



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:00 PM UTC

PDB ID : 1ZQR / pdb_00001zqr
Title : DNA POLYMERASE BETA (E.C.2.7.7.7)/DNA COMPLEX, SOAKED IN THE PRESENCE OF NICL2
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-04-12
Resolution : 3.70 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

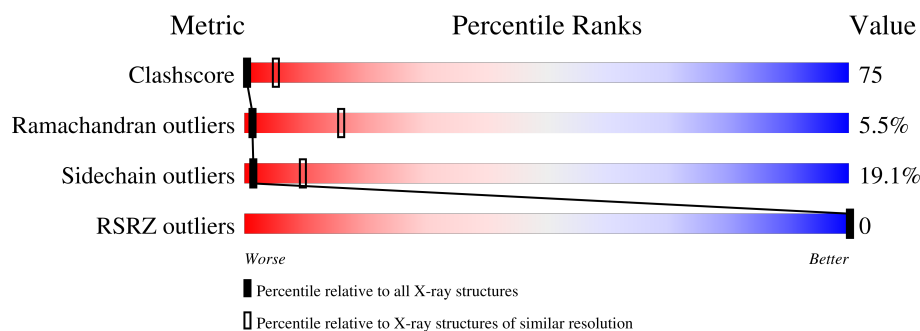
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	25% 12% 62%
2	P	7	57% 43%
3	A	335	15% 47% 30% 5% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3058 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 NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ni	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	16	Total	O	0	0
			16	16		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	23	Total 23	O 23	0	0
6	A	104	Total 104	O 104	0	0

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.

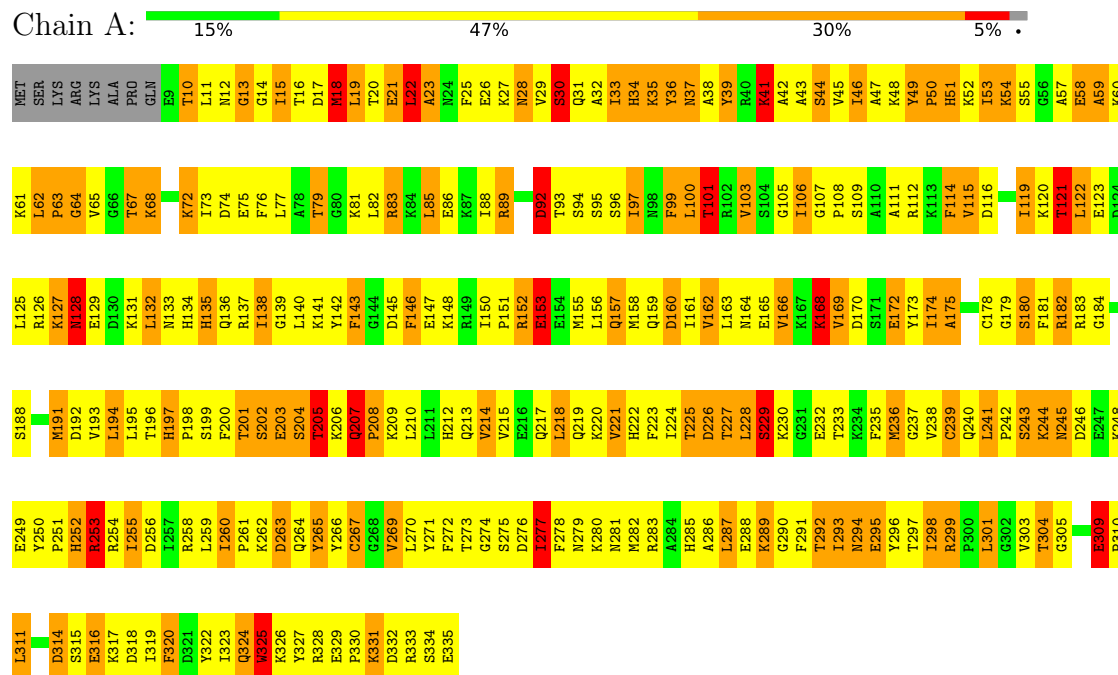
- Molecule 1: DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3')



- 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	179.69Å 57.50Å 47.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.70 20.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	70.0 (20.00-3.70) 53.8 (20.00-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 2.63Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.173 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	2.8	Xtriage
Anisotropy	4.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	4.21 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3058	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% 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: NI, 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	1.44	2/162 (1.2%)	3.08	10/249 (4.0%)
2	P	1.36	2/160 (1.2%)	2.90	8/243 (3.3%)
3	A	1.47	10/2672 (0.4%)	2.33	142/3590 (4.0%)
All	All	1.46	14/2994 (0.5%)	2.42	160/4082 (3.9%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	128	ASN	CA-C	-8.30	1.43	1.53
3	A	101	THR	C-O	-6.48	1.16	1.24
3	A	253	ARG	CA-C	-6.27	1.45	1.52
1	T	6	DG	C3'-O3'	-6.16	1.24	1.42
2	P	1	DT	OP3-P	5.87	1.60	1.48
3	A	57	ALA	N-CA	-5.33	1.39	1.46
3	A	58	GLU	CD-OE1	5.33	1.35	1.25
3	A	15	ILE	CA-C	-5.27	1.46	1.52
3	A	54	LYS	N-CA	-5.22	1.39	1.45
3	A	96	SER	CA-C	-5.22	1.46	1.52
3	A	220	LYS	C-N	-5.21	1.28	1.33
1	T	6	DG	O3'-P	-5.18	1.53	1.61
3	A	63	PRO	N-CA	-5.14	1.41	1.46
2	P	5	DA	C3'-C2'	5.06	1.63	1.52

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	6	DG	C4-N9-C1'	-21.98	94.03	127.00
1	T	6	DG	C8-N9-C1'	20.47	157.70	127.00
1	T	7	DA	C4-N9-C1'	-18.82	98.83	127.05
2	P	7	DG	C4-N9-C1'	-18.52	99.22	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	1	DT	C6-N1-C1'	-18.19	92.06	119.35
2	P	7	DG	C8-N9-C1'	17.97	153.95	127.00
1	T	7	DA	C8-N9-C1'	17.93	153.94	127.05
2	P	1	DT	C2-N1-C1'	17.61	145.76	119.35
3	A	49	TYR	CA-C-N	15.25	134.77	119.82
3	A	49	TYR	C-N-CA	15.25	134.77	119.82
1	T	4	DT	C6-N1-C1'	-13.90	98.50	119.35
1	T	4	DT	C2-N1-C1'	13.24	139.21	119.35
2	P	5	DA	C4-N9-C1'	12.90	146.40	127.05
2	P	5	DA	C8-N9-C1'	-12.78	107.88	127.05
2	P	6	DT	C6-N1-C1'	-10.66	103.36	119.35
3	A	146	PHE	CA-CB-CG	-10.45	103.35	113.80
3	A	116	ASP	CA-CB-CG	-10.39	102.21	112.60
3	A	99	PHE	CA-CB-CG	-10.30	103.50	113.80
2	P	6	DT	C2-N1-C1'	10.27	134.75	119.35
1	T	3	DT	C2-N1-C1'	-9.28	105.43	119.35
3	A	49	TYR	O-C-N	9.13	129.25	121.31
3	A	92	ASP	CB-CA-C	8.87	125.01	110.81
3	A	51	HIS	CA-CB-CG	8.87	122.67	113.80
1	T	3	DT	C6-N1-C1'	8.74	132.46	119.35
3	A	157	GLN	N-CA-CB	8.66	122.56	110.01
3	A	115	VAL	N-CA-C	8.33	119.13	110.72
3	A	192	ASP	CA-C-N	-8.28	111.85	123.11
3	A	192	ASP	C-N-CA	-8.28	111.85	123.11
3	A	269	VAL	CA-C-N	8.20	131.61	120.54
3	A	269	VAL	C-N-CA	8.20	131.61	120.54
