



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:31 PM UTC

PDB ID : 7ICQ / pdb_00007icq
Title : DNA POLYMERASE BETA (E.C.2.7.7.7)/DNA COMPLEX, SOAKED IN
THE PRESENCE OF ZNCL2
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-04-19
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
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

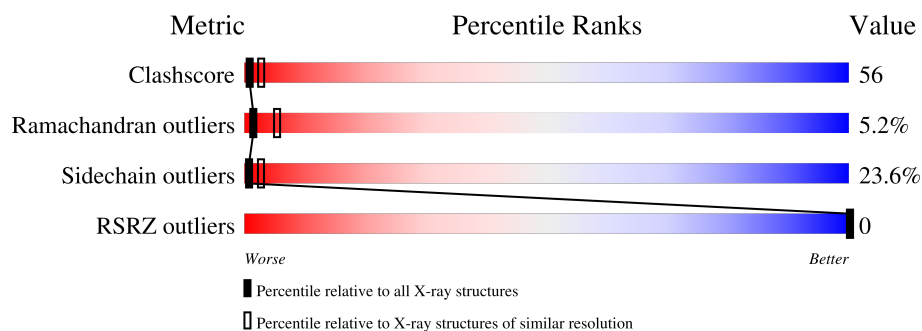
1 Overall quality at a glance

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	7	
2	P	6	
3	A	335	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3023 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*CP*TP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	7	Total	C	N	O	P	0	0	0
			122	58	20	38	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	6	Total	C	N	O	P	0	0	0
			126	59	25	36	6			

- 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	26	0	0
			2623	1657	458	499	9			

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	11	Total	O	0	0
			11	11		

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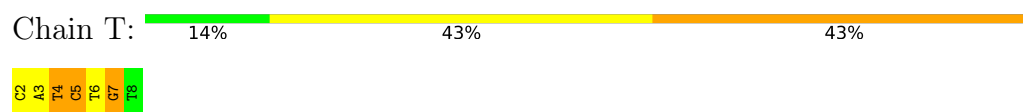
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	21	Total 21	O 21	0	0
6	A	117	Total 117	O 117	0	0

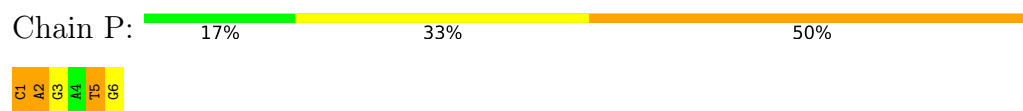
3 Residue-property plots

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.

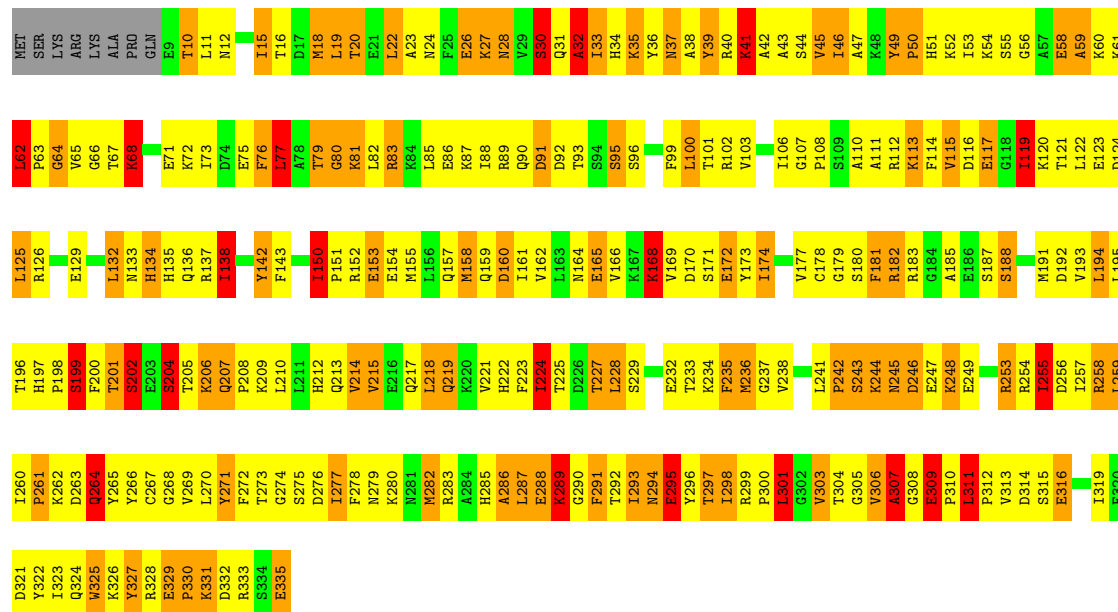
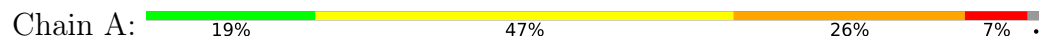
- Molecule 1: DNA (5'-D(*CP*AP*TP*CP*TP*GP*T)-3')



- Molecule 2: DNA (5'-D(*CP*AP*GP*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	178.94Å 57.80Å 48.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.0 (20.00-2.90) 89.3 (20.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.70Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.159 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 312.2	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	0.95	EDS
Total number of atoms	3023	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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: ZN, 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	1.14	0/135	2.50	12/207 (5.8%)
2	P	1.39	2/141 (1.4%)	2.31	10/214 (4.7%)
3	A	1.72	30/2672 (1.1%)	2.16	103/3590 (2.9%)
All	All	1.68	32/2948 (1.1%)	2.19	125/4011 (3.1%)

