.97	0.64
3:A:285:HIS:NE2	6:A:583:HOH:O	2.29	0.64
3:A:155:MET:HE2	3:A:188:SER:HB2	1.80	0.64
3:A:155:MET:HE3	3:A:181:PHE:HB2	1.79	0.64
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.29	0.64
3:A:12:ASN:HD21	3:A:53:ILE:H	1.46	0.63
3:A:18:MET:HE2	3:A:82:LEU:HD22	1.78	0.63
3:A:327:TYR:HD1	3:A:328:ARG:N	1.97	0.63
3:A:300:PRO:HD3	3:A:311:LEU:HD22	1.82	0.62
3:A:188:SER:HB3	6:A:522:HOH:O	2.00	0.62
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.80	0.62
3:A:323:ILE:C	3:A:324:GLN:HG2	2.25	0.62
3:A:248:LYS:O	3:A:248:LYS:HG2	1.99	0.61
3:A:119:ILE:HG22	3:A:124:ASP:HB3	1.82	0.61
3:A:243:SER:HB3	3:A:249:GLU:HA	1.82	0.61
3:A:277:ILE:HG12	3:A:335:GLU:HA	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:41:LYS:HD3	3:A:42:ALA:N	2.15	0.61
3:A:270:LEU:HD13	3:A:316:GLU:OE2	2.01	0.61
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.83	0.60
3:A:83:ARG:O	3:A:86:GLU:N	2.34	0.60
3:A:41:LYS:NZ	3:A:64:GLY:O	2.30	0.59
3:A:291:PHE:CD1	3:A:300:PRO:HA	2.37	0.59
3:A:286:ALA:O	3:A:291:PHE:HB2	2.02	0.59
3:A:11:LEU:H	3:A:11:LEU:CD2	2.13	0.59
3:A:124:ASP:O	3:A:128:ASN:ND2	2.35	0.59
3:A:26:GLU:HG3	3:A:35:LYS:HB3	1.84	0.59
3:A:291:PHE:HD1	3:A:300:PRO:HA	1.67	0.59
3:A:178:CYS:SG	3:A:194:LEU:HD23	2.42	0.58
3:A:182:ARG:NH2	3:A:316:GLU:OE1	2.35	0.58
3:A:180:SER:HB3	3:A:183:ARG:NH2	2.12	0.58
3:A:253:ARG:HH11	3:A:253:ARG:CG	2.17	0.58
3:A:202:SER:HG	3:A:263:ASP:CG	2.11	0.58
3:A:80:GLY:O	3:A:81:LYS:HG2	2.04	0.57
3:A:191:MET:HG2	3:A:255:ILE:HG13	1.86	0.57
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.39	0.57
3:A:302:GLY:N	3:A:307:ALA:HB3	2.19	0.57
3:A:152:ARG:NE	3:A:184:GLY:O	2.36	0.56
3:A:201:THR:HA	3:A:261:PRO:HB3	1.88	0.56
3:A:23:ALA:O	3:A:36:TYR:HD2	1.87	0.56
3:A:73:ILE:HG22	3:A:77:LEU:CD2	2.35	0.56
3:A:172:GLU:CG	3:A:198:PRO:HG2	2.36	0.56
3:A:260:ILE:HG22	3:A:261:PRO:N	2.20	0.56
3:A:200:PHE:CE2	3:A:261:PRO:HD3	2.41	0.55
3:A:303:VAL:C	3:A:305:GLY:H	2.13	0.55
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.88	0.55
3:A:172:GLU:HG2	3:A:198:PRO:HG2	1.89	0.55
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.41	0.55
3:A:180:SER:CB	3:A:183:ARG:HH21	2.13	0.55
3:A:28:ASN:ND2	3:A:28:ASN:N	2.47	0.55
3:A:302:GLY:HA3	3:A:307:ALA:HB2	1.88	0.54
3:A:309:GLU:H	3:A:310:PRO:HD3	1.72	0.54
3:A:326:LYS:O	3:A:326:LYS:HG3	2.05	0.54
3:A:32:ALA:O	3:A:36:TYR:HB3	2.08	0.54
3:A:18:MET:HE3	3:A:76:PHE:HB2	1.88	0.54
3:A:150:ILE:HG12	3:A:253:ARG:HG2	1.89	0.54
3:A:82:LEU:HD23	3:A:85:LEU:HB2	1.89	0.54
3:A:259:LEU:HD12	3:A:260:ILE:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:254:ARG:CZ	3:A:254:ARG:HB3	2.38	0.54
1:T:1:DC:H2''	1:T:2:DA:OP2	2.08	0.53
3:A:93:THR:HG22	3:A:94:SER:N	2.22	0.53
3:A:157:GLN:HG3	3:A:241:LEU:CD1	2.38	0.53
3:A:279:ASN:O	3:A:283:ARG:N	2.30	0.53