3	A	105	GLY	N-CA-C	-8.18	104.83	113.58
3	A	92	ASP	CA-CB-CG	8.15	120.75	112.60
3	A	168	LYS	N-CA-CB	8.06	121.95	109.94
1	T	2	DA	C4-N9-C1'	-7.98	115.07	127.05
3	A	121	THR	N-CA-C	7.91	120.54	109.31
3	A	20	THR	N-CA-CB	7.86	121.91	110.20
3	A	227	THR	N-CA-CB	7.79	123.47	110.77
3	A	143	PHE	CA-CB-CG	7.77	121.57	113.80
3	A	64	GLY	CA-C-N	-7.65	113.11	122.90
3	A	64	GLY	C-N-CA	-7.65	113.11	122.90
1	T	2	DA	C8-N9-C1'	7.48	138.27	127.05
3	A	15	ILE	N-CA-CB	7.47	121.28	110.52
3	A	74	ASP	N-CA-CB	7.41	121.00	110.12
3	A	318	ASP	CA-CB-CG	-7.38	105.22	112.60
3	A	153	GLU	N-CA-C	-7.28	102.13	111.02
3	A	21	GLU	N-CA-C	-7.21	103.42	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	267	CYS	CB-CA-C	-7.17	99.62	110.88
3	A	192	ASP	CA-CB-CG	7.17	119.77	112.60
3	A	57	ALA	N-CA-CB	-7.09	99.43	110.06
3	A	95	SER	O-C-N	7.02	131.93	122.59
3	A	114	PHE	N-CA-CB	7.01	120.58	110.06
3	A	157	GLN	CB-CA-C	6.85	121.64	110.88
3	A	17	ASP	CB-CA-C	6.83	121.69	110.90
3	A	41	LYS	N-CA-CB	6.82	119.89	110.01
3	A	225	THR	CA-C-N	-6.76	111.64	122.53
3	A	225	THR	C-N-CA	-6.76	111.64	122.53
3	A	229	SER	N-CA-CB	6.72	121.85	110.49
3	A	22	LEU	CA-C-N	6.60	129.45	120.54
3	A	22	LEU	C-N-CA	6.60	129.45	120.54
3	A	172	GLU	CA-C-N	6.56	130.88	121.50
3	A	172	GLU	C-N-CA	6.56	130.88	121.50
3	A	205	THR	N-CA-CB	6.52	121.51	110.49
3	A	239	CYS	N-CA-CB	6.51	121.49	111.46
3	A	213	GLN	CA-C-N	6.51	129.38	120.46
3	A	213	GLN	C-N-CA	6.51	129.38	120.46
3	A	193	VAL	N-CA-C	6.45	116.92	107.37
3	A	64	GLY	CA-C-O	6.38	125.27	118.95
3	A	50	PRO	CB-CA-C	-6.37	102.33	111.62
3	A	168	LYS	CB-CA-C	6.36	120.99	110.81
3	A	114	PHE	CA-CB-CG	-6.36	107.44	113.80
3	A	224	ILE	CA-C-N	-6.36	112.26	122.24
3	A	224	ILE	C-N-CA	-6.36	112.26	122.24
3	A	269	VAL	O-C-N	6.31	128.44	121.94
3	A	53	ILE	N-CA-CB	6.22	121.50	111.23
3	A	63	PRO	N-CA-C	-6.21	100.59	112.01
3	A	28	ASN	CA-CB-CG	-6.17	106.42	112.60
3	A	252	HIS	CA-C-N	-6.17	113.24	122.74
3	A	252	HIS	C-N-CA	-6.17	113.24	122.74
3	A	162	VAL	N-CA-C	6.11	117.58	110.62
3	A	166	VAL	N-CA-C	-6.10	103.95	110.36
3	A	222	HIS	CA-CB-CG	-6.10	107.70	113.80
3	A	309	GLU	CA-C-N	6.05	127.40	119.84
3	A	309	GLU	C-N-CA	6.05	127.40	119.84
3	A	194	LEU	N-CA-CB	6.04	119.00	109.71
3	A	54	LYS	CB-CA-C	6.03	119.20	109.07
3	A	15	ILE	O-C-N	5.98	129.67	121.90
3	A	21	GLU	CB-CG-CD	-5.97	102.45	112.60
3	A	207	GLN	CA-C-N	5.97	126.12	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	207	GLN	C-N-CA	5.97	126.12	119.32
3	A	54	LYS	N-CA-CB	-5.96	102.39	110.67
3	A	260	ILE	CB-CA-C	-5.95	100.53	111.36
3	A	53	ILE	CB-CA-C	5.93	121.01	111.29
3	A	67	THR	N-CA-C	5.88	118.64	111.82
3	A	30	SER	CA-C-N	-5.84	113.38	122.67
3	A	30	SER	C-N-CA	-5.84	113.38	122.67
3	A	96	SER	CA-C-O	-5.84	114.65	120.90
3	A	106	ILE	CA-C-N	5.82	131.00	121.87
3	A	106	ILE	C-N-CA	5.82	131.00	121.87
3	A	191	MET	N-CA-CB	5.79	119.60	110.23
3	A	263	ASP	CA-CB-CG	-5.75	106.85	112.60
3	A	226	ASP	CA-CB-CG	5.74	118.34	112.60
3	A	139	GLY	N-CA-C	-5.73	105.85	112.73
3	A	39	TYR	N-CA-C	5.72	119.08	111.75
3	A	18	MET	CA-C-N	5.72	128.51	120.28
3	A	18	MET	C-N-CA	5.72	128.51	120.28
3	A	169	VAL	CB-CA-C	5.71	120.66	111.29
3	A	68	LYS	N-CA-CB	5.71	118.34	110.07
3	A	299	ARG	CA-C-N	5.71	125.47	119.76
3	A	299	ARG	C-N-CA	5.71	125.47	119.76
3	A	59	ALA	O-C-N	5.70	128.18	122.08
3	A	101	THR	CA-CB-OG1	5.65	118.08	109.60
3	A	72	LYS	CB-CA-C	5.65	119.75	110.88
3	A	35	LYS	O-C-N	5.63	127.94	122.09
3	A	160	ASP	O-C-N	5.62	130.06	122.59
3	A	85	LEU	CA-C-N	5.61	128.26	120.29
3	A	85	LEU	C-N-CA	5.61	128.26	120.29
3	A	320	PHE	CA-CB-CG	-5.58	108.22	113.80
3	A	34	HIS	CA-CB-CG	-5.53	108.27	113.80
3	A	219	GLN	O-C-N	5.53	128.06	122.09
3	A	152	ARG	O-C-N	5.51	128.48	122.20
3	A	74	ASP	CA-CB-CG	5.49	118.09	112.60
3	A	281	ASN	CA-CB-CG	5.46	118.06	112.60