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	3	0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	1	DC	OP3-P	7.28	1.63	1.48
3	A	232	GLU	CA-C	-7.25	1.42	1.52
3	A	138	ILE	CA-CB	-7.17	1.46	1.54
3	A	119	ILE	CA-C	-7.12	1.44	1.52
3	A	24	ASN	C-N	-6.85	1.24	1.33
3	A	160	ASP	C-O	-6.71	1.16	1.24
3	A	227	THR	C-O	-6.35	1.16	1.24
3	A	125	LEU	CA-C	-6.12	1.45	1.52
3	A	165	GLU	C-O	-6.07	1.16	1.24
3	A	171	SER	CA-C	-6.01	1.44	1.52
3	A	55	SER	C-N	-6.01	1.26	1.33
3	A	115	VAL	CA-CB	-5.93	1.46	1.54
3	A	215	VAL	CA-CB	-5.79	1.47	1.54
3	A	76	PHE	N-CA	-5.72	1.39	1.46
3	A	65	VAL	CA-CB	-5.70	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	224	ILE	CA-CB	-5.68	1.47	1.54
3	A	35	LYS	CA-C	-5.62	1.45	1.52
3	A	160	ASP	C-N	-5.51	1.26	1.33
3	A	234	LYS	CA-C	-5.51	1.45	1.52
3	A	91	ASP	CA-C	-5.45	1.45	1.52
3	A	119	ILE	CA-CB	-5.32	1.47	1.54
3	A	58	GLU	CD-OE1	5.30	1.35	1.25
3	A	330	PRO	N-CA	-5.29	1.40	1.47
3	A	116	ASP	N-CA	-5.25	1.39	1.46
2	P	5	DT	C1'-N1	5.18	1.65	1.49
3	A	39	TYR	CA-C	-5.17	1.45	1.52
3	A	255	ILE	CA-CB	-5.17	1.47	1.54
3	A	66	GLY	CA-C	-5.14	1.45	1.52
3	A	261	PRO	CA-C	-5.06	1.46	1.52
3	A	129	GLU	CD-OE1	5.04	1.34	1.25
3	A	159	GLN	N-CA	-5.04	1.40	1.46
3	A	90	GLN	CA-C	-5.03	1.47	1.53

