



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:17 AM UTC

PDB ID : 9ICP / pdb_00009icp
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SIX BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF PYROPHOSPHATE (1 MILLIMOLAR) AND MGCL2 (5 MILLIMOLAR)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1995-12-16
Resolution : 3.10 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

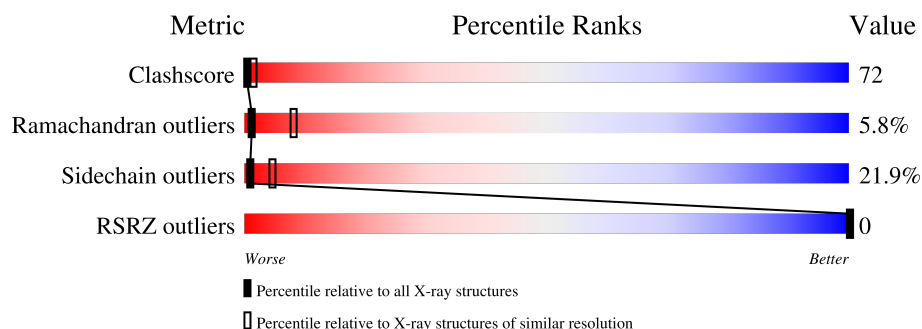
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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

There are 5 unique types of molecules in this entry. The entry contains 3022 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		

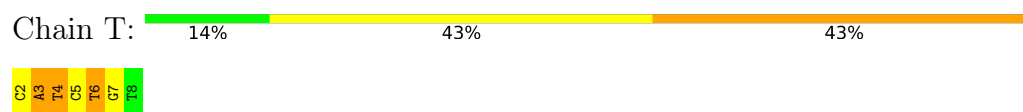
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	T	10	Total	O	0	0
			10	10		
5	P	23	Total	O	0	0
			23	23		
5	A	116	Total	O	0	0
			116	116		

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.

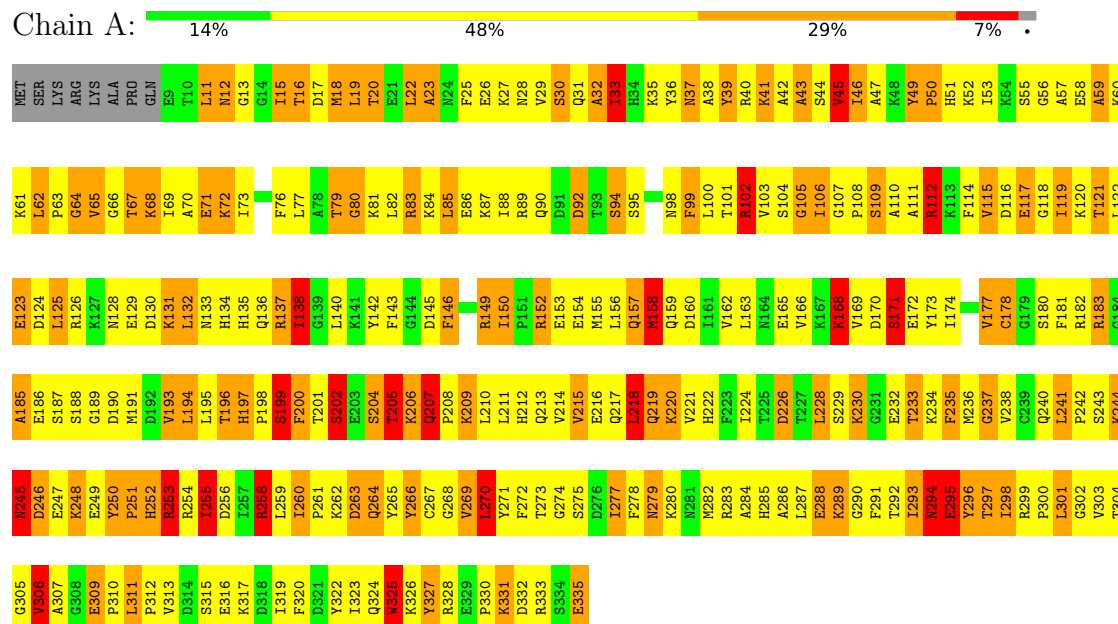
- Molecule 1: DNA (5'-D(*CP*AP*TP*CP*TP*GP*T)-3')



- 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	178.66Å 57.82Å 48.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	91.0 (20.00-3.10) 89.9 (20.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.68Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.165 , (Not available) 0.158 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 320.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3022	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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

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	2.10	5/207 (2.4%)
2	P	1.31	1/141 (0.7%)	3.25	14/214 (6.5%)
3	A	1.59	22/2672 (0.8%)	2.23	125/3590 (3.5%)
All	All	1.56	23/2948 (0.8%)	2.29	144/4011 (3.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	2	0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	228	LEU	CA-C	-7.08	1.43	1.53
3	A	15	ILE	CA-C	-7.06	1.44	1.52
2	P	1	DC	OP3-P	6.55	1.61	1.48
3	A	106	ILE	N-CA	-6.36	1.39	1.46
3	A	294	ASN	CA-C	-6.16	1.45	1.52
3	A	94	SER	N-CA	-6.13	1.38	1.46
3	A	268	GLY	CA-C	-6.06	1.45	1.52
3	A	51	HIS	CA-C	-5.66	1.45	1.53
3	A	146	PHE	CA-C	-5.58	1.45	1.52
3	A	66	GLY	N-CA	-5.52	1.40	1.45
3	A	199	SER	N-CA	-5.47	1.38	1.46
3	A	229	SER	N-CA	-5.47	1.39	1.46
3	A	157	GLN	C-N	5.36	1.40	1.33
3	A	39	TYR	CA-C	-5.33	1.45	1.52
3	A	65	VAL	N-CA	-5.31	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	116	ASP	CA-C	-5.28	1.45	1.52
3	A	119	ILE	CA-CB	-5.28	1.47	1.54
3	A	119	ILE	CA-C	-5.25	1.46	1.52
3	A	115	VAL	CA-CB	-5.25	1.47	1.54
3	A	215	VAL	CA-C	-5.21	1.46	1.52
3	A	252	HIS	CE1-NE2	5.11	1.37	1.32
3	A	310	PRO	N-CA	-5.11	1.41	1.47
3	A	306	VAL	N-CA	-5.03	1.40	1.46

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	5	DT	C2-N1-C1'	19.55	148.67	119.35
2	P	5	DT	C6-N1-C1'	-18.96	90.91	119.35
2	P	3	DG	C8-N9-C1'	14.40	148.59	127.00
3	A	99	PHE	CA-CB-CG	-13.31	100.48	113.80
2	P	3	DG	C4-N9-C1'	-12.40	108.39	127.00