3	A	265	TYR	CA-C-N	5.45	127.85	120.38
3	A	265	TYR	C-N-CA	5.45	127.85	120.38
3	A	103	VAL	N-CA-CB	-5.45	106.01	111.90
3	A	277	ILE	N-CA-CB	5.43	118.73	110.58
3	A	21	GLU	CB-CA-C	-5.37	101.87	110.79
3	A	23	ALA	CA-C-N	5.36	127.46	120.28
3	A	23	ALA	C-N-CA	5.36	127.46	120.28
3	A	151	PRO	N-CA-CB	5.34	108.08	103.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	197	HIS	CA-C-N	5.33	125.39	119.32
3	A	197	HIS	C-N-CA	5.33	125.39	119.32
3	A	83	ARG	N-CA-CB	5.31	117.76	110.07
3	A	54	LYS	CA-C-O	5.29	124.63	118.97
3	A	175	ALA	CB-CA-C	-5.29	99.86	109.38
3	A	115	VAL	N-CA-CB	5.24	118.44	110.58
3	A	208	PRO	CB-CA-C	-5.21	103.57	112.64
3	A	180	SER	N-CA-C	5.21	118.42	111.75
3	A	194	LEU	CA-C-N	-5.21	115.13	122.94
3	A	194	LEU	C-N-CA	-5.21	115.13	122.94
3	A	65	VAL	N-CA-CB	5.20	117.30	111.21
3	A	236	MET	CA-C-N	-5.20	111.23	121.41
3	A	236	MET	C-N-CA	-5.20	111.23	121.41
3	A	241	LEU	O-C-N	5.18	129.05	121.54
3	A	115	VAL	CB-CA-C	-5.17	105.09	112.22
3	A	205	THR	N-CA-C	5.16	121.79	110.80
3	A	224	ILE	CA-CB-CG1	-5.15	101.64	110.40
3	A	10	THR	N-CA-CB	5.13	119.15	110.49
3	A	252	HIS	CB-CA-C	5.12	117.53	109.84
3	A	180	SER	CA-C-N	5.12	127.10	120.44
3	A	180	SER	C-N-CA	5.12	127.10	120.44
3	A	241	LEU	N-CA-CB	5.12	117.89	110.32
3	A	23	ALA	N-CA-C	5.11	117.24	111.11
3	A	292	THR	N-CA-CB	5.10	119.38	110.81
3	A	325	TRP	N-CA-CB	-5.07	103.14	110.70
3	A	255	ILE	N-CA-CB	5.07	118.50	111.05
3	A	132	LEU	CB-CA-C	-5.06	100.94	109.50
3	A	20	THR	N-CA-C	-5.03	105.50	111.69
3	A	68	LYS	CB-CA-C	5.03	118.84	110.90
3	A	184	GLY	N-CA-C	5.02	121.06	115.08

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	9	0
2	P	144	0	81	17	0
3	A	2623	0	2641	407	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	104	0	0	22	0
6	P	23	0	0	5	0
6	T	16	0	0	5	0
All	All	3058	0	2802	427	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 75.

All (427) 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:6:DT:H2''	2:P:7:DG:H5''	1.20	1.11
2:P:5:DA:H2''	2:P:6:DT:H5''	1.32	1.06
3:A:155:MET:HE2	3:A:188:SER:HB2	1.40	1.04
3:A:243:SER:HB3	3:A:249:GLU:HA	1.39	1.01
3:A:245:ASN:HD22	3:A:245:ASN:N	1.54	1.00
3:A:201:THR:HA	3:A:261:PRO:HB3	1.43	0.99
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.44	0.97
1:T:6:DG:H2''	1:T:7:DA:C8	1.99	0.96
3:A:138:ILE:HG21	3:A:228:LEU:HD11	1.44	0.96
3:A:245:ASN:H	3:A:245:ASN:ND2	1.62	0.94
3:A:254:ARG:HH11	3:A:255:ILE:H	1.08	0.94
3:A:197:HIS:ND1	3:A:199:SER:HB3	1.84	0.93
3:A:41:LYS:HE2	3:A:64:GLY:HA3	1.50	0.93
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.50	0.92
3:A:197:HIS:HD1	3:A:199:SER:HB3	1.35	0.91
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.51	0.91
3:A:114:PHE:HB3	3:A:119:ILE:HB	1.48	0.90
2:P:5:DA:H2''	2:P:6:DT:C5'	2.01	0.89
3:A:254:ARG:NH1	3:A:255:ILE:H	1.71	0.87
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.57	0.87
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.38	0.85
3:A:19:LEU:HB3	3:A:43:ALA:HB2	1.58	0.84
3:A:141:LYS:HE2	3:A:142:TYR:CZ	2.13	0.83
3:A:27:LYS:HG3	3:A:28:ASN:ND2	1.95	0.81
3:A:18:MET:CE	3:A:76:PHE:HB2	2.10	0.81
3:A:15:ILE:HB	3:A:46:ILE:HD11	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.62	0.81
3:A:18:MET:HE2	3:A:82:LEU:HD13	1.61	0.80
3:A:285:HIS:HD2	3:A:323:ILE:HD12	1.45	0.80
3:A:111:ALA:O	3:A:115:VAL:HG23	1.81	0.80
3:A:138:ILE:HD12	3:A:228:LEU:CD1	2.11	0.80
3:A:18:MET:HE2	3:A:82:LEU:HD22	1.63	0.80
3:A:209:LYS:HA	3:A:212:HIS:HB2	1.62	0.80
3:A:150:ILE:CG2	3:A:158:MET:HE1	2.11	0.79
3:A:330:PRO:HA	3:A:333:ARG:CG	2.12	0.79
3:A:214:VAL:O	3:A:218:LEU:HD13	1.83	0.79
3:A:201:THR:HA	3:A:261:PRO:CB	2.12	0.78
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.11	0.78
2:P:3:DT:H1'	6:P:511:HOH:O	1.81	0.78
3:A:197:HIS:CE1	3:A:199:SER:HB3	2.18	0.78