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	4	DT	C6-N1-C1'	-13.28	99.43	119.35
1	T	4	DT	C2-N1-C1'	12.56	138.20	119.35
2	P	5	DT	C2-N1-C1'	12.24	137.70	119.35
2	P	5	DT	C6-N1-C1'	-11.96	101.41	119.35
3	A	272	PHE	CA-CB-CG	-10.63	103.17	113.80
3	A	49	TYR	CA-C-N	10.19	132.58	119.84
3	A	49	TYR	C-N-CA	10.19	132.58	119.84
1	T	5	DC	C2-N1-C1'	10.01	134.72	119.70
3	A	40	ARG	N-CA-C	9.94	121.87	111.14
1	T	5	DC	C6-N1-C1'	-9.80	105.00	119.70
3	A	65	VAL	N-CA-CB	9.61	123.13	111.60
3	A	64	GLY	N-CA-C	-9.29	103.13	115.21
3	A	34	HIS	CA-CB-CG	-9.11	104.69	113.80
3	A	20	THR	CB-CA-C	8.52	124.25	110.88
3	A	20	THR	N-CA-CB	8.52	122.36	110.01
3	A	28	ASN	N-CA-C	8.51	120.33	111.14
3	A	222	HIS	CB-CA-C	-7.93	99.11	111.39
3	A	117	GLU	N-CA-C	-7.78	101.59	113.89
3	A	32	ALA	N-CA-C	7.67	127.14	110.80
2	P	5	DT	P-O5'-C5'	-7.62	108.57	120.00
3	A	99	PHE	CA-CB-CG	-7.56	106.24	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	271	TYR	CA-CB-CG	-7.47	100.45	113.90
3	A	313	VAL	N-CA-C	7.43	118.51	108.11
3	A	296	TYR	N-CA-C	7.36	122.55	113.50
3	A	266	TYR	N-CA-C	7.32	120.19	111.33
3	A	168	LYS	N-CA-CB	7.25	120.77	110.12
3	A	286	ALA	CA-C-N	7.07	129.75	120.28
3	A	286	ALA	C-N-CA	7.07	129.75	120.28
2	P	3	DG	P-O3'-C3'	7.03	130.74	120.20
3	A	329	GLU	N-CA-C	-7.02	100.39	110.08
3	A	96	SER	O-C-N	6.97	129.25	122.07
3	A	291	PHE	N-CA-C	6.93	118.64	108.86
3	A	92	ASP	N-CA-CB	6.92	120.30	110.12
3	A	30	SER	CA-C-N	-6.87	111.33	122.26
3	A	30	SER	C-N-CA	-6.87	111.33	122.26
3	A	83	ARG	N-CA-CB	6.85	119.91	109.91
1	T	6	DT	C6-N1-C1'	-6.67	109.34	119.35
1	T	7	DG	C4-N9-C1'	-6.55	117.18	127.00
3	A	199	SER	N-CA-CB	-6.51	99.50	110.49
3	A	238	VAL	CA-C-N	-6.42	112.09	122.36
3	A	238	VAL	C-N-CA	-6.42	112.09	122.36
3	A	193	VAL	N-CA-C	6.41	117.53	108.36
3	A	335	GLU	N-CA-CB	6.40	121.39	110.50
3	A	62	LEU	CA-C-N	6.33	126.83	119.99
3	A	62	LEU	C-N-CA	6.33	126.83	119.99
3	A	28	ASN	CA-CB-CG	-6.26	106.34	112.60
3	A	181	PHE	CB-CA-C	-6.21	100.13	110.68
3	A	201	THR	N-CA-CB	-6.17	102.18	111.56
2	P	1	DC	C6-N1-C1'	-6.17	110.45	119.70
2	P	2	DA	C4-N9-C1'	6.16	136.29	127.05
3	A	243	SER	CB-CA-C	6.12	119.44	110.26
3	A	50	PRO	CB-CA-C	-6.10	101.49	111.56
3	A	86	GLU	CB-CA-C	6.07	120.86	110.79
3	A	161	ILE	N-CA-C	6.07	116.23	110.53
3	A	171	SER	O-C-N	6.06	129.31	122.22
3	A	181	PHE	CA-C-N	6.05	128.89	120.29
3	A	181	PHE	C-N-CA	6.05	128.89	120.29
3	A	214	VAL	N-CA-CB	6.05	119.66	110.58
3	A	309	GLU	CA-C-N	6.00	127.33	119.84
3	A	309	GLU	C-N-CA	6.00	127.33	119.84
3	A	242	PRO	CB-CA-C	-5.97	101.70	111.56
3	A	286	ALA	O-C-N	5.90	128.38	122.12
2	P	2	DA	C8-N9-C1'	-5.87	118.24	127.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	2	DC	C2-N1-C1'	5.85	128.48	119.70
3	A	215	VAL	CA-CB-CG1	-5.84	100.47	110.40
3	A	246	ASP	N-CA-C	5.84	123.23	110.80
2	P	2	DA	P-O5'-C5'	-5.79	111.32	120.00
3	A	116	ASP	CA-CB-CG	-5.78	106.82	112.60
3	A	87	LYS	CA-C-N	5.77	128.62	120.42
3	A	87	LYS	C-N-CA	5.77	128.62	120.42
3	A	96	SER	N-CA-C	5.73	117.20	111.07
3	A	225	THR	N-CA-C	5.70	120.25	113.12
3	A	41	LYS	N-CA-C	-5.66	105.19	111.36
3	A	174	ILE	N-CA-CB	5.64	119.32	112.10
3	A	68	LYS	O-C-N	5.64	128.10	122.12
3	A	87	LYS	CB-CA-C	5.63	120.14	110.79
3	A	116	ASP	N-CA-C	-5.62	106.64	112.93
3	A	86	GLU	N-CA-CB	5.59	118.34	110.12
3	A	77	LEU	N-CA-C	-5.57	105.12	111.14
3	A	142	TYR	CB-CA-C	-5.53	102.54	111.28
3	A	312	PRO	CA-C-N	5.53	130.38	123.14
3	A	312	PRO	C-N-CA	5.53	130.38	123.14
1	T	3	DA	N9-C1'-C2'	5.51	121.77	113.50
2	P	2	DA	C4'-C3'-C2'	-5.50	94.15	102.40
3	A	297	THR	N-CA-C	5.48	115.77	108.38
3	A	266	TYR	CA-CB-CG	-5.46	104.08	113.90
1	T	4	DT	P-O3'-C3'	5.44	128.36	120.20
1	T	2	DC	C6-N1-C1'	-5.39	111.61	119.70
3	A	59	ALA	O-C-N	5.38	127.62	122.07
3	A	49	TYR	O-C-N	5.37	127.49	121.32
3	A	26	GLU	O-C-N	5.35	127.65	122.09
2	P	1	DC	C2-N1-C1'	5.35	127.72	119.70
3	A	311	LEU	N-CA-C	-5.34	102.71	110.08
3	A	34	HIS	CA-C-N	5.34	127.38	120.44
3	A	34	HIS	C-N-CA	5.34	127.38	120.44
3	A	160	ASP	CA-CB-CG	-5.33	107.27	112.60
3	A	327	TYR	N-CA-CB	5.33	117.88	109.83
3	A	158	MET	CA-C-O	5.28	126.13	120.70
3	A	307	ALA	CB-CA-C	5.27	120.91	110.42
3	A	264	GLN	CB-CG-CD	-5.27	103.64	112.60
3	A	223	PHE	CA-CB-CG	-5.26	108.54	113.80
3	A	92	ASP	CB-CA-C	5.25	119.51	110.79
3	A	261	PRO	N-CA-C	-5.23	102.90	110.80
3	A	257	ILE	CA-CB-CG2	-5.19	101.68	110.50
3	A	303	VAL	CB-CA-C	5.17	118.59	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	296	TYR	CB-CA-C	-5.12	99.96	109.29
3	A	150	ILE	N-CA-CB	5.11	117.83	111.39
3	A	233	THR	O-C-N	5.11	127.34	121.93
1	T	3	DA	P-O5'-C5'	5.10	127.65	120.00
3	A	115	VAL	CA-C-O	5.10	125.98	120.47
3	A	107	GLY	N-CA-C	-5.09	101.95	112.34
3	A	241	LEU	CA-C-N	5.09	126.21	119.84
3	A	241	LEU	C-N-CA	5.09	126.21	119.84
3	A	65	VAL	O-C-N	5.09	129.67	122.59
1	T	7	DG	C8-N9-C1'	5.08	134.62	127.00
3	A	102	ARG	CD-NE-CZ	-5.07	117.30	124.40
3	A	123	GLU	CB-CA-C	5.07	118.83	110.88
3	A	301	LEU	N-CA-C	5.06	117.01	108.96
3	A	295	GLU	CB-CG-CD	5.05	121.19	112.60
3	A	241	LEU	C-N-CD	-5.05	104.30	125.00
3	A	134	HIS	ND1-CE1-NE2	5.04	113.44	108.40
3	A	88	ILE	CB-CA-C	-5.03	105.28	112.22
3	A	90	GLN	O-C-N	5.02	128.04	122.11
3	A	316	GLU	CA-C-N	5.01	127.26	120.65
3	A	316	GLU	C-N-CA	5.01	127.26	120.65

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	20	THR	CA
3	A	32	ALA	CA
3	A	246	ASP	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	122	0	69	2	0
2	P	126	0	68	6	0
3	A	2623	0	2641	301	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	117	0	0	17	0
6	P	21	0	0	1	0
6	T	11	0	0	1	0
All	All	3023	0	2778	309	1

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 56.