3	A	49	TYR	CA-C-N	11.43	131.22	119.56
3	A	49	TYR	C-N-CA	11.43	131.22	119.56
2	P	4	DA	C8-N9-C1'	-10.15	111.83	127.05
2	P	4	DA	C4-N9-C1'	9.73	141.64	127.05
3	A	310	PRO	N-CA-CB	9.61	111.86	103.31
1	T	6	DT	C2-N1-C1'	-9.56	105.01	119.35
3	A	310	PRO	N-CA-C	9.29	125.63	111.14
3	A	193	VAL	N-CA-C	9.16	120.92	107.37
3	A	296	TYR	N-CA-C	9.06	123.64	112.23
3	A	146	PHE	CA-CB-CG	-8.94	104.86	113.80
1	T	6	DT	C6-N1-C1'	8.94	132.75	119.35
3	A	272	PHE	CA-CB-CG	-8.44	105.36	113.80
3	A	149	ARG	CA-C-N	-8.43	116.87	122.60
3	A	149	ARG	C-N-CA	-8.43	116.87	122.60
2	P	5	DT	N1-C1'-C2'	8.37	126.06	113.50
3	A	152	ARG	N-CA-CB	8.27	124.47	110.49
3	A	207	GLN	CA-C-N	8.26	129.05	119.47
3	A	207	GLN	C-N-CA	8.26	129.05	119.47
2	P	4	DA	P-O3'-C3'	8.13	132.40	120.20
2	P	4	DA	C4'-C3'-O3'	-7.95	98.08	110.00
3	A	310	PRO	CB-CA-C	7.69	121.38	111.46
3	A	49	TYR	O-C-N	7.49	129.93	121.32
2	P	2	DA	P-O5'-C5'	-7.45	108.82	120.00
3	A	268	GLY	N-CA-C	-7.45	103.79	112.73
3	A	87	LYS	CA-C-N	7.38	130.56	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	87	LYS	C-N-CA	7.38	130.56	120.46
3	A	270	LEU	O-C-N	7.36	129.96	122.08
3	A	130	ASP	CA-CB-CG	7.36	119.96	112.60
3	A	253	ARG	CD-NE-CZ	7.22	134.51	124.40
3	A	269	VAL	N-CA-CB	7.22	119.00	110.55
3	A	83	ARG	N-CA-CB	7.21	120.46	110.01
3	A	240	GLN	N-CA-C	7.18	119.30	108.46
3	A	327	TYR	N-CA-CB	6.99	120.55	109.51
3	A	150	ILE	N-CA-C	6.97	113.90	107.56
3	A	251	PRO	CA-C-N	-6.95	110.18	122.07
3	A	251	PRO	C-N-CA	-6.95	110.18	122.07
3	A	270	LEU	CA-C-N	6.83	129.76	120.54
3	A	270	LEU	C-N-CA	6.83	129.76	120.54
3	A	177	VAL	N-CA-C	6.83	113.51	106.21
3	A	255	ILE	N-CA-C	6.76	117.85	108.12
3	A	115	VAL	O-C-N	6.75	128.78	121.83
3	A	138	ILE	N-CA-CB	-6.75	103.02	110.51
3	A	325	TRP	N-CA-CB	-6.73	100.42	111.66
3	A	263	ASP	CA-CB-CG	-6.72	105.88	112.60
3	A	215	VAL	N-CA-CB	6.68	118.37	110.55
3	A	116	ASP	N-CA-C	-6.68	104.39	112.54
3	A	50	PRO	CA-C-N	-6.67	110.79	123.32
3	A	50	PRO	C-N-CA	-6.67	110.79	123.32
3	A	272	PHE	CA-C-N	6.64	129.47	120.44
3	A	272	PHE	C-N-CA	6.64	129.47	120.44
3	A	237	GLY	CA-C-N	6.63	132.16	122.94
3	A	237	GLY	C-N-CA	6.63	132.16	122.94
3	A	241	LEU	O-C-N	6.59	126.91	121.31
3	A	117	GLU	N-CA-C	-6.58	105.00	113.16
3	A	15	ILE	N-CA-CB	6.55	118.21	110.55
3	A	152	ARG	CD-NE-CZ	-6.52	115.28	124.40
3	A	230	LYS	N-CA-CB	6.45	121.38	110.87
3	A	237	GLY	O-C-N	6.45	131.08	122.70
3	A	109	SER	N-CA-C	-6.45	103.16	111.02
3	A	266	TYR	CA-CB-CG	-6.44	102.31	113.90
3	A	297	THR	CB-CA-C	-6.42	98.68	111.91
3	A	33	ILE	N-CA-CB	-6.38	102.49	110.47
3	A	222	HIS	CB-CA-C	-6.33	99.48	111.06
3	A	313	VAL	N-CA-C	6.25	116.88	107.75
3	A	92	ASP	N-CA-CB	6.21	119.38	110.06
3	A	250	TYR	N-CA-C	6.14	118.76	110.29
3	A	197	HIS	CB-CA-C	6.13	118.25	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	57	ALA	N-CA-CB	-6.11	99.82	109.78
3	A	277	ILE	N-CA-CB	6.10	117.28	110.51
3	A	99	PHE	N-CA-C	6.08	117.59	110.97
3	A	40	ARG	CB-CA-C	6.06	120.29	110.96
3	A	168	LYS	N-CA-CB	6.00	118.88	109.94
3	A	245	ASN	CB-CA-C	5.99	120.39	111.17