3:A:277:ILE:HG13	3:A:335:GLU:HB2	1.89	0.53
3:A:295:GLU:H	3:A:295:GLU:CD	2.17	0.53
3:A:270:LEU:CD2	3:A:319:ILE:HG21	2.39	0.52
3:A:11:LEU:HD23	3:A:11:LEU:N	2.16	0.52
3:A:241:LEU:HB2	3:A:250:TYR:CD2	2.45	0.52
3:A:293:ILE:HD13	3:A:298:ILE:CG1	2.22	0.52
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.58	0.52
3:A:26:GLU:HB2	3:A:36:TYR:HB2	1.91	0.51
3:A:41:LYS:HD3	3:A:42:ALA:H	1.75	0.51
3:A:28:ASN:N	3:A:28:ASN:HD22	1.94	0.51
3:A:254:ARG:NH2	3:A:256:ASP:OD1	2.38	0.51
3:A:69:ILE:O	3:A:73:ILE:HG13	2.10	0.51
3:A:254:ARG:HH11	3:A:255:ILE:N	2.04	0.51
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.39	0.51
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.91	0.51
2:P:5:DA:H5''	3:A:107:GLY:N	2.26	0.51
3:A:183:ARG:HH11	3:A:275:SER:CA	2.21	0.51
3:A:269:VAL:O	3:A:273:THR:OG1	2.27	0.51
3:A:245:ASN:H	3:A:245:ASN:HD22	0.75	0.51
3:A:204:SER:O	3:A:204:SER:OG	2.28	0.51
3:A:189:GLY:N	4:A:338:SO4:O3	2.29	0.50
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.41	0.50
3:A:195:LEU:O	3:A:260:ILE:N	2.44	0.50
3:A:330:PRO:CA	3:A:333:ARG:HG2	2.42	0.50
3:A:31:GLN:HB2	3:A:112:ARG:NH1	2.27	0.50
3:A:294:ASN:HB2	3:A:295:GLU:OE1	2.12	0.50
3:A:302:GLY:H	3:A:307:ALA:HB3	1.75	0.50
1:T:5:DA:H1'	6:T:564:HOH:O	2.12	0.50
3:A:18:MET:HE2	3:A:82:LEU:CD1	2.37	0.50
2:P:5:DA:H2''	2:P:6:DT:H71	1.94	0.50
3:A:245:ASN:ND2	3:A:245:ASN:N	2.30	0.50
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.94	0.50
3:A:294:ASN:ND2	3:A:297:THR:H	2.10	0.50
3:A:330:PRO:O	3:A:333:ARG:HG2	2.11	0.50
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.47	0.49
3:A:201:THR:HA	3:A:261:PRO:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:277:ILE:HD11	3:A:334:SER:O	2.12	0.49
3:A:133:ASN:O	3:A:137:ARG:HG3	2.12	0.49
3:A:263:ASP:O	3:A:264:GLN:HG2	2.13	0.49
3:A:170:ASP:OD1	3:A:171:SER:N	2.46	0.49
3:A:310:PRO:HB3	6:A:626:HOH:O	2.11	0.49
2:P:6:DT:H2''	2:P:7:DG:C8	2.48	0.49
3:A:282:MET:HE3	6:A:555:HOH:O	2.12	0.48
3:A:239:CYS:O	3:A:240:GLN:HB2	2.13	0.48
3:A:155:MET:CE	3:A:181:PHE:HB2	2.43	0.48
3:A:328:ARG:O	3:A:333:ARG:NE	2.28	0.48
3:A:111:ALA:O	3:A:115:VAL:HG23	2.13	0.48
3:A:270:LEU:CD2	3:A:282:MET:HE1	2.42	0.48
3:A:148:LYS:HB3	6:A:620:HOH:O	2.13	0.48
3:A:59:ALA:C	3:A:65:VAL:HG21	2.38	0.48
3:A:277:ILE:HG13	3:A:335:GLU:CB	2.44	0.48
1:T:6:DG:C2'	1:T:7:DA:C8	2.96	0.48
3:A:119:ILE:HG22	3:A:124:ASP:CB	2.43	0.48
3:A:286:ALA:HB1	3:A:291:PHE:HB2	1.95	0.48
3:A:150:ILE:N	3:A:188:SER:O	2.32	0.47
2:P:5:DA:P	3:A:107:GLY:HA3	2.54	0.47
3:A:182:ARG:HG2	3:A:273:THR:CG2	2.44	0.47
3:A:217:GLN:HA	3:A:217:GLN:HE21	1.77	0.47
3:A:317:LYS:HE3	3:A:321:ASP:OD1	2.13	0.47
3:A:83:ARG:HA	3:A:86:GLU:HG2	1.96	0.47
3:A:88:ILE:HG22	3:A:89:ARG:N	2.25	0.47
3:A:121:THR:O	3:A:124:ASP:HB2	2.15	0.47