All (309) 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:23:ALA:HB2	3:A:39:TYR:HB2	1.33	1.06
3:A:155:MET:HA	3:A:158:MET:HE3	1.41	1.01
3:A:201:THR:HA	3:A:261:PRO:HB3	1.49	0.92
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.51	0.90
3:A:11:LEU:HD23	3:A:11:LEU:H	1.35	0.90
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.55	0.88
3:A:12:ASN:HD21	3:A:53:ILE:H	1.21	0.88
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.04	0.88
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.56	0.87
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.57	0.87
3:A:300:PRO:HD3	3:A:311:LEU:HD13	1.57	0.87
3:A:218:LEU:CB	3:A:224:ILE:HD12	2.05	0.87
2:P:1:DC:H2"	2:P:2:DA:H5"	1.56	0.86
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.56	0.86
3:A:12:ASN:HB3	3:A:46:ILE:CD1	2.06	0.85
3:A:68:LYS:HB2	3:A:68:LYS:NZ	1.91	0.85
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.14	0.83
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.08	0.83
3:A:194:LEU:HD11	3:A:258:ARG:HD3	1.59	0.83
3:A:197:HIS:ND1	3:A:199:SER:HB3	1.95	0.82
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.09	0.82
3:A:277:ILE:HG13	3:A:335:GLU:HB3	1.63	0.81
3:A:245:ASN:N	3:A:245:ASN:HD22	1.79	0.81
3:A:289:LYS:HD2	3:A:324:GLN:OE1	1.82	0.80
3:A:218:LEU:HB3	3:A:224:ILE:HD12	1.65	0.78
3:A:18:MET:HE1	3:A:76:PHE:CB	2.13	0.78
3:A:271:TYR:HB2	6:A:592:HOH:O	1.83	0.78
3:A:286:ALA:HA	3:A:323:ILE:HG21	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:23:ALA:CB	3:A:39:TYR:HB2	2.12	0.76
3:A:255:ILE:HG12	3:A:256:ASP:N	2.01	0.76
3:A:68:LYS:O	3:A:72:LYS:HE3	1.86	0.75
3:A:254:ARG:NH1	3:A:255:ILE:H	1.83	0.75
3:A:44:SER:O	3:A:47:ALA:HB3	1.86	0.75
3:A:245:ASN:HD22	3:A:245:ASN:H	1.35	0.75
3:A:194:LEU:CD1	3:A:258:ARG:HD3	2.17	0.75
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.16	0.74
3:A:286:ALA:HA	3:A:323:ILE:CG2	2.16	0.74
3:A:294:ASN:HB2	3:A:295:GLU:OE2	1.88	0.74
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.53	0.74
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.69	0.73
3:A:212:HIS:HB3	6:A:541:HOH:O	1.87	0.73
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.69	0.73
3:A:172:GLU:HG2	3:A:198:PRO:HG2	1.68	0.73
3:A:218:LEU:HB2	3:A:224:ILE:HD12	1.71	0.73
3:A:155:MET:HE3	3:A:188:SER:OG	1.89	0.73
3:A:254:ARG:HH11	3:A:255:ILE:H	1.36	0.72
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.25	0.72
3:A:270:LEU:HD21	3:A:282:MET:HE2	1.72	0.72
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.72	0.72
1:T:4:DT:H2''	1:T:5:DC:O5'	1.90	0.71
2:P:2:DA:C8	2:P:2:DA:H5'	2.26	0.71
2:P:1:DC:C2'	2:P:2:DA:H5''	2.21	0.70
3:A:201:THR:HA	3:A:261:PRO:CB	2.19	0.70
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.73	0.70
3:A:182:ARG:HH11	3:A:273:THR:HG21	1.56	0.70
3:A:262:LYS:O	3:A:262:LYS:HG3	1.91	0.70
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.89	0.69
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.90	0.69
3:A:152:ARG:HA	3:A:155:MET:HB2	1.74	0.69
3:A:31:GLN:N	6:A:641:HOH:O	2.26	0.69
3:A:59:ALA:O	3:A:62:LEU:HB2	1.92	0.69
3:A:331:LYS:HD2	3:A:332:ASP:N	2.07	0.69
3:A:119:ILE:HG22	3:A:124:ASP:HB3	1.75	0.68
3:A:182:ARG:HG2	3:A:273:THR:HG23	1.75	0.67
3:A:108:PRO:O	3:A:112:ARG:HG3	1.94	0.67
3:A:113:LYS:O	3:A:117:GLU:HG3	1.95	0.67
3:A:202:SER:HB2	3:A:263:ASP:OD2	1.94	0.67
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.30	0.67
3:A:277:ILE:HG13	3:A:335:GLU:CB	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:155:MET:HE3	3:A:188:SER:CB	2.26	0.66
3:A:80:GLY:O	3:A:81:LYS:HG2	1.96	0.66