3	A	17	ASP	N-CA-C	5.92	117.61	111.03
3	A	64	GLY	N-CA-C	-5.88	106.37	114.67
3	A	229	SER	CB-CA-C	5.86	121.28	109.68
3	A	229	SER	N-CA-CB	5.85	121.71	111.13
3	A	105	GLY	CA-C-N	-5.84	115.07	122.43
3	A	105	GLY	C-N-CA	-5.84	115.07	122.43
3	A	102	ARG	CD-NE-CZ	-5.83	116.23	124.40
3	A	169	VAL	N-CA-C	5.81	116.55	110.62
3	A	50	PRO	CB-CA-C	-5.80	103.61	111.85
3	A	209	LYS	O-C-N	5.80	128.27	122.12
3	A	137	ARG	CB-CA-C	5.79	119.92	110.95
3	A	45	VAL	N-CA-C	5.74	116.38	110.82
3	A	158	MET	CB-CA-C	-5.74	101.63	110.81
3	A	268	GLY	O-C-N	5.74	127.70	122.19
3	A	253	ARG	N-CA-C	5.73	118.91	109.85
3	A	23	ALA	N-CA-CB	5.73	118.54	110.12
3	A	105	GLY	CA-C-O	5.72	125.22	119.27
3	A	28	ASN	N-CA-C	5.70	117.35	111.03
3	A	116	ASP	CA-C-N	-5.67	112.11	122.38
3	A	116	ASP	C-N-CA	-5.67	112.11	122.38
2	P	1	DC	P-O3'-C3'	5.65	128.68	120.20
3	A	99	PHE	CA-C-N	5.65	127.84	120.28
3	A	99	PHE	C-N-CA	5.65	127.84	120.28
3	A	279	ASN	O-C-N	5.64	127.90	122.03
3	A	272	PHE	N-CA-C	5.62	118.17	111.71
3	A	215	VAL	O-C-N	5.62	127.41	121.91
3	A	218	LEU	CB-CA-C	5.59	120.07	110.79
3	A	119	ILE	CB-CA-C	-5.56	104.02	110.91
1	T	3	DA	P-O3'-C3'	5.54	128.52	120.20
3	A	43	ALA	CB-CA-C	5.54	121.44	110.42
1	T	5	DC	C6-N1-C1'	5.52	127.98	119.70
3	A	186	GLU	N-CA-C	5.52	119.11	112.38
1	T	4	DT	P-O5'-C5'	-5.44	111.83	120.00
3	A	12	ASN	CB-CA-C	5.44	119.75	110.56
3	A	246	ASP	N-CA-C	5.42	122.34	110.80
3	A	196	THR	N-CA-CB	5.42	120.11	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	294	ASN	N-CA-C	-5.40	100.91	108.96
3	A	121	THR	CA-CB-CG2	-5.37	101.37	110.50
3	A	115	VAL	CA-CB-CG1	-5.37	101.28	110.40
3	A	258	ARG	N-CA-C	5.33	117.77	108.76
3	A	200	PHE	N-CA-C	5.30	117.04	108.34
3	A	335	GLU	N-CA-CB	5.30	119.51	110.50
2	P	5	DT	C5-C4-O4	5.29	130.53	122.60
3	A	71	GLU	N-CA-CB	-5.29	101.16	109.78
3	A	20	THR	N-CA-CB	5.28	118.47	110.28
3	A	112	ARG	O-C-N	5.26	127.71	122.08
3	A	65	VAL	CB-CA-C	5.26	117.33	110.96
3	A	202	SER	N-CA-CB	-5.25	101.62	110.49
3	A	51	HIS	CA-C-N	-5.25	115.56	122.85
3	A	51	HIS	C-N-CA	-5.25	115.56	122.85
3	A	171	SER	N-CA-CB	5.24	118.69	110.46
3	A	272	PHE	O-C-N	5.23	128.34	122.22
3	A	226	ASP	CA-CB-CG	-5.23	107.37	112.60
3	A	59	ALA	O-C-N	5.20	127.65	122.03
2	P	2	DA	C8-N9-C1'	-5.20	119.25	127.05
2	P	5	DT	P-O3'-C3'	5.20	128.00	120.20
3	A	195	LEU	N-CA-C	5.19	117.88	109.06
3	A	295	GLU	CB-CA-C	5.18	120.73	110.42
3	A	197	HIS	N-CA-CB	-5.15	103.61	110.77
3	A	98	ASN	CA-CB-CG	-5.13	107.47	112.60
3	A	123	GLU	CB-CA-C	5.12	119.55	110.85
3	A	295	GLU	CB-CG-CD	5.08	121.24	112.60
3	A	15	ILE	CB-CA-C	-5.08	105.47	111.97
3	A	286	ALA	CA-C-N	5.03	127.42	120.29
3	A	286	ALA	C-N-CA	5.03	127.42	120.29
3	A	260	ILE	CB-CA-C	-5.01	102.24	111.36

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	152	ARG	CA
3	A	310	PRO	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	7	0
2	P	126	0	67	20	0
3	A	2623	0	2641	380	1
4	A	2	0	0	0	0
5	A	116	0	0	22	0
5	P	23	0	0	4	0
5	T	10	0	0	3	0
All	All	3022	0	2777	398	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 72.