3:A:311:LEU:HB3	3:A:322:TYR:HE2	1.79	0.47
3:A:121:THR:HG23	3:A:124:ASP:CG	2.40	0.47
3:A:212:HIS:N	3:A:212:HIS:CD2	2.79	0.47
3:A:36:TYR:CD1	3:A:36:TYR:C	2.90	0.47
3:A:99:PHE:CD1	3:A:99:PHE:C	2.92	0.47
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.96	0.47
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.59	0.46
3:A:308:GLY:O	3:A:309:GLU:HB2	2.16	0.46
3:A:288:GLU:C	3:A:290:GLY:H	2.23	0.46
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.49	0.46
3:A:278:PHE:HB2	3:A:333:ARG:O	2.15	0.46
3:A:159:GLN:O	3:A:159:GLN:HG2	2.09	0.46
3:A:195:LEU:O	3:A:259:LEU:HD12	2.16	0.46
3:A:207:GLN:HB2	6:A:625:HOH:O	2.15	0.46
2:P:5:DA:H2''	2:P:6:DT:H5'	1.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:25:PHE:CE2	3:A:88:ILE:HG12	2.51	0.46
3:A:157:GLN:HG3	3:A:241:LEU:HD11	1.96	0.46
3:A:15:ILE:HG21	3:A:46:ILE:HD13	1.97	0.46
3:A:182:ARG:NH1	3:A:273:THR:CG2	2.79	0.46
3:A:327:TYR:CD1	3:A:328:ARG:N	2.82	0.46
3:A:127:LYS:HB2	3:A:128:ASN:ND2	2.31	0.45
3:A:182:ARG:HH11	3:A:273:THR:CG2	2.30	0.45
2:P:5:DA:C2'	2:P:6:DT:H71	2.45	0.45
3:A:108:PRO:O	3:A:112:ARG:HG3	2.16	0.45
3:A:200:PHE:O	3:A:261:PRO:HA	2.15	0.45
3:A:244:LYS:H	3:A:244:LYS:HG2	1.60	0.45
3:A:259:LEU:HD12	3:A:260:ILE:N	2.31	0.45
3:A:294:ASN:O	3:A:296:TYR:N	2.49	0.45
1:T:5:DA:H2	2:P:3:DT:O2	1.99	0.45
3:A:320:PHE:CE1	3:A:328:ARG:HG3	2.51	0.45
3:A:75:GLU:O	3:A:79:THR:HG23	2.17	0.45
3:A:89:ARG:HD3	3:A:89:ARG:C	2.41	0.45
3:A:280:LYS:O	3:A:283:ARG:HB2	2.17	0.45
3:A:228:LEU:HB2	3:A:236:MET:O	2.16	0.45
3:A:129:GLU:HG2	3:A:137:ARG:HD3	1.99	0.45
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.98	0.45
3:A:194:LEU:HD12	3:A:194:LEU:HA	1.40	0.45
3:A:195:LEU:HA	3:A:195:LEU:HD12	1.72	0.45
3:A:204:SER:O	3:A:206:LYS:N	2.51	0.44
3:A:255:ILE:HG12	3:A:256:ASP:N	2.31	0.44
2:P:2:DC:H2'	2:P:2:DC:O5'	2.18	0.44
3:A:294:ASN:ND2	6:A:593:HOH:O	2.50	0.44
3:A:209:LYS:HA	3:A:209:LYS:HD3	1.32	0.44
3:A:41:LYS:O	3:A:45:VAL:HG13	2.18	0.44
3:A:191:MET:HE3	3:A:191:MET:HB2	1.72	0.44
3:A:155:MET:CA	3:A:158:MET:HE3	2.45	0.44
3:A:243:SER:OG	3:A:249:GLU:HG3	2.18	0.44
2:P:1:DT:H72	6:P:571:HOH:O	2.18	0.44
3:A:41:LYS:HE2	3:A:64:GLY:HA2	1.99	0.44
3:A:306:VAL:HG22	6:A:650:HOH:O	2.17	0.44
3:A:15:ILE:CG2	3:A:46:ILE:CD1	2.96	0.44
3:A:25:PHE:CD1	3:A:25:PHE:C	2.95	0.44
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.31	0.44
3:A:180:SER:HA	3:A:183:ARG:HE	1.82	0.44
3:A:155:MET:HE2	3:A:188:SER:OG	2.18	0.43
3:A:253:ARG:HH11	3:A:253:ARG:HG3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:232:GLU:O	3:A:233:THR:HG23	2.18	0.43
3:A:27:LYS:HG3	3:A:28:ASN:N	2.33	0.43
3:A:241:LEU:HA	3:A:242:PRO:HD2	1.69	0.43
3:A:266:TYR:HB2	3:A:313:VAL:HG11	2.00	0.43
3:A:280:LYS:O	3:A:284:ALA:N	2.43	0.43
3:A:293:ILE:HA	6:A:593:HOH:O	2.17	0.43