3:A:253:ARG:NH1	6:A:503:HOH:O	2.28	0.65
3:A:254:ARG:NH1	3:A:255:ILE:N	2.44	0.65
3:A:244:LYS:CB	3:A:245:ASN:HD22	2.10	0.65
3:A:68:LYS:HB2	3:A:68:LYS:HZ1	1.62	0.64
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.11	0.64
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.44	0.64
3:A:276:ASP:O	3:A:280:LYS:HG3	1.98	0.64
3:A:32:ALA:HB1	3:A:35:LYS:HB2	1.80	0.63
3:A:178:CYS:SG	3:A:194:LEU:HD23	2.39	0.63
3:A:292:THR:O	3:A:298:ILE:HA	1.97	0.63
3:A:16:THR:HG23	3:A:46:ILE:HG13	1.79	0.63
3:A:41:LYS:HE2	3:A:64:GLY:HA2	1.80	0.63
3:A:28:ASN:HD22	3:A:28:ASN:N	1.96	0.62
3:A:217:GLN:NE2	3:A:217:GLN:HA	2.14	0.62
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.34	0.62
3:A:182:ARG:HH11	3:A:182:ARG:CG	2.12	0.62
3:A:330:PRO:HA	3:A:333:ARG:CG	2.27	0.62
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.30	0.62
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.30	0.62
3:A:306:VAL:HG23	3:A:307:ALA:N	2.14	0.61
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.64	0.61
3:A:295:GLU:CD	3:A:295:GLU:H	2.07	0.61
3:A:242:PRO:HG2	6:A:589:HOH:O	1.99	0.61
3:A:179:GLY:O	3:A:182:ARG:HB3	2.01	0.61
3:A:132:LEU:HB3	3:A:136:GLN:HB3	1.83	0.61
3:A:298:ILE:HG22	6:A:578:HOH:O	2.01	0.61
1:T:7:DG:N3	6:T:634:HOH:O	2.31	0.60
3:A:278:PHE:HB2	3:A:333:ARG:O	2.02	0.60
3:A:95:SER:HB3	6:A:639:HOH:O	2.01	0.60
3:A:16:THR:O	3:A:20:THR:HG23	2.01	0.59
3:A:267:CYS:SG	3:A:297:THR:HA	2.42	0.58
3:A:27:LYS:HB3	3:A:36:TYR:CD1	2.38	0.58
3:A:293:ILE:HD12	3:A:298:ILE:HG13	1.85	0.58
3:A:157:GLN:HE22	3:A:244:LYS:NZ	2.01	0.58
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.18	0.58
3:A:325:TRP:HD1	6:A:583:HOH:O	1.86	0.58
3:A:79:THR:O	3:A:81:LYS:N	2.36	0.58
3:A:33:ILE:O	3:A:37:ASN:HB2	2.04	0.58
3:A:49:TYR:CZ	3:A:51:HIS:HB2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:166:VAL:O	3:A:169:VAL:HG12	2.04	0.57
3:A:23:ALA:O	3:A:36:TYR:HD1	1.86	0.57
3:A:286:ALA:O	3:A:291:PHE:HB2	2.05	0.57
3:A:85:LEU:O	3:A:89:ARG:HG3	2.05	0.57
3:A:243:SER:HB3	3:A:249:GLU:HA	1.87	0.56
3:A:202:SER:HB2	3:A:263:ASP:CG	2.30	0.56
3:A:286:ALA:CA	3:A:323:ILE:HG21	2.33	0.56
3:A:41:LYS:HD3	3:A:42:ALA:H	1.71	0.56
3:A:288:GLU:C	3:A:290:GLY:H	2.14	0.56
3:A:155:MET:HE3	3:A:188:SER:HB2	1.87	0.56
3:A:16:THR:HG23	3:A:46:ILE:CG1	2.36	0.55
3:A:254:ARG:HH11	3:A:255:ILE:N	2.02	0.55
3:A:43:ALA:O	3:A:47:ALA:HB2	2.07	0.55
3:A:11:LEU:H	3:A:11:LEU:CD2	2.14	0.55
3:A:177:VAL:O	3:A:182:ARG:HD3	2.06	0.55
3:A:248:LYS:O	3:A:248:LYS:HG2	2.05	0.55
3:A:151:PRO:HG2	3:A:154:GLU:HG3	1.88	0.55
3:A:288:GLU:O	3:A:290:GLY:N	2.39	0.55
3:A:192:ASP:OD1	3:A:258:ARG:NH1	2.40	0.55
3:A:18:MET:HE1	3:A:76:PHE:CG	2.42	0.54
3:A:237:GLY:O	3:A:254:ARG:NH1	2.40	0.54
3:A:12:ASN:ND2	3:A:53:ILE:H	1.99	0.54
3:A:121:THR:O	3:A:124:ASP:HB2	2.07	0.54
3:A:319:ILE:O	3:A:322:TYR:HB2	2.07	0.54
3:A:75:GLU:O	3:A:79:THR:HG23	2.07	0.54
3:A:207:GLN:HB3	3:A:210:LEU:HD12	1.89	0.54
3:A:182:ARG:HG2	3:A:273:THR:CG2	2.38	0.53
3:A:183:ARG:HD3	3:A:273:THR:O	2.08	0.53
3:A:292:THR:C	3:A:293:ILE:HD13	2.34	0.53
3:A:295:GLU:HA	6:A:592:HOH:O	2.08	0.53
3:A:42:ALA:O	3:A:46:ILE:HG23	2.09	0.53
3:A:155:MET:HA	3:A:158:MET:CE	2.25	0.53
3:A:200:PHE:CE2	3:A:261:PRO:HD3	2.42	0.53
3:A:200:PHE:HB2	3:A:210:LEU:CD1	2.38	0.53
3:A:111:ALA:O	3:A:115:VAL:HG23	2.08	0.53
3:A:114:PHE:HB3	3:A:119:ILE:HB	1.90	0.53
3:A:182:ARG:HH11	3:A:273:THR:CG2	2.20	0.53
3:A:277:ILE:CG1	3:A:335:GLU:HB3	2.35	0.53
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.38	0.53
3:A:120:LYS:N	3:A:124:ASP:OD2	2.29	0.53