All (398) 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	1.27	1.08
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.50	1.07
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.41	1.02
3:A:301:LEU:HD11	3:A:306:VAL:HA	1.41	1.02
3:A:177:VAL:HG22	3:A:193:VAL:HG22	1.46	0.97
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.07	0.97
3:A:62:LEU:HD12	3:A:63:PRO:HD2	1.46	0.97
3:A:285:HIS:CE1	3:A:289:LYS:HE3	2.00	0.96
3:A:245:ASN:N	3:A:245:ASN:HD22	1.57	0.95
3:A:201:THR:HA	3:A:261:PRO:HB2	1.50	0.94
3:A:245:ASN:HD22	3:A:245:ASN:H	1.12	0.93
2:P:2:DA:C8	2:P:2:DA:H5'	2.05	0.92
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.02	0.88
3:A:16:THR:HG23	3:A:46:ILE:HG12	1.55	0.86
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.55	0.86
3:A:201:THR:HA	3:A:261:PRO:CB	2.04	0.86
3:A:155:MET:HE3	3:A:188:SER:HB2	1.58	0.85
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.57	0.85
3:A:101:THR:HA	3:A:106:ILE:HG22	1.59	0.85
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:157:GLN:HE22	3:A:244:LYS:NZ	1.77	0.83
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.60	0.82
3:A:12:ASN:HB3	3:A:46:ILE:CD1	2.10	0.82
3:A:202:SER:HB2	3:A:263:ASP:CG	2.04	0.82
3:A:282:MET:HE3	3:A:323:ILE:HD11	1.62	0.81
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.77	0.80
3:A:197:HIS:CE1	3:A:198:PRO:HD2	2.17	0.80
3:A:16:THR:HG23	3:A:46:ILE:CG1	2.11	0.80
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.17	0.80
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.29	0.80
3:A:68:LYS:HB2	3:A:68:LYS:NZ	1.98	0.79
3:A:157:GLN:HE22	3:A:244:LYS:HZ1	1.28	0.79
3:A:18:MET:HG2	3:A:19:LEU:N	1.96	0.78
3:A:157:GLN:NE2	3:A:244:LYS:NZ	2.31	0.78
3:A:294:ASN:HB2	3:A:295:GLU:OE2	1.83	0.77
3:A:278:PHE:HB2	3:A:333:ARG:O	1.83	0.77
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.12	0.77
3:A:41:LYS:HE2	3:A:64:GLY:HA2	1.66	0.77
3:A:111:ALA:O	3:A:115:VAL:HG23	1.84	0.77
3:A:128:ASN:HB3	3:A:131:LYS:HD2	1.65	0.77
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.20	0.76
3:A:293:ILE:HD13	3:A:298:ILE:CG1	2.13	0.76
3:A:49:TYR:CE2	3:A:53:ILE:HG13	2.20	0.76
3:A:15:ILE:O	3:A:19:LEU:HD22	1.86	0.76
3:A:15:ILE:CG2	3:A:46:ILE:HD13	2.16	0.76
3:A:218:LEU:HB2	3:A:224:ILE:HD12	1.67	0.76
3:A:298:ILE:O	3:A:311:LEU:HB2	1.86	0.75
3:A:197:HIS:ND1	3:A:198:PRO:HD2	2.00	0.75
3:A:218:LEU:CB	3:A:224:ILE:HD12	2.16	0.75
3:A:244:LYS:HB2	3:A:245:ASN:HD22	1.51	0.75
2:P:3:DG:H1'	5:P:511:HOH:O	1.86	0.75
3:A:44:SER:O	3:A:47:ALA:HB3	1.87	0.75
3:A:150:ILE:HG21	3:A:158:MET:CE	2.17	0.74
3:A:260:ILE:HG22	3:A:261:PRO:HD2	1.69	0.74
3:A:197:HIS:HE1	3:A:199:SER:HB2	1.52	0.74
3:A:38:ALA:O	3:A:41:LYS:HD3	1.88	0.74
3:A:271:TYR:HB2	5:A:592:HOH:O	1.88	0.74
3:A:157:GLN:NE2	3:A:244:LYS:HZ1	1.86	0.73
3:A:41:LYS:O	3:A:45:VAL:HG13	1.88	0.73
3:A:68:LYS:O	3:A:72:LYS:HE3	1.89	0.73
3:A:182:ARG:HG2	3:A:273:THR:CG2	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:328:ARG:HB3	3:A:332:ASP:OD1	1.89	0.72
3:A:245:ASN:N	3:A:245:ASN:ND2	2.31	0.72
3:A:18:MET:O	3:A:22:LEU:HD22	1.90	0.72
3:A:289:LYS:HD2	3:A:324:GLN:OE1	1.89	0.72
3:A:59:ALA:O	3:A:62:LEU:HB2	1.90	0.72
3:A:15:ILE:HG21	3:A:46:ILE:HD13	1.71	0.71
3:A:182:ARG:HG2	3:A:273:THR:HG23	1.71	0.70