3:A:250:TYR:HB3	6:A:577:HOH:O	2.18	0.43
3:A:309:GLU:O	3:A:311:LEU:HD13	2.18	0.43
3:A:287:LEU:HA	3:A:287:LEU:HD13	1.64	0.43
3:A:309:GLU:N	3:A:310:PRO:HD3	2.33	0.43
3:A:327:TYR:CD1	3:A:327:TYR:C	2.95	0.43
3:A:31:GLN:HE21	3:A:112:ARG:CZ	2.31	0.43
3:A:267:CYS:O	3:A:271:TYR:HB2	2.19	0.43
3:A:128:ASN:HB3	3:A:131:LYS:HG3	2.00	0.43
3:A:128:ASN:ND2	3:A:128:ASN:N	2.67	0.42
3:A:128:ASN:C	3:A:130:ASP:N	2.76	0.42
3:A:183:ARG:HE	3:A:183:ARG:HB2	1.67	0.42
3:A:26:GLU:O	3:A:30:SER:O	2.36	0.42
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.34	0.42
3:A:209:LYS:HA	3:A:212:HIS:HB2	2.01	0.42
3:A:253:ARG:CG	3:A:253:ARG:NH1	2.80	0.42
3:A:303:VAL:C	3:A:305:GLY:N	2.78	0.42
3:A:172:GLU:HG3	3:A:198:PRO:HG2	2.01	0.42
3:A:182:ARG:HB3	3:A:273:THR:HG23	2.01	0.42
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.52	0.42
3:A:122:LEU:HD22	3:A:126:ARG:NH2	2.35	0.42
3:A:126:ARG:C	3:A:128:ASN:N	2.77	0.42
3:A:133:ASN:C	3:A:133:ASN:ND2	2.78	0.42
3:A:172:GLU:HB3	3:A:197:HIS:CD2	2.54	0.42
3:A:56:GLY:O	3:A:59:ALA:HB3	2.20	0.42
3:A:154:GLU:HB3	3:A:158:MET:HE2	2.01	0.42
3:A:330:PRO:C	3:A:333:ARG:HG2	2.45	0.42
3:A:156:LEU:HD23	3:A:156:LEU:HA	1.79	0.42
3:A:243:SER:O	3:A:244:LYS:O	2.37	0.42
1:T:2:DA:H2"	1:T:3:DT:OP2	2.20	0.41
3:A:15:ILE:HG12	3:A:73:ILE:HG23	2.01	0.41
3:A:18:MET:CE	3:A:76:PHE:HB2	2.49	0.41
3:A:132:LEU:HB3	3:A:136:GLN:HB2	2.02	0.41
3:A:260:ILE:HG23	3:A:260:ILE:HD12	1.65	0.41
3:A:126:ARG:C	3:A:128:ASN:H	2.28	0.41
3:A:157:GLN:HG3	3:A:241:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:68:LYS:O	3:A:71:GLU:HB3	2.20	0.41
3:A:125:LEU:HD23	3:A:125:LEU:HA	1.86	0.41
3:A:15:ILE:CG2	3:A:46:ILE:HD13	2.49	0.41
3:A:302:GLY:HA3	3:A:307:ALA:CB	2.50	0.41
3:A:18:MET:HG2	3:A:22:LEU:HD23	2.02	0.41
3:A:180:SER:HB2	3:A:185:ALA:CB	2.48	0.41
3:A:18:MET:HE3	3:A:76:PHE:CB	2.50	0.41
3:A:260:ILE:CG2	3:A:261:PRO:CD	2.99	0.41
3:A:303:VAL:O	3:A:305:GLY:N	2.54	0.41
1:T:4:DT:H2"	1:T:5:DA:H8	1.86	0.41
3:A:18:MET:HE2	3:A:82:LEU:CD2	2.49	0.41
3:A:133:ASN:HD22	3:A:135:HIS:H	1.68	0.41
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.55	0.41
3:A:150:ILE:CD1	3:A:190:ASP:HA	2.51	0.41
3:A:184:GLY:O	3:A:185:ALA:O	2.38	0.41
3:A:54:LYS:HA	3:A:54:LYS:HD2	1.67	0.40
3:A:224:ILE:HG22	3:A:225:THR:N	2.31	0.40
3:A:253:ARG:HH11	3:A:253:ARG:HG2	1.86	0.40
3:A:309:GLU:HA	3:A:310:PRO:HD2	1.89	0.40
3:A:200:PHE:O	3:A:262:LYS:N	2.49	0.40
3:A:259:LEU:HD12	3:A:259:LEU:HA	1.70	0.40
3:A:260:ILE:HG22	3:A:261:PRO:CD	2.51	0.40
3:A:37:ASN:HD22	3:A:37:ASN:HA	1.70	0.40
3:A:62:LEU:HA	3:A:62:LEU:HD12	1.77	0.40
3:A:304:THR:H	3:A:304:THR:HG23	1.28	0.40
3:A:22:LEU:HA	3:A:22:LEU:HD13	1.47	0.40
3:A:244:LYS:C	3:A:246:ASP:H	2.29	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%)	272 (84%)	37 (11%)	16 (5%)	1 6