3:A:315:SER:OG	3:A:316:GLU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:58:GLU:O	3:A:61:LYS:HB2	2.08	0.52
3:A:162:VAL:O	3:A:166:VAL:HG23	2.09	0.52
3:A:279:ASN:O	3:A:283:ARG:N	2.34	0.52
3:A:133:ASN:O	3:A:137:ARG:HG3	2.09	0.52
3:A:195:LEU:O	3:A:260:ILE:N	2.41	0.52
3:A:208:PRO:O	3:A:212:HIS:HD2	1.93	0.52
3:A:150:ILE:O	3:A:187:SER:HA	2.10	0.52
3:A:306:VAL:HG23	3:A:307:ALA:H	1.75	0.52
3:A:16:THR:CG2	3:A:46:ILE:HG13	2.40	0.52
3:A:80:GLY:C	3:A:81:LYS:HG2	2.35	0.51
3:A:200:PHE:HB2	6:A:625:HOH:O	2.10	0.51
3:A:243:SER:CB	3:A:249:GLU:HA	2.41	0.51
3:A:41:LYS:O	3:A:45:VAL:HG13	2.09	0.51
3:A:201:THR:HG23	3:A:204:SER:HB3	1.93	0.51
3:A:201:THR:CG2	3:A:204:SER:HB3	2.41	0.51
3:A:150:ILE:HD13	3:A:253:ARG:HG2	1.93	0.51
3:A:155:MET:CE	3:A:188:SER:HB2	2.41	0.51
3:A:309:GLU:OE1	3:A:309:GLU:HA	2.10	0.51
3:A:134:HIS:HE1	3:A:227:THR:O	1.93	0.51
3:A:26:GLU:OE1	3:A:26:GLU:HA	2.10	0.50
3:A:26:GLU:HA	3:A:30:SER:OG	2.11	0.50
3:A:49:TYR:CE2	3:A:51:HIS:HB2	2.47	0.50
3:A:303:VAL:C	3:A:305:GLY:H	2.18	0.50
3:A:35:LYS:O	3:A:38:ALA:HB3	2.10	0.50
3:A:152:ARG:NH2	3:A:181:PHE:O	2.44	0.50
3:A:41:LYS:O	3:A:44:SER:HB3	2.12	0.50
3:A:206:LYS:O	3:A:207:GLN:HB2	2.11	0.50
3:A:236:MET:HG2	3:A:254:ARG:NH2	2.26	0.50
3:A:327:TYR:CD1	3:A:328:ARG:N	2.79	0.50
6:P:568:HOH:O	3:A:110:ALA:HB2	2.11	0.50
3:A:236:MET:HG2	3:A:254:ARG:HH22	1.77	0.50
3:A:12:ASN:CB	3:A:46:ILE:HD12	2.31	0.50
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.47	0.50
3:A:229:SER:HB3	6:A:513:HOH:O	2.12	0.50
3:A:38:ALA:O	3:A:41:LYS:HD3	2.13	0.49
3:A:27:LYS:HG3	3:A:28:ASN:HD22	1.77	0.49
3:A:166:VAL:CG1	3:A:173:TYR:HB3	2.43	0.49
3:A:207:GLN:O	3:A:210:LEU:HB2	2.12	0.49
3:A:59:ALA:O	3:A:62:LEU:N	2.34	0.49
3:A:115:VAL:C	3:A:117:GLU:H	2.20	0.49
3:A:18:MET:CE	3:A:76:PHE:HB2	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:103:VAL:HG22	3:A:143:PHE:CE2	2.48	0.48
3:A:259:LEU:O	3:A:260:ILE:HD13	2.12	0.48
2:P:5:DT:H2"	2:P:6:DG:C8	2.48	0.48
3:A:157:GLN:NE2	3:A:244:LYS:NZ	2.61	0.48
3:A:164:ASN:O	3:A:168:LYS:HG2	2.13	0.48
3:A:288:GLU:OE1	3:A:288:GLU:HA	1.89	0.48
3:A:79:THR:C	3:A:81:LYS:H	2.21	0.48
3:A:72:LYS:HG2	3:A:82:LEU:HD11	1.96	0.48
3:A:68:LYS:O	3:A:71:GLU:HB3	2.14	0.47
3:A:218:LEU:N	3:A:218:LEU:HD13	2.29	0.47
3:A:205:THR:O	3:A:206:LYS:O	2.33	0.47
3:A:122:LEU:O	3:A:126:ARG:HG3	2.15	0.47
3:A:201:THR:CA	3:A:261:PRO:HB3	2.34	0.47
3:A:298:ILE:HG21	3:A:322:TYR:HD2	1.79	0.47
3:A:11:LEU:HD23	3:A:11:LEU:N	2.12	0.47
3:A:194:LEU:HD12	3:A:258:ARG:HG2	1.97	0.47
3:A:151:PRO:HB2	3:A:153:GLU:HG2	1.97	0.47
3:A:155:MET:O	3:A:158:MET:HB2	2.15	0.46
3:A:22:LEU:HD13	3:A:85:LEU:CD1	2.45	0.46
3:A:273:THR:O	3:A:273:THR:HG22	2.13	0.46
3:A:18:MET:CE	3:A:76:PHE:CG	2.99	0.46
3:A:282:MET:HG2	6:A:555:HOH:O	2.15	0.46
3:A:157:GLN:HE22	3:A:244:LYS:HZ1	1.63	0.46
3:A:218:LEU:N	3:A:218:LEU:CD1	2.78	0.46
3:A:11:LEU:CD2	3:A:11:LEU:N	2.77	0.46
3:A:85:LEU:HD12	3:A:85:LEU:HA	1.74	0.46
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.98	0.46
3:A:182:ARG:HG2	3:A:182:ARG:NH1	2.25	0.46
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.50	0.46
3:A:196:THR:OG1	3:A:197:HIS:N	2.48	0.45
3:A:292:THR:O	3:A:293:ILE:HD13	2.16	0.45
3:A:15:ILE:O	3:A:19:LEU:HD22	2.16	0.45
3:A:157:GLN:O	3:A:160:ASP:HB3	2.17	0.45
3:A:243:SER:OG	3:A:249:GLU:HG3	2.17	0.45
3:A:15:ILE:HD11	3:A:77:LEU:CD1	2.47	0.45
3:A:30:SER:HB3	6:A:561:HOH:O	2.17	0.45
3:A:209:LYS:O	3:A:213:GLN:HG3	2.17	0.45
3:A:306:VAL:CG2	3:A:307:ALA:N	2.78	0.45
3:A:41:LYS:HD3	3:A:42:ALA:N	2.32	0.45
3:A:169:VAL:HG13	3:A:170:ASP:N	2.32	0.45