3:A:162:VAL:O	3:A:166:VAL:HG23	1.90	0.70
3:A:99:PHE:HD2	3:A:100:LEU:HD12	1.57	0.70
3:A:285:HIS:HE1	3:A:289:LYS:HE3	1.56	0.70
3:A:89:ARG:HB2	5:A:645:HOH:O	1.92	0.69
3:A:119:ILE:HG21	3:A:125:LEU:HD23	1.73	0.69
3:A:26:GLU:OE1	3:A:32:ALA:HB3	1.91	0.69
3:A:68:LYS:HB2	3:A:68:LYS:HZ1	1.54	0.69
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.73	0.69
2:P:5:DT:OP2	3:A:109:SER:HB3	1.90	0.69
3:A:244:LYS:HB2	3:A:245:ASN:ND2	2.08	0.69
1:T:6:DT:H5''	5:T:547:HOH:O	1.92	0.68
2:P:5:DT:H2''	2:P:6:DG:H5'	1.75	0.68
3:A:114:PHE:HD1	3:A:119:ILE:HD12	1.57	0.68
3:A:31:GLN:N	5:A:641:HOH:O	2.27	0.68
3:A:81:LYS:HZ3	3:A:86:GLU:HB3	1.58	0.67
3:A:295:GLU:HA	5:A:592:HOH:O	1.93	0.67
3:A:114:PHE:CD1	3:A:119:ILE:HD12	2.30	0.67
3:A:291:PHE:CD1	3:A:300:PRO:HA	2.30	0.67
3:A:241:LEU:HB2	3:A:250:TYR:CD2	2.30	0.67
5:P:568:HOH:O	3:A:110:ALA:HB2	1.95	0.66
3:A:119:ILE:HG22	3:A:124:ASP:HB3	1.76	0.66
3:A:251:PRO:HG2	3:A:253:ARG:NH2	2.11	0.66
2:P:2:DA:N7	5:P:598:HOH:O	2.29	0.66
3:A:292:THR:O	3:A:298:ILE:HA	1.95	0.66
2:P:3:DG:N3	5:P:511:HOH:O	2.29	0.65
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.25	0.65
3:A:43:ALA:O	3:A:47:ALA:HB2	1.96	0.65
3:A:92:ASP:O	3:A:95:SER:HB2	1.96	0.65
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.29	0.65
3:A:266:TYR:N	5:A:508:HOH:O	2.29	0.65
3:A:285:HIS:O	3:A:288:GLU:N	2.30	0.64
3:A:52:LYS:HE2	5:A:554:HOH:O	1.96	0.64
3:A:157:GLN:O	3:A:160:ASP:HB3	1.98	0.64
3:A:11:LEU:H	3:A:11:LEU:CD2	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:120:LYS:N	3:A:124:ASP:OD2	2.29	0.63
3:A:279:ASN:O	3:A:283:ARG:N	2.29	0.63
3:A:278:PHE:HZ	3:A:320:PHE:CZ	2.15	0.63
3:A:81:LYS:NZ	3:A:86:GLU:HB3	2.13	0.63
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.39	0.63
3:A:12:ASN:HA	5:A:642:HOH:O	1.97	0.63
3:A:35:LYS:O	3:A:38:ALA:HB3	1.99	0.63
3:A:319:ILE:O	3:A:322:TYR:HB2	1.99	0.63
3:A:250:TYR:HB3	5:A:577:HOH:O	1.98	0.62
3:A:165:GLU:HA	3:A:168:LYS:HG3	1.80	0.62
3:A:180:SER:HB2	3:A:185:ALA:HB2	1.82	0.62
2:P:5:DT:P	3:A:109:SER:HB3	2.39	0.62
3:A:11:LEU:HD23	3:A:12:ASN:H	1.65	0.62
3:A:259:LEU:O	3:A:260:ILE:HD13	1.98	0.62
3:A:33:ILE:HG21	5:A:616:HOH:O	2.00	0.61
3:A:182:ARG:HH22	3:A:316:GLU:CD	2.08	0.61
3:A:100:LEU:HD11	3:A:120:LYS:O	1.99	0.61
3:A:100:LEU:O	3:A:106:ILE:HG21	2.01	0.61
3:A:243:SER:OG	3:A:249:GLU:HA	2.00	0.61
3:A:295:GLU:CD	3:A:295:GLU:H	2.09	0.61
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.82	0.61
3:A:158:MET:O	3:A:162:VAL:HG23	1.99	0.60
3:A:183:ARG:HH11	3:A:275:SER:HA	1.66	0.60
3:A:212:HIS:HB3	5:A:541:HOH:O	2.01	0.60
3:A:280:LYS:O	3:A:284:ALA:N	2.32	0.60
3:A:282:MET:HG3	3:A:323:ILE:CD1	2.32	0.60
3:A:282:MET:HE3	3:A:323:ILE:CD1	2.31	0.60
3:A:217:GLN:HE22	3:A:220:LYS:HD3	1.66	0.60
3:A:42:ALA:O	3:A:45:VAL:N	2.32	0.60
3:A:11:LEU:H	3:A:11:LEU:HD23	1.67	0.60
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.32	0.60
3:A:60:LYS:HE2	3:A:67:THR:CA	2.32	0.60
3:A:255:ILE:HG12	3:A:256:ASP:N	2.15	0.60
1:T:2:DC:H2"	1:T:3:DA:C8	2.37	0.60
3:A:182:ARG:NH2	3:A:316:GLU:OE1	2.34	0.60
3:A:197:HIS:CE1	3:A:199:SER:HB2	2.37	0.60
3:A:266:TYR:HA	3:A:269:VAL:HB	1.84	0.60
2:P:1:DC:H2"	2:P:2:DA:H5"	1.84	0.59
3:A:331:LYS:HD2	3:A:332:ASP:N	2.17	0.59
3:A:234:LYS:HB2	5:A:538:HOH:O	2.02	0.59