3:A:254:ARG:HH11	3:A:255:ILE:N	1.80	0.77
3:A:18:MET:CE	3:A:82:LEU:HD13	2.14	0.77
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.48	0.76
3:A:180:SER:CA	3:A:183:ARG:HH21	1.98	0.76
3:A:245:ASN:HD22	3:A:245:ASN:H	0.80	0.76
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.67	0.75
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.68	0.75
3:A:174:ILE:HB	3:A:196:THR:HG22	1.68	0.75
3:A:255:ILE:HG12	3:A:256:ASP:N	2.01	0.74
3:A:18:MET:HE3	3:A:76:PHE:HB2	1.68	0.74
3:A:236:MET:HG3	3:A:256:ASP:OD1	1.87	0.74
3:A:163:LEU:HD22	3:A:175:ALA:HB3	1.67	0.74
3:A:147:GLU:HG3	6:A:514:HOH:O	1.87	0.74
3:A:138:ILE:HG21	3:A:228:LEU:CD1	2.18	0.74
3:A:250:TYR:HB3	6:A:568:HOH:O	1.87	0.74
3:A:180:SER:HA	3:A:183:ARG:HH21	1.52	0.74
3:A:201:THR:CA	3:A:261:PRO:HB3	2.17	0.73
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.23	0.73
3:A:82:LEU:HD23	3:A:85:LEU:HB2	1.71	0.73
3:A:26:GLU:HA	3:A:30:SER:OG	1.89	0.72
3:A:253:ARG:HG3	3:A:253:ARG:HH11	1.54	0.72
3:A:53:ILE:HG21	3:A:59:ALA:HB2	1.72	0.72
3:A:165:GLU:HA	3:A:168:LYS:CG	2.19	0.72
3:A:93:THR:O	3:A:97:ILE:HG13	1.90	0.72
3:A:99:PHE:HD2	3:A:100:LEU:HD13	1.54	0.72
3:A:202:SER:N	3:A:261:PRO:HB3	2.06	0.71
3:A:108:PRO:O	3:A:112:ARG:HG3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:103:VAL:CB	3:A:106:ILE:HD12	2.21	0.71
3:A:285:HIS:CD2	3:A:323:ILE:HD12	2.26	0.71
3:A:128:ASN:HB3	3:A:131:LYS:HG3	1.73	0.70
3:A:254:ARG:NH1	3:A:255:ILE:N	2.38	0.70
3:A:271:TYR:HB2	6:A:580:HOH:O	1.89	0.70
3:A:277:ILE:HG13	3:A:335:GLU:HB2	1.73	0.70
3:A:138:ILE:CG2	3:A:228:LEU:HD11	2.21	0.70
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.27	0.70
3:A:174:ILE:O	3:A:195:LEU:HD12	1.92	0.70
3:A:165:GLU:HB3	3:A:217:GLN:CG	2.22	0.69
3:A:299:ARG:HG2	3:A:310:PRO:N	2.06	0.69
3:A:18:MET:O	3:A:21:GLU:HB2	1.91	0.69
3:A:259:LEU:HD12	3:A:260:ILE:H	1.58	0.69
3:A:255:ILE:HG12	3:A:256:ASP:H	1.56	0.69
3:A:282:MET:HB2	3:A:325:TRP:CZ3	2.28	0.69
3:A:29:VAL:HG21	3:A:94:SER:CB	2.22	0.69
3:A:46:ILE:HD12	3:A:46:ILE:O	1.92	0.69
3:A:140:LEU:HB3	6:A:607:HOH:O	1.93	0.68
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.76	0.68
3:A:138:ILE:HD12	3:A:228:LEU:HD12	1.75	0.68
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.59	0.68
2:P:5:DA:C2'	2:P:6:DT:H5''	2.18	0.68
3:A:152:ARG:HA	3:A:155:MET:HB2	1.75	0.68
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.29	0.67
3:A:207:GLN:HB3	3:A:210:LEU:HD12	1.75	0.67
3:A:73:ILE:HG22	3:A:77:LEU:HD22	1.75	0.67
1:T:3:DT:H1'	6:T:603:HOH:O	1.94	0.67
1:T:6:DG:H5''	6:T:545:HOH:O	1.94	0.67
3:A:19:LEU:HD23	3:A:43:ALA:CA	2.25	0.67
3:A:276:ASP:O	3:A:280:LYS:HG3	1.94	0.66
3:A:25:PHE:CE1	3:A:88:ILE:HG12	2.30	0.66
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.31	0.66
2:P:4:DA:H1'	6:P:583:HOH:O	1.96	0.65
3:A:155:MET:CE	3:A:188:SER:HB2	2.22	0.65
3:A:162:VAL:O	3:A:166:VAL:HG23	1.96	0.65
3:A:266:TYR:HA	3:A:269:VAL:HB	1.77	0.65
3:A:11:LEU:HD23	3:A:11:LEU:H	1.60	0.65
3:A:135:HIS:HB2	6:A:584:HOH:O	1.97	0.65
2:P:6:DT:C2'	2:P:7:DG:H5''	2.13	0.64
3:A:298:ILE:N	6:A:569:HOH:O	2.31	0.64
3:A:58:GLU:O	3:A:61:LYS:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:292:THR:HG22	3:A:299:ARG:O	1.97	0.64
2:P:5:DA:O5'	3:A:107:GLY:HA3	1.97	0.63
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.27	0.63
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.28	0.63
3:A:50:PRO:HG2	3:A:51:HIS:CD2	2.33	0.63
3:A:294:ASN:O	3:A:296:TYR:N	2.30	0.63
3:A:207:GLN:HB3	3:A:210:LEU:CD1	2.28	0.63
3:A:44:SER:O	3:A:47:ALA:HB3	1.99	0.63
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.79	0.63
3:A:202:SER:H	3:A:261:PRO:HB3	1.62	0.62
3:A:253:ARG:HH11	3:A:253:ARG:CG	2.12	0.62
3:A:327:TYR:HD1	3:A:328:ARG:N	1.97	0.62
3:A:18:MET:HG3	3:A:85:LEU:HD22	1.81	0.62
3:A:27:LYS:HB2	3:A:36:TYR:CD2	2.35	0.62