3:A:178:CYS:SG	3:A:194:LEU:CD2	3.04	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:217:GLN:NE2	3:A:217:GLN:CA	2.78	0.44
3:A:331:LYS:CD	3:A:332:ASP:N	2.78	0.44
3:A:133:ASN:ND2	3:A:135:HIS:H	2.15	0.44
3:A:182:ARG:NH1	3:A:182:ARG:CG	2.76	0.44
3:A:62:LEU:HD12	3:A:63:PRO:HD2	1.98	0.44
3:A:27:LYS:CG	3:A:28:ASN:N	2.80	0.44
3:A:32:ALA:O	3:A:36:TYR:HB3	2.17	0.44
3:A:308:GLY:O	3:A:309:GLU:HB2	2.17	0.44
3:A:326:LYS:HG3	3:A:326:LYS:O	2.18	0.44
3:A:264:GLN:HE21	3:A:264:GLN:HB3	1.38	0.44
3:A:287:LEU:HA	3:A:287:LEU:HD13	1.64	0.44
3:A:150:ILE:N	3:A:188:SER:O	2.42	0.44
3:A:221:VAL:H	3:A:221:VAL:HG22	1.54	0.44
3:A:309:GLU:HA	3:A:310:PRO:HD2	1.73	0.44
3:A:60:LYS:C	3:A:62:LEU:N	2.75	0.44
3:A:150:ILE:HD13	3:A:253:ARG:CG	2.48	0.44
3:A:191:MET:HG2	3:A:255:ILE:HG13	2.00	0.43
3:A:198:PRO:C	3:A:200:PHE:H	2.26	0.43
3:A:265:TYR:O	3:A:269:VAL:HG23	2.18	0.43
3:A:270:LEU:HD22	3:A:319:ILE:HD13	2.00	0.43
3:A:152:ARG:HB3	6:A:530:HOH:O	2.17	0.43
3:A:289:LYS:HA	3:A:289:LYS:HD3	1.50	0.43
3:A:56:GLY:O	3:A:59:ALA:N	2.52	0.43
3:A:194:LEU:N	3:A:194:LEU:HD13	2.27	0.43
3:A:197:HIS:ND1	3:A:198:PRO:HD2	2.33	0.43
3:A:253:ARG:CG	3:A:253:ARG:HH11	2.31	0.43
3:A:301:LEU:HD12	3:A:301:LEU:HA	1.53	0.43
3:A:194:LEU:HD12	3:A:194:LEU:HA	1.45	0.43
3:A:299:ARG:HB3	3:A:300:PRO:HD2	2.00	0.43
3:A:138:ILE:HG22	3:A:142:TYR:CD2	2.53	0.43
3:A:228:LEU:HD12	3:A:228:LEU:HA	1.60	0.43
3:A:10:THR:O	3:A:10:THR:HG23	2.18	0.43
3:A:133:ASN:HD22	3:A:135:HIS:H	1.67	0.43
3:A:255:ILE:O	3:A:255:ILE:HG23	2.17	0.43
3:A:327:TYR:HD1	3:A:328:ARG:H	1.67	0.42
3:A:197:HIS:CG	3:A:198:PRO:CD	3.00	0.42
3:A:36:TYR:CD2	3:A:36:TYR:C	2.96	0.42
3:A:321:ASP:O	3:A:324:GLN:N	2.47	0.42
3:A:26:GLU:HG3	3:A:35:LYS:HB3	2.02	0.42
3:A:100:LEU:HA	3:A:100:LEU:HD12	1.23	0.42
3:A:100:LEU:N	3:A:100:LEU:HD13	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:15:ILE:HG21	3:A:46:ILE:HD13	2.00	0.42
3:A:244:LYS:HB2	3:A:245:ASN:HD22	1.84	0.42
3:A:125:LEU:HD23	3:A:125:LEU:HA	1.43	0.42
3:A:289:LYS:HG3	3:A:323:ILE:O	2.20	0.42
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.55	0.42
3:A:166:VAL:HG12	3:A:173:TYR:CB	2.49	0.42
3:A:174:ILE:HG21	3:A:174:ILE:HD13	1.68	0.42
3:A:210:LEU:HB3	3:A:259:LEU:HD21	2.02	0.42
3:A:213:GLN:HG2	6:A:644:HOH:O	2.20	0.42
3:A:322:TYR:HD1	3:A:322:TYR:HA	1.53	0.42
3:A:44:SER:HB2	6:A:608:HOH:O	2.20	0.41
3:A:115:VAL:C	3:A:117:GLU:N	2.78	0.41
3:A:138:ILE:HG22	3:A:142:TYR:HD2	1.85	0.41
3:A:27:LYS:HG3	3:A:28:ASN:N	2.27	0.41
2:P:2:DA:H5'	2:P:2:DA:H2'	1.50	0.41
3:A:197:HIS:CE1	3:A:199:SER:HB3	2.53	0.41
3:A:15:ILE:HG12	3:A:73:ILE:HG23	2.03	0.41
3:A:119:ILE:HG22	3:A:124:ASP:CB	2.46	0.41
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.36	0.41
3:A:274:GLY:HA3	3:A:275:SER:HA	1.86	0.41
3:A:333:ARG:NH1	6:A:584:HOH:O	2.39	0.41
3:A:215:VAL:O	3:A:219:GLN:HG3	2.21	0.41
2:P:2:DA:H5'	2:P:2:DA:H8	1.79	0.41
3:A:133:ASN:ND2	3:A:135:HIS:N	2.69	0.41
3:A:150:ILE:HD11	3:A:253:ARG:HG2	2.02	0.41
3:A:301:LEU:HD12	3:A:307:ALA:O	2.21	0.41
3:A:36:TYR:CD2	3:A:37:ASN:N	2.89	0.41
3:A:41:LYS:HE2	3:A:64:GLY:HA3	2.02	0.40
3:A:268:GLY:O	3:A:271:TYR:HB3	2.19	0.40
3:A:285:HIS:CE1	3:A:289:LYS:HE3	2.55	0.40
3:A:213:GLN:HE21	3:A:213:GLN:HB2	1.64	0.40
3:A:235:PHE:CD1	3:A:235:PHE:C	2.95	0.40
3:A:166:VAL:CG1	3:A:173:TYR:CB	2.99	0.40
3:A:206:LYS:HA	3:A:206:LYS:HD3	1.88	0.40
3:A:28:ASN:N	3:A:28:ASN:ND2	2.67	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:83:ARG:NH1	3:A:117:GLU:CB[3_558]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	325/335 (97%)	275 (85%)	33 (10%)	17 (5%)	1 5