3:A:126:ARG:O	3:A:129:GLU:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:228:LEU:HB2	3:A:236:MET:O	2.02	0.59
3:A:63:PRO:C	3:A:65:VAL:H	2.09	0.59
3:A:150:ILE:HB	3:A:155:MET:CE	2.33	0.59
3:A:16:THR:CG2	3:A:46:ILE:HG12	2.31	0.58
3:A:293:ILE:HG23	3:A:298:ILE:HB	1.85	0.58
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.25	0.58
3:A:301:LEU:HD11	3:A:306:VAL:CA	2.27	0.58
3:A:253:ARG:NH2	5:A:620:HOH:O	2.36	0.58
2:P:2:DA:H5'	2:P:2:DA:H8	1.66	0.58
3:A:23:ALA:O	3:A:36:TYR:HD2	1.87	0.58
3:A:99:PHE:HD2	3:A:100:LEU:CD1	2.16	0.58
3:A:159:GLN:O	3:A:163:LEU:HG	2.03	0.58
3:A:183:ARG:NH1	3:A:275:SER:HA	2.19	0.58
3:A:202:SER:HB2	3:A:263:ASP:OD2	2.03	0.58
3:A:103:VAL:HG22	3:A:143:PHE:CE1	2.38	0.58
3:A:331:LYS:HD2	3:A:331:LYS:C	2.29	0.58
3:A:132:LEU:HD23	3:A:132:LEU:N	2.18	0.57
3:A:200:PHE:O	3:A:262:LYS:N	2.30	0.57
3:A:133:ASN:O	3:A:137:ARG:HG3	2.04	0.57
3:A:233:THR:HG22	3:A:259:LEU:HB3	1.86	0.57
3:A:150:ILE:HB	3:A:155:MET:HE2	1.87	0.57
2:P:4:DA:H2'	2:P:5:DT:H71	1.84	0.57
3:A:326:LYS:HG3	3:A:326:LYS:O	2.04	0.57
3:A:60:LYS:HE2	3:A:67:THR:N	2.20	0.57
3:A:254:ARG:HH11	3:A:255:ILE:N	2.02	0.57
3:A:327:TYR:HD1	3:A:328:ARG:N	2.02	0.57
3:A:215:VAL:O	3:A:219:GLN:HG3	2.05	0.57
3:A:18:MET:HG3	3:A:22:LEU:CD2	2.35	0.56
3:A:294:ASN:HD22	3:A:294:ASN:H	1.53	0.56
3:A:86:GLU:O	3:A:90:GLN:HG3	2.05	0.56
3:A:106:ILE:HD11	3:A:125:LEU:HD11	1.86	0.56
3:A:172:GLU:HB3	3:A:198:PRO:CD	2.34	0.56
3:A:68:LYS:O	3:A:71:GLU:HB3	2.05	0.56
3:A:150:ILE:N	3:A:188:SER:O	2.29	0.56
3:A:79:THR:O	3:A:81:LYS:N	2.29	0.56
3:A:81:LYS:NZ	3:A:86:GLU:OE1	2.34	0.56
3:A:254:ARG:NH2	3:A:256:ASP:OD1	2.36	0.56
1:T:3:DA:H1'	5:T:617:HOH:O	2.04	0.55
3:A:212:HIS:CE1	3:A:230:LYS:HD2	2.41	0.55
3:A:218:LEU:HB3	3:A:224:ILE:HD12	1.88	0.55
3:A:316:GLU:CD	3:A:333:ARG:HH12	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:5:DT:OP2	3:A:108:PRO:HD2	2.07	0.55
3:A:29:VAL:HG21	3:A:94:SER:OG	2.07	0.55
3:A:248:LYS:O	3:A:248:LYS:HG2	2.06	0.55
3:A:154:GLU:O	3:A:158:MET:HG2	2.07	0.55
2:P:5:DT:H2''	2:P:6:DG:C5'	2.35	0.55
3:A:44:SER:HB2	5:A:608:HOH:O	2.06	0.55
3:A:152:ARG:CA	3:A:155:MET:HB2	2.37	0.55
2:P:4:DA:H5''	3:A:109:SER:OG	2.06	0.55
3:A:18:MET:HE2	3:A:82:LEU:HD22	1.88	0.54
3:A:157:GLN:NE2	3:A:244:LYS:HZ3	2.04	0.54
3:A:150:ILE:HG12	3:A:253:ARG:HG2	1.89	0.54
3:A:129:GLU:O	3:A:129:GLU:HG2	2.08	0.54
3:A:33:ILE:O	3:A:37:ASN:HB2	2.07	0.54
3:A:134:HIS:CE1	3:A:138:ILE:HD11	2.43	0.54
3:A:254:ARG:NH1	3:A:255:ILE:N	2.56	0.54
3:A:132:LEU:HB3	3:A:136:GLN:HB3	1.90	0.53
3:A:201:THR:HG23	3:A:204:SER:HB3	1.90	0.53
3:A:270:LEU:HD23	3:A:319:ILE:HD13	1.89	0.53
2:P:5:DT:P	3:A:107:GLY:HA3	2.48	0.53
3:A:108:PRO:O	3:A:112:ARG:HG2	2.08	0.53
3:A:103:VAL:HG12	3:A:104:SER:N	2.24	0.53
3:A:65:VAL:HG13	3:A:69:ILE:HG21	1.90	0.53
3:A:197:HIS:CE1	3:A:199:SER:H	2.27	0.53
2:P:1:DC:H2''	2:P:2:DA:C5'	2.39	0.52
3:A:101:THR:HA	3:A:106:ILE:CG2	2.37	0.52
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.44	0.52
3:A:309:GLU:OE1	3:A:309:GLU:HA	2.10	0.52
3:A:36:TYR:CD1	3:A:37:ASN:N	2.78	0.52
3:A:115:VAL:O	3:A:118:GLY:N	2.41	0.52
3:A:278:PHE:HZ	3:A:320:PHE:CE1	2.27	0.52
3:A:294:ASN:HD22	3:A:294:ASN:N	2.05	0.52
3:A:76:PHE:O	3:A:79:THR:O	2.28	0.52
3:A:173:TYR:OH	3:A:213:GLN:NE2	2.43	0.52