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	185	ALA
3	A	205	THR
3	A	244	LYS
3	A	246	ASP
3	A	247	GLU
3	A	295	GLU
3	A	309	GLU
3	A	80	GLY
3	A	204	SER
3	A	304	THR
3	A	206	LYS
3	A	10	THR
3	A	310	PRO
3	A	207	GLN
3	A	289	LYS
3	A	13	GLY

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 2

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

Mol	Chain	Res	Type
3	A	10	THR
3	A	11	LEU
3	A	18	MET
3	A	19	LEU
3	A	22	LEU

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Mol	Chain	Res	Type
3	A	27	LYS
3	A	30	SER
3	A	36	TYR
3	A	37	ASN
3	A	41	LYS
3	A	45	VAL
3	A	46	ILE
3	A	52	LYS
3	A	54	LYS
3	A	61	LYS
3	A	62	LEU
3	A	65	VAL
3	A	67	THR
3	A	77	LEU
3	A	79	THR
3	A	81	LYS
3	A	89	ARG
3	A	94	SER
3	A	95	SER
3	A	100	LEU
3	A	101	THR
3	A	119	ILE
3	A	121	THR
3	A	122	LEU
3	A	128	ASN
3	A	132	LEU
3	A	133	ASN
3	A	138	ILE
3	A	153	GLU
3	A	168	LYS
3	A	169	VAL
3	A	191	MET
3	A	194	LEU
3	A	201	THR
3	A	213	GLN
3	A	214	VAL
3	A	218	LEU
3	A	226	ASP
3	A	228	LEU
3	A	245	ASN
3	A	248	LYS
3	A	251	PRO

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Mol	Chain	Res	Type
3	A	253	ARG
3	A	255	ILE
3	A	256	ASP
3	A	263	ASP
3	A	270	LEU
3	A	273	THR
3	A	277	ILE
3	A	279	ASN
3	A	287	LEU
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	306	VAL
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	325	TRP
3	A	331	LYS
3	A	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) 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	51	HIS
3	A	128	ASN
3	A	133	ASN
3	A	136	GLN
3	A	157	GLN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	245	ASN
3	A	252	HIS
3	A	264	GLN
3	A	279	ASN

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Mol	Chain	Res	Type
3	A	294	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no 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	0.85	0	6,6,6	0.90	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	338	SO4	1	0

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%)	0.27	1 (12%) 8 7	21, 43, 65, 92	1 (12%)
2	P	7/7 (100%)	-0.59	1 (14%) 6 5	21, 24, 36, 99	0
3	A	325/335 (97%)	-0.71	2 (0%) 85 81	6, 33, 85, 100	0
All	All	340/350 (97%)	-0.68	4 (1%) 76 69	6, 33, 86, 100	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	1	DC	6.0
2	P	7	DG	2.6
3	A	246	ASP	2.4
3	A	304	THR	2.3

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($\text{\AA}^2$)	Q<0.9
4	SO4	A	338	5/5	0.76	0.21	70,70,70,70	5
5	NA	A	342	1/1	0.89	0.10	69,69,69,69	0
5	NA	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.