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	32	ALA
3	A	185	ALA
3	A	202	SER
3	A	206	LYS
3	A	207	GLN
3	A	244	LYS
3	A	246	ASP
3	A	247	GLU
3	A	289	LYS
3	A	307	ALA
3	A	309	GLU
3	A	10	THR
3	A	80	GLY
3	A	199	SER
3	A	91	ASP
3	A	304	THR
3	A	204	SER

5.3.2 Protein sidechains [i](#)

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%)	220 (76%)	68 (24%)	1 3

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	41	LYS
3	A	45	VAL
3	A	46	ILE
3	A	52	LYS
3	A	54	LYS
3	A	62	LEU
3	A	67	THR
3	A	68	LYS
3	A	77	LEU
3	A	79	THR
3	A	81	LYS
3	A	93	THR
3	A	95	SER
3	A	100	LEU
3	A	101	THR
3	A	113	LYS
3	A	119	ILE
3	A	132	LEU
3	A	138	ILE
3	A	150	ILE
3	A	153	GLU
3	A	168	LYS
3	A	172	GLU
3	A	180	SER
3	A	182	ARG
3	A	188	SER
3	A	194	LEU
3	A	202	SER
3	A	204	SER
3	A	214	VAL

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Mol	Chain	Res	Type
3	A	218	LEU
3	A	219	GLN
3	A	224	ILE
3	A	228	LEU
3	A	235	PHE
3	A	236	MET
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE
3	A	258	ARG
3	A	259	LEU
3	A	264	GLN
3	A	277	ILE
3	A	282	MET
3	A	287	LEU
3	A	288	GLU
3	A	289	LYS
3	A	293	ILE
3	A	294	ASN
3	A	295	GLU
3	A	298	ILE
3	A	301	LEU
3	A	306	VAL
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	325	TRP
3	A	329	GLU
3	A	331	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	28	ASN
3	A	31	GLN
3	A	37	ASN
3	A	90	GLN
3	A	98	ASN
3	A	133	ASN
3	A	134	HIS

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Mol	Chain	Res	Type
3	A	136	GLN
3	A	157	GLN
3	A	159	GLN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	219	GLN
3	A	245	ASN
3	A	252	HIS
3	A	264	GLN
3	A	279	ASN
3	A	281	ASN
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, 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	7/7 (100%)	-1.19	0 100 100	22, 35, 63, 100	0
2	P	6/6 (100%)	-1.47	0 100 100	21, 30, 30, 38	0
3	A	324/335 (96%)	-1.00	0 100 100	6, 36, 84, 100	0
All	All	337/348 (96%)	-1.02	0 100 100	6, 35, 85, 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
5	ZN	A	343	1/1	0.95	0.08	93,93,93,93	0
4	NA	A	341	1/1	0.96	0.06	34,34,34,34	0
4	NA	A	342	1/1	0.97	0.06	31,31,31,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.