3:A:177:VAL:HG12	3:A:177:VAL:O	2.09	0.52
3:A:19:LEU:HD23	3:A:43:ALA:HB2	1.93	0.51
3:A:115:VAL:C	3:A:118:GLY:H	2.18	0.51
3:A:262:LYS:O	3:A:262:LYS:HG3	2.10	0.51
3:A:55:SER:O	3:A:58:GLU:HB3	2.10	0.51
3:A:189:GLY:HA2	5:A:523:HOH:O	2.11	0.51
3:A:241:LEU:HB2	3:A:250:TYR:CG	2.46	0.51
3:A:145:ASP:CG	3:A:252:HIS:H	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:60:LYS:HE2	3:A:67:THR:HA	1.93	0.51
3:A:182:ARG:HG2	3:A:273:THR:HG21	1.92	0.51
3:A:282:MET:HG3	3:A:323:ILE:HD11	1.93	0.51
3:A:298:ILE:O	3:A:298:ILE:HG23	2.11	0.51
3:A:300:PRO:HD3	3:A:311:LEU:HD13	1.93	0.51
3:A:22:LEU:HB3	3:A:39:TYR:CE2	2.46	0.51
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.41	0.50
3:A:283:ARG:NH2	3:A:294:ASN:HA	2.26	0.50
3:A:327:TYR:CD1	3:A:328:ARG:N	2.79	0.50
3:A:206:LYS:O	3:A:207:GLN:HB2	2.11	0.50
3:A:172:GLU:HB3	3:A:198:PRO:HD3	1.94	0.50
3:A:196:THR:OG1	3:A:197:HIS:N	2.44	0.50
1:T:3:DA:C2	2:P:5:DT:N3	2.79	0.50
3:A:198:PRO:C	3:A:200:PHE:H	2.20	0.49
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.93	0.49
3:A:201:THR:HA	3:A:261:PRO:HB3	1.90	0.49
3:A:205:THR:O	3:A:206:LYS:O	2.30	0.49
3:A:241:LEU:O	3:A:250:TYR:HD2	1.96	0.49
3:A:65:VAL:HG13	3:A:69:ILE:CG2	2.42	0.49
3:A:106:ILE:HG22	3:A:106:ILE:O	2.10	0.49
3:A:237:GLY:O	3:A:254:ARG:NH1	2.46	0.49
3:A:265:TYR:O	3:A:269:VAL:N	2.35	0.49
3:A:282:MET:CE	3:A:319:ILE:HG22	2.42	0.49
3:A:297:THR:HG22	5:A:626:HOH:O	2.12	0.49
3:A:73:ILE:CG2	3:A:77:LEU:HD13	2.42	0.49
3:A:149:ARG:NH2	3:A:187:SER:O	2.36	0.49
3:A:26:GLU:HG3	3:A:35:LYS:HB3	1.93	0.49
3:A:150:ILE:CG2	3:A:155:MET:HE2	2.43	0.49
3:A:261:PRO:HG2	3:A:264:GLN:HG3	1.95	0.49
3:A:303:VAL:C	3:A:305:GLY:H	2.21	0.49
3:A:170:ASP:OD1	3:A:171:SER:N	2.46	0.49
3:A:114:PHE:HD1	3:A:119:ILE:CD1	2.26	0.48
3:A:158:MET:HB2	3:A:191:MET:HE1	1.95	0.48
3:A:174:ILE:O	3:A:265:TYR:OH	2.29	0.48
3:A:282:MET:CE	3:A:323:ILE:HD11	2.40	0.48
3:A:235:PHE:HZ	3:A:237:GLY:HA3	1.70	0.48
3:A:123:GLU:HG3	5:A:623:HOH:O	2.12	0.48
3:A:173:TYR:CE1	3:A:197:HIS:CD2	3.01	0.48
3:A:209:LYS:O	3:A:213:GLN:HG3	2.13	0.48
3:A:326:LYS:HD2	5:A:657:HOH:O	2.12	0.48
3:A:12:ASN:HB3	3:A:46:ILE:HD11	1.90	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:142:TYR:O	3:A:146:PHE:HB2	2.13	0.48
3:A:201:THR:CG2	3:A:204:SER:HB3	2.43	0.48
3:A:299:ARG:HB3	3:A:300:PRO:HD2	1.95	0.48
3:A:12:ASN:O	3:A:46:ILE:HD11	2.14	0.48
3:A:333:ARG:HD3	5:A:584:HOH:O	2.13	0.48
3:A:108:PRO:HA	3:A:111:ALA:HB3	1.96	0.48
3:A:31:GLN:O	3:A:33:ILE:N	2.48	0.47
3:A:60:LYS:CE	3:A:67:THR:HB	2.43	0.47
3:A:177:VAL:CG2	3:A:193:VAL:HG22	2.33	0.47
3:A:270:LEU:HA	3:A:316:GLU:OE2	2.15	0.47
3:A:285:HIS:CD2	3:A:325:TRP:CD1	3.02	0.47
3:A:267:CYS:HB2	3:A:295:GLU:O	2.14	0.47
3:A:288:GLU:O	3:A:290:GLY:N	2.47	0.47
3:A:55:SER:OG	3:A:58:GLU:HB2	2.15	0.47
3:A:288:GLU:OE1	3:A:288:GLU:HA	2.04	0.47
2:P:6:DG:OP1	3:A:105:GLY:N	2.47	0.47
3:A:261:PRO:HG2	3:A:264:GLN:CG	2.45	0.47
3:A:291:PHE:HD1	3:A:300:PRO:HA	1.75	0.47
3:A:19:LEU:CB	3:A:43:ALA:HB2	2.45	0.47
3:A:173:TYR:CD1	3:A:197:HIS:HB2	2.50	0.47
3:A:16:THR:O	3:A:20:THR:HG23	2.15	0.47
1:T:3:DA:H2	2:P:5:DT:O2	1.98	0.46
2:P:1:DC:H2'	2:P:2:DA:C8	2.50	0.46
3:A:103:VAL:HG22	3:A:143:PHE:CD1	2.50	0.46
3:A:150:ILE:CB	3:A:155:MET:HE2	2.45	0.46
1:T:6:DT:H2''	1:T:7:DG:C8	2.50	0.46