3:A:282:MET:O	3:A:285:HIS:HB3	1.99	0.62
3:A:19:LEU:HD23	3:A:43:ALA:HB2	1.81	0.62
3:A:263:ASP:O	3:A:264:GLN:HG2	1.99	0.62
3:A:121:THR:OG1	3:A:122:LEU:N	2.32	0.61
3:A:161:ILE:O	3:A:164:ASN:HB2	1.99	0.61
3:A:254:ARG:NH1	3:A:255:ILE:O	2.33	0.61
3:A:92:ASP:HB3	6:A:629:HOH:O	2.01	0.61
3:A:133:ASN:O	3:A:137:ARG:HG3	1.99	0.61
3:A:299:ARG:HG2	3:A:310:PRO:CA	2.30	0.61
3:A:331:LYS:HG2	3:A:332:ASP:N	2.11	0.61
3:A:295:GLU:HA	6:A:580:HOH:O	2.01	0.61
3:A:217:GLN:O	3:A:221:VAL:HG13	2.01	0.60
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.36	0.60
3:A:41:LYS:HD3	3:A:42:ALA:H	1.66	0.60
3:A:122:LEU:HD11	3:A:143:PHE:CD2	2.35	0.60
3:A:277:ILE:CG1	3:A:335:GLU:HB2	2.31	0.60
1:T:1:DC:H2''	1:T:2:DA:OP2	2.02	0.60
3:A:159:GLN:O	3:A:163:LEU:HG	2.02	0.60
3:A:99:PHE:HD2	3:A:100:LEU:CD1	2.14	0.60
3:A:323:ILE:C	3:A:324:GLN:HG2	2.27	0.59
3:A:55:SER:O	3:A:58:GLU:HB3	2.02	0.59
3:A:103:VAL:O	3:A:106:ILE:N	2.30	0.59
3:A:181:PHE:HA	6:A:530:HOH:O	2.01	0.59
3:A:277:ILE:HD11	3:A:335:GLU:HB3	1.84	0.59
3:A:228:LEU:HB2	3:A:236:MET:O	2.03	0.59
3:A:204:SER:O	3:A:206:LYS:N	2.35	0.59
3:A:18:MET:HE2	3:A:82:LEU:CD2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:299:ARG:HG2	3:A:310:PRO:HA	1.86	0.58
3:A:83:ARG:HA	3:A:86:GLU:HG2	1.86	0.58
3:A:183:ARG:HD3	3:A:273:THR:O	2.02	0.58
3:A:182:ARG:HG2	3:A:182:ARG:NH1	2.10	0.58
3:A:29:VAL:HG21	3:A:94:SER:OG	2.04	0.57
3:A:150:ILE:N	3:A:188:SER:O	2.30	0.57
3:A:270:LEU:CD2	3:A:319:ILE:HD13	2.34	0.57
3:A:201:THR:HA	3:A:261:PRO:CA	2.34	0.57
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.18	0.57
3:A:15:ILE:CB	3:A:46:ILE:HD11	2.32	0.57
3:A:25:PHE:CD1	3:A:88:ILE:HD13	2.39	0.57
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.40	0.57
3:A:114:PHE:HB3	3:A:119:ILE:CB	2.28	0.57
3:A:30:SER:HA	6:A:553:HOH:O	2.05	0.56
3:A:241:LEU:HB2	3:A:250:TYR:CD2	2.40	0.56
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.41	0.56
2:P:5:DA:P	3:A:109:SER:HB3	2.46	0.56
3:A:225:THR:HG21	6:A:520:HOH:O	2.04	0.56
3:A:259:LEU:O	3:A:260:ILE:HD13	2.05	0.56
3:A:270:LEU:HD22	3:A:319:ILE:CD1	2.36	0.56
3:A:23:ALA:O	3:A:36:TYR:HD2	1.88	0.56
3:A:18:MET:HE2	3:A:82:LEU:CD1	2.33	0.56
1:T:3:DT:H2''	1:T:4:DT:C5'	2.35	0.56
3:A:22:LEU:HB3	3:A:39:TYR:CE1	2.40	0.56
3:A:238:VAL:HG12	3:A:239:CYS:H	1.70	0.56
3:A:188:SER:HB3	6:A:522:HOH:O	2.06	0.56
3:A:316:GLU:O	3:A:320:PHE:HD2	1.88	0.56
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.87	0.56
3:A:172:GLU:HB3	3:A:197:HIS:NE2	2.21	0.56
3:A:180:SER:HA	3:A:183:ARG:NH2	2.21	0.56
1:T:3:DT:H2''	1:T:4:DT:H5'	1.88	0.55
3:A:29:VAL:CG2	3:A:94:SER:HA	2.36	0.55
3:A:278:PHE:HB2	3:A:333:ARG:O	2.05	0.55
3:A:244:LYS:C	3:A:246:ASP:H	2.13	0.55
3:A:181:PHE:HD1	6:A:530:HOH:O	1.88	0.55
1:T:4:DT:H1'	6:T:527:HOH:O	2.05	0.55
3:A:72:LYS:HG2	3:A:82:LEU:HD11	1.89	0.55
3:A:34:HIS:O	3:A:38:ALA:N	2.39	0.55
3:A:22:LEU:HB3	3:A:39:TYR:CD1	2.42	0.55
3:A:289:LYS:HD3	3:A:289:LYS:N	2.16	0.55
3:A:132:LEU:HB2	3:A:137:ARG:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:260:ILE:HG22	3:A:261:PRO:N	2.21	0.54
3:A:293:ILE:HA	6:A:581:HOH:O	2.08	0.54
3:A:13:GLY:O	3:A:15:ILE:N	2.41	0.54
3:A:129:GLU:HG2	3:A:137:ARG:HD3	1.89	0.54
3:A:142:TYR:O	3:A:146:PHE:HB2	2.08	0.54
3:A:201:THR:C	3:A:261:PRO:HB3	2.32	0.54
3:A:100:LEU:HD11	3:A:120:LYS:O	2.08	0.54
3:A:207:GLN:O	3:A:210:LEU:HB2	2.08	0.54
3:A:174:ILE:HB	3:A:196:THR:CG2	2.38	0.54
2:P:5:DA:H1'	6:P:559:HOH:O	2.07	0.53
2:P:6:DT:C4	2:P:7:DG:C6	2.96	0.53
3:A:132:LEU:HD23	3:A:132:LEU:N	2.23	0.53
2:P:5:DA:C5'	3:A:107:GLY:HA3	2.38	0.53
3:A:29:VAL:HA	3:A:97:ILE:HD12	1.90	0.53
3:A:19:LEU:HD23	3:A:43:ALA:N	2.24	0.53
3:A:103:VAL:HG11	3:A:106:ILE:CD1	2.39	0.53
3:A:170:ASP:HB3	3:A:173:TYR:CD2	2.44	0.53
3:A:259:LEU:HD12	3:A:260:ILE:N	2.23	0.53
3:A:165:GLU:OE1	3:A:168:LYS:NZ	2.33	0.53
3:A:13:GLY:O	3:A:16:THR:N	2.42	0.53
2:P:5:DA:P	3:A:107:GLY:HA3	2.49	0.53
3:A:128:ASN:N	3:A:128:ASN:HD22	2.06	0.53
3:A:283:ARG:HG3	6:A:550:HOH:O	2.09	0.53
6:T:545:HOH:O	3:A:133:ASN:HB2	2.08	0.52
3:A:19:LEU:HD23	3:A:43:ALA:CB	2.39	0.52
3:A:235:PHE:CE1	3:A:237:GLY:N	2.77	0.52
3:A:200:PHE:CD2	3:A:259:LEU:HG	2.44	0.52
3:A:241:LEU:HB2	3:A:250:TYR:CG	2.44	0.52
3:A:18:MET:HG2	3:A:22:LEU:HD23	1.91	0.52
3:A:200:PHE:CE2	3:A:259:LEU:HG	2.45	0.52
3:A:265:TYR:CD2	3:A:269:VAL:HG21	2.45	0.52
3:A:36:TYR:CD1	3:A:37:ASN:N	2.78	0.52
3:A:201:THR:HA	3:A:261:PRO:HA	1.92	0.52
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.39	0.52
3:A:155:MET:HA	3:A:158:MET:HE3	1.91	0.52
3:A:275:SER:N	3:A:278:PHE:HB3	2.25	0.52
3:A:258:ARG:NH2	3:A:272:PHE:CZ	2.78	0.52
3:A:29:VAL:HG21	3:A:94:SER:HA	1.92	0.51
3:A:203:GLU:O	3:A:205:THR:N	2.43	0.51
3:A:134:HIS:O	3:A:137:ARG:HB2	2.10	0.51
3:A:270:LEU:HD22	3:A:319:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:165:GLU:O	3:A:169:VAL:HG12	2.10	0.51
3:A:15:ILE:O	3:A:19:LEU:HB2	2.11	0.51
3:A:59:ALA:O	3:A:62:LEU:HB2	2.10	0.51
3:A:180:SER:CB	3:A:183:ARG:HH21	2.24	0.51
2:P:6:DT:OP1	3:A:106:ILE:O	2.29	0.51
3:A:243:SER:O	3:A:244:LYS:O	2.29	0.51
3:A:271:TYR:CE1	3:A:283:ARG:NH2	2.79	0.51
3:A:26:GLU:O	3:A:30:SER:O	2.28	0.51
3:A:209:LYS:CA	3:A:212:HIS:HB2	2.37	0.51
3:A:271:TYR:CD1	3:A:283:ARG:NH2	2.79	0.51
3:A:158:MET:HB3	3:A:191:MET:HE3	1.92	0.51
3:A:238:VAL:HG12	3:A:239:CYS:N	2.26	0.51
3:A:31:GLN:N	6:A:553:HOH:O	2.43	0.50
3:A:253:ARG:HD3	6:A:521:HOH:O	2.11	0.50
3:A:294:ASN:HB2	3:A:295:GLU:OE1	2.11	0.50
3:A:41:LYS:NZ	3:A:64:GLY:O	2.29	0.50
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.26	0.50
3:A:200:PHE:C	3:A:201:THR:HG22	2.36	0.50
3:A:41:LYS:HD3	3:A:42:ALA:N	2.26	0.50
3:A:153:GLU:O	3:A:156:LEU:HB2	2.11	0.50
3:A:228:LEU:O	3:A:229:SER:HB3	2.11	0.50
3:A:282:MET:HB2	3:A:325:TRP:HZ3	1.75	0.50
3:A:22:LEU:HD22	3:A:85:LEU:HD13	1.94	0.50
3:A:240:GLN:NE2	3:A:250:TYR:O	2.44	0.50
3:A:288:GLU:C	3:A:290:GLY:H	2.19	0.50
3:A:152:ARG:NH2	3:A:181:PHE:O	2.38	0.50
3:A:294:ASN:N	3:A:294:ASN:HD22	2.09	0.50
3:A:209:LYS:O	3:A:212:HIS:HB2	2.12	0.50
3:A:252:HIS:ND1	6:A:579:HOH:O	2.23	0.50
3:A:26:GLU:HB3	3:A:32:ALA:HB3	1.94	0.50
3:A:157:GLN:O	3:A:160:ASP:HB3	2.12	0.50
3:A:329:GLU:O	3:A:333:ARG:HG2	2.12	0.50
3:A:207:GLN:OE1	3:A:210:LEU:HD11	2.12	0.50
3:A:15:ILE:CD1	3:A:73:ILE:HG21	2.42	0.49
3:A:48:LYS:HG3	6:A:594:HOH:O	2.12	0.49
3:A:196:THR:HB	3:A:265:TYR:CD1	2.48	0.49
3:A:294:ASN:ND2	6:A:581:HOH:O	2.44	0.49
3:A:166:VAL:CG1	3:A:173:TYR:HB3	2.43	0.49
3:A:235:PHE:CG	3:A:236:MET:N	2.80	0.49
3:A:59:ALA:O	3:A:62:LEU:N	2.28	0.49
3:A:22:LEU:HD21	3:A:82:LEU:CD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:141:LYS:HE2	3:A:142:TYR:CE1	2.48	0.48
3:A:199:SER:O	3:A:199:SER:OG	2.31	0.48
3:A:103:VAL:HB	3:A:106:ILE:HB	1.96	0.48
3:A:123:GLU:O	3:A:127:LYS:HG2	2.14	0.48
3:A:278:PHE:HE1	3:A:325:TRP:CZ3	2.31	0.48
3:A:295:GLU:OE1	3:A:295:GLU:N	2.41	0.48
3:A:309:GLU:HA	3:A:310:PRO:HD2	1.67	0.48
3:A:29:VAL:HG21	3:A:94:SER:CA	2.43	0.48
3:A:11:LEU:H	3:A:11:LEU:CD2	2.26	0.48
3:A:103:VAL:CG1	3:A:106:ILE:HD12	2.43	0.48
1:T:4:DT:H73	6:T:645:HOH:O	2.13	0.48
3:A:126:ARG:O	3:A:128:ASN:N	2.47	0.48
3:A:243:SER:CB	3:A:249:GLU:HA	2.28	0.48
3:A:270:LEU:HA	3:A:316:GLU:OE2	2.13	0.48
2:P:2:DC:H1'	6:P:617:HOH:O	2.13	0.48
3:A:133:ASN:HD21	3:A:135:HIS:HB3	1.79	0.48
3:A:200:PHE:O	3:A:261:PRO:HA	2.14	0.48
3:A:326:LYS:O	3:A:328:ARG:HG2	2.13	0.48
3:A:115:VAL:O	3:A:115:VAL:HG12	2.14	0.48
3:A:328:ARG:HB2	3:A:333:ARG:HD3	1.94	0.48
3:A:16:THR:HG21	3:A:47:ALA:HB2	1.95	0.47
3:A:22:LEU:HA	3:A:22:LEU:HD13	1.57	0.47
3:A:19:LEU:HD23	3:A:43:ALA:HA	1.96	0.47
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.42	0.47
3:A:103:VAL:CG1	3:A:106:ILE:HG13	2.44	0.47
3:A:135:HIS:O	3:A:138:ILE:N	2.47	0.47
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.53	0.47
3:A:182:ARG:HH11	3:A:273:THR:HG21	1.79	0.47
3:A:41:LYS:O	3:A:44:SER:HB3	2.13	0.47
3:A:314:ASP:O	3:A:315:SER:HB2	2.14	0.47
3:A:303:VAL:C	3:A:305:GLY:H	2.22	0.47
3:A:195:LEU:O	3:A:259:LEU:HD12	2.15	0.47
3:A:282:MET:HG3	3:A:323:ILE:HD11	1.96	0.47
3:A:32:ALA:HB1	3:A:35:LYS:HB2	1.96	0.47
3:A:101:THR:HA	3:A:106:ILE:HG22	1.97	0.47
3:A:150:ILE:HG22	3:A:155:MET:HG2	1.96	0.47
3:A:162:VAL:CG2	3:A:223:PHE:CE2	2.98	0.47
3:A:103:VAL:O	3:A:103:VAL:HG12	2.14	0.47
3:A:180:SER:HA	3:A:183:ARG:HE	1.79	0.47
3:A:15:ILE:CG2	3:A:46:ILE:HD11	2.45	0.47
3:A:145:ASP:HA	3:A:148:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:245:ASN:N	3:A:245:ASN:ND2	2.31	0.46
3:A:22:LEU:HD21	3:A:82:LEU:HD21	1.96	0.46
3:A:103:VAL:O	3:A:106:ILE:HB	2.15	0.46
3:A:114:PHE:O	3:A:119:ILE:HG12	2.15	0.46
3:A:279:ASN:HD22	3:A:279:ASN:HA	1.39	0.46
3:A:132:LEU:HB3	3:A:136:GLN:HB2	1.97	0.46
3:A:196:THR:OG1	3:A:262:LYS:HA	2.16	0.46
3:A:283:ARG:HG2	3:A:293:ILE:HB	1.98	0.46
3:A:99:PHE:CD2	3:A:100:LEU:CD1	2.98	0.46
3:A:103:VAL:HG11	3:A:106:ILE:HD12	1.98	0.46
3:A:212:HIS:N	3:A:212:HIS:CD2	2.82	0.46
3:A:25:PHE:CD1	3:A:88:ILE:CD1	2.99	0.46
3:A:79:THR:C	3:A:81:LYS:H	2.24	0.46
3:A:274:GLY:HA3	3:A:275:SER:HA	1.75	0.46
3:A:287:LEU:HD13	3:A:287:LEU:HA	1.62	0.46
3:A:259:LEU:C	3:A:260:ILE:HG12	2.39	0.46
3:A:330:PRO:HA	3:A:333:ARG:HG2	1.96	0.46
3:A:255:ILE:CG1	3:A:256:ASP:H	2.27	0.45
3:A:152:ARG:HH11	3:A:152:ARG:HD3	1.62	0.45
3:A:278:PHE:CE1	3:A:325:TRP:HZ3	2.34	0.45
3:A:158:MET:HB3	3:A:191:MET:CE	2.47	0.45
3:A:255:ILE:O	3:A:256:ASP:OD1	2.34	0.45
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.97	0.45
3:A:33:ILE:O	3:A:37:ASN:HB2	2.17	0.45
3:A:62:LEU:HD12	3:A:62:LEU:HA	1.73	0.45
3:A:11:LEU:HD23	3:A:11:LEU:N	2.26	0.45
3:A:141:LYS:HE2	3:A:142:TYR:OH	2.16	0.45
3:A:158:MET:HE2	6:A:521:HOH:O	2.17	0.45
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.52	0.45
3:A:270:LEU:HD23	3:A:319:ILE:HD13	1.99	0.44
3:A:76:PHE:O	3:A:79:THR:O	2.35	0.44
3:A:289:LYS:HD3	3:A:289:LYS:HA	1.54	0.44
3:A:127:LYS:HB3	3:A:127:LYS:HE3	1.81	0.44
3:A:253:ARG:CG	3:A:253:ARG:NH1	2.78	0.44
3:A:299:ARG:HG2	3:A:309:GLU:C	2.42	0.44
3:A:29:VAL:HG22	3:A:97:ILE:HD12	1.99	0.44
3:A:254:ARG:HH12	3:A:255:ILE:C	2.24	0.44
2:P:5:DA:H5"	3:A:107:GLY:HA3	2.00	0.44
3:A:103:VAL:HG12	3:A:106:ILE:HG13	2.00	0.44
3:A:292:THR:C	3:A:293:ILE:HD13	2.43	0.44
3:A:265:TYR:CE2	3:A:269:VAL:HG21	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:12:ASN:HD22	3:A:12:ASN:HA	1.54	0.43
3:A:36:TYR:CD1	3:A:36:TYR:C	2.95	0.43
3:A:235:PHE:CD1	3:A:236:MET:N	2.86	0.43
3:A:180:SER:HB3	3:A:183:ARG:HH21	1.82	0.43
3:A:208:PRO:HB3	3:A:232:GLU:HB2	2.00	0.43
3:A:15:ILE:HD11	3:A:73:ILE:HG21	2.00	0.43
3:A:127:LYS:C	3:A:128:ASN:HD22	2.26	0.43
3:A:140:LEU:HD12	3:A:140:LEU:O	2.17	0.43
3:A:183:ARG:HH11	3:A:275:SER:HB3	1.83	0.43
3:A:299:ARG:CD	3:A:310:PRO:HD3	2.48	0.43
3:A:267:CYS:SG	3:A:297:THR:HA	2.59	0.43
3:A:27:LYS:HG3	3:A:28:ASN:HD21	1.79	0.43
3:A:46:ILE:HD13	3:A:53:ILE:HD12	2.01	0.43
3:A:100:LEU:HD21	3:A:120:LYS:O	2.19	0.43
3:A:228:LEU:HD12	3:A:228:LEU:HA	1.84	0.43
3:A:258:ARG:NH2	3:A:272:PHE:HZ	2.17	0.43
3:A:128:ASN:N	3:A:128:ASN:ND2	2.67	0.43
3:A:41:LYS:HZ1	3:A:64:GLY:C	2.20	0.43
3:A:271:TYR:CD2	3:A:271:TYR:C	2.97	0.42
3:A:129:GLU:O	3:A:137:ARG:NE	2.44	0.42
3:A:11:LEU:HA	3:A:52:LYS:NZ	2.34	0.42
3:A:12:ASN:HD21	3:A:53:ILE:H	1.66	0.42
3:A:25:PHE:CD2	3:A:25:PHE:C	2.95	0.42
3:A:180:SER:HB3	3:A:183:ARG:NH2	2.34	0.42
3:A:277:ILE:HG12	3:A:335:GLU:HA	2.01	0.42
3:A:18:MET:O	3:A:22:LEU:N	2.42	0.42
3:A:255:ILE:CG1	3:A:256:ASP:N	2.78	0.42
3:A:265:TYR:O	3:A:269:VAL:N	2.44	0.42
3:A:15:ILE:CG2	3:A:46:ILE:CD1	2.98	0.42
3:A:122:LEU:CD1	3:A:143:PHE:CE2	3.03	0.42
3:A:13:GLY:C	3:A:15:ILE:N	2.77	0.42
3:A:122:LEU:CD2	3:A:140:LEU:HD11	2.49	0.42
3:A:282:MET:HG3	3:A:323:ILE:CD1	2.50	0.42
3:A:82:LEU:HB3	3:A:85:LEU:CB	2.44	0.42
3:A:237:GLY:N	3:A:255:ILE:O	2.47	0.42
3:A:158:MET:CB	3:A:191:MET:HE3	2.49	0.42
3:A:37:ASN:HD22	3:A:37:ASN:HA	1.55	0.42
3:A:179:GLY:O	3:A:182:ARG:HB3	2.20	0.42
3:A:201:THR:O	3:A:203:GLU:N	2.53	0.42
3:A:259:LEU:CD1	3:A:260:ILE:H	2.28	0.42
3:A:277:ILE:HD11	3:A:334:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:293:ILE:CD1	3:A:298:ILE:CD1	2.97	0.42
2:P:3:DT:H4'	6:P:563:HOH:O	2.19	0.41
3:A:227:THR:HG21	3:A:230:LYS:HB2	2.01	0.41
3:A:146:PHE:CE2	3:A:254:ARG:HD3	2.55	0.41
3:A:165:GLU:CA	3:A:168:LYS:HG2	2.32	0.41
3:A:240:GLN:HG2	3:A:241:LEU:N	2.35	0.41
3:A:315:SER:C	3:A:317:LYS:N	2.78	0.41
3:A:89:ARG:HD3	3:A:89:ARG:C	2.46	0.41
3:A:277:ILE:HD11	3:A:335:GLU:CB	2.49	0.41
3:A:75:GLU:CD	6:A:590:HOH:O	2.63	0.41
3:A:99:PHE:CD2	3:A:100:LEU:HD13	2.44	0.41
3:A:100:LEU:HD13	3:A:100:LEU:N	2.35	0.41
3:A:250:TYR:HA	3:A:251:PRO:HD3	1.92	0.41
3:A:15:ILE:HD13	3:A:73:ILE:HD13	2.03	0.41
3:A:126:ARG:C	3:A:128:ASN:N	2.79	0.41
3:A:127:LYS:C	3:A:128:ASN:ND2	2.79	0.41
3:A:270:LEU:HD22	3:A:319:ILE:HD12	2.02	0.41
3:A:270:LEU:HD21	3:A:282:MET:HE1	2.02	0.41
3:A:301:LEU:HA	3:A:301:LEU:HD12	1.47	0.41
3:A:29:VAL:HG22	3:A:94:SER:HA	2.02	0.41
3:A:62:LEU:HD12	3:A:63:PRO:HD2	2.03	0.41
3:A:150:ILE:HG12	3:A:253:ARG:HG2	2.02	0.41
3:A:119:ILE:HG21	3:A:125:LEU:HD23	2.03	0.40
3:A:266:TYR:O	3:A:270:LEU:HB2	2.21	0.40
3:A:311:LEU:HD12	3:A:311:LEU:HA	1.71	0.40
3:A:122:LEU:HD21	3:A:140:LEU:HD11	2.03	0.40
3:A:214:VAL:CG2	3:A:215:VAL:N	2.81	0.40
1:T:1:DC:H6	1:T:1:DC:H2'	1.53	0.40
3:A:228:LEU:HD22	3:A:237:GLY:O	2.21	0.40
3:A:260:ILE:CG2	3:A:261:PRO:N	2.82	0.40
3:A:277:ILE:CG1	3:A:335:GLU:CB	2.99	0.40
3:A:303:VAL:C	3:A:305:GLY:N	2.80	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%)	263 (81%)	44 (14%)	18 (6%)	1	16

All (18) 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	295	GLU
3	A	13	GLY
3	A	14	GLY
3	A	60	LYS
3	A	127	LYS
3	A	229	SER
3	A	298	ILE
3	A	135	HIS
3	A	304	THR
3	A	316	GLU
3	A	207	GLN
3	A	289	LYS
3	A	309	GLU
3	A	242	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%)	233 (81%)	55 (19%)	1	10

All (55) 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	30	SER
3	A	33	ILE
3	A	36	TYR
3	A	37	ASN
3	A	41	LYS
3	A	44	SER
3	A	45	VAL
3	A	46	ILE
3	A	54	LYS
3	A	62	LEU
3	A	67	THR
3	A	68	LYS
3	A	79	THR
3	A	89	ARG
3	A	92	ASP
3	A	97	ILE
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	138	ILE
3	A	153	GLU
3	A	168	LYS
3	A	174	ILE
3	A	182	ARG
3	A	201	THR
3	A	203	GLU
3	A	214	VAL
3	A	218	LEU
3	A	221	VAL
3	A	226	ASP
3	A	228	LEU
3	A	233	THR
3	A	243	SER
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG

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Mol	Chain	Res	Type
3	A	277	ILE
3	A	287	LEU
3	A	293	ILE
3	A	294	ASN
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	331	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) 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	217	GLN
3	A	245	ASN
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, 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%)	0.07	0 100 100	12, 45, 75, 100	0
2	P	7/7 (100%)	-0.17	0 100 100	6, 22, 46, 76	0
3	A	325/335 (97%)	-0.58	0 100 100	3, 38, 88, 100	0
All	All	340/350 (97%)	-0.56	0 100 100	3, 38, 89, 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	NI	A	343	1/1	0.83	0.07	29,29,29,29	0
5	NA	A	341	1/1	0.92	0.35	60,60,60,60	0
4	NI	A	340	1/1	0.97	0.08	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.