3:A:58:GLU:O	3:A:61:LYS:HG3	2.15	0.46
3:A:152:ARG:O	3:A:156:LEU:HD12	2.15	0.46
3:A:80:GLY:O	3:A:81:LYS:HG2	2.15	0.46
3:A:327:TYR:CD1	3:A:327:TYR:C	2.94	0.46
3:A:32:ALA:HB1	3:A:35:LYS:HB2	1.98	0.46
3:A:315:SER:OG	3:A:316:GLU:N	2.49	0.46
3:A:67:THR:O	3:A:70:ALA:HB3	2.16	0.46
3:A:212:HIS:ND1	3:A:230:LYS:HD3	2.31	0.45
3:A:100:LEU:CD1	3:A:100:LEU:N	2.79	0.45
3:A:114:PHE:CD1	3:A:119:ILE:CD1	2.99	0.45
3:A:194:LEU:HD12	3:A:194:LEU:HA	1.44	0.45
1:T:4:DT:H5'	5:T:617:HOH:O	2.16	0.45
3:A:172:GLU:HG2	3:A:198:PRO:HG3	1.98	0.45
3:A:303:VAL:O	3:A:305:GLY:N	2.49	0.45
3:A:212:HIS:CE1	3:A:230:LYS:CD	2.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:208:PRO:HB3	3:A:232:GLU:HB2	1.98	0.45
3:A:259:LEU:HD12	3:A:259:LEU:HA	1.34	0.45
3:A:100:LEU:C	3:A:106:ILE:HG21	2.42	0.45
3:A:49:TYR:HE2	3:A:53:ILE:HG13	1.74	0.45
3:A:183:ARG:NH1	3:A:275:SER:CB	2.79	0.45
3:A:264:GLN:HB3	3:A:296:TYR:O	2.17	0.45
3:A:132:LEU:N	3:A:132:LEU:CD2	2.79	0.45
3:A:211:LEU:HB2	3:A:259:LEU:HD22	1.98	0.45
3:A:49:TYR:CD2	3:A:53:ILE:HG13	2.52	0.45
3:A:274:GLY:HA3	3:A:275:SER:HA	1.78	0.45
3:A:18:MET:HG3	3:A:22:LEU:HD21	1.99	0.44
3:A:73:ILE:HG22	3:A:77:LEU:HD13	1.99	0.44
3:A:84:LYS:HD2	5:A:524:HOH:O	2.16	0.44
3:A:191:MET:HB2	3:A:191:MET:HE3	1.68	0.44
3:A:258:ARG:HG2	3:A:260:ILE:HD11	1.99	0.44
3:A:37:ASN:HD22	3:A:37:ASN:HA	1.44	0.44
3:A:166:VAL:HG12	3:A:173:TYR:HB2	1.98	0.44
3:A:182:ARG:CG	3:A:273:THR:HG23	2.43	0.44
3:A:132:LEU:HA	3:A:136:GLN:HE21	1.82	0.44
3:A:49:TYR:CE2	3:A:53:ILE:CG1	2.98	0.44
3:A:165:GLU:OE2	3:A:168:LYS:HD3	2.18	0.44
3:A:81:LYS:NZ	3:A:86:GLU:CB	2.81	0.44
3:A:181:PHE:HA	5:A:530:HOH:O	2.17	0.44
3:A:201:THR:OG1	3:A:202:SER:N	2.51	0.44
3:A:206:LYS:HE3	3:A:232:GLU:OE2	2.18	0.44
3:A:278:PHE:CZ	3:A:320:PHE:HZ	2.36	0.44
3:A:60:LYS:HE3	3:A:67:THR:HB	1.99	0.44
3:A:224:ILE:HA	3:A:238:VAL:O	2.18	0.44
3:A:18:MET:C	3:A:22:LEU:HD22	2.43	0.44
3:A:25:PHE:CE2	3:A:88:ILE:HG12	2.53	0.44
3:A:115:VAL:O	3:A:115:VAL:HG12	2.17	0.44
3:A:11:LEU:HD23	3:A:12:ASN:N	2.32	0.43
3:A:27:LYS:HB3	3:A:36:TYR:CD2	2.53	0.43
3:A:183:ARG:HD3	3:A:273:THR:O	2.18	0.43
3:A:228:LEU:HA	3:A:228:LEU:HD23	1.26	0.43
3:A:301:LEU:HD12	3:A:302:GLY:N	2.33	0.43
3:A:82:LEU:HA	3:A:82:LEU:HD12	1.80	0.43
3:A:244:LYS:CB	3:A:245:ASN:ND2	2.78	0.43
3:A:243:SER:OG	3:A:249:GLU:HG3	2.19	0.43
3:A:99:PHE:CD2	3:A:100:LEU:HD12	2.44	0.43
3:A:233:THR:HB	5:A:538:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:49:TYR:HA	3:A:50:PRO:HD2	1.39	0.43
3:A:207:GLN:O	3:A:210:LEU:HB2	2.19	0.43
3:A:261:PRO:HB2	3:A:263:ASP:OD1	2.18	0.43
3:A:317:LYS:HG3	5:A:501:HOH:O	2.18	0.43
3:A:241:LEU:HA	3:A:242:PRO:HD3	1.86	0.43
3:A:150:ILE:HG21	3:A:155:MET:HE2	2.00	0.42
3:A:301:LEU:CD1	3:A:306:VAL:HA	2.30	0.42
3:A:238:VAL:HA	3:A:253:ARG:O	2.19	0.42
3:A:271:TYR:CE1	3:A:283:ARG:NH2	2.88	0.42
3:A:11:LEU:CD2	3:A:11:LEU:N	2.78	0.42
3:A:103:VAL:CG1	3:A:104:SER:N	2.83	0.42
3:A:121:THR:H	3:A:121:THR:HG23	1.57	0.42
3:A:206:LYS:HD3	3:A:206:LYS:HA	1.81	0.42
3:A:285:HIS:O	3:A:288:GLU:HB2	2.18	0.42
3:A:311:LEU:HA	3:A:312:PRO:HD3	1.74	0.42
3:A:166:VAL:HG12	3:A:173:TYR:CB	2.49	0.42
3:A:216:GLU:O	3:A:220:LYS:N	2.52	0.42
3:A:306:VAL:O	3:A:307:ALA:HB2	2.19	0.42
3:A:102:ARG:HH11	3:A:102:ARG:HD3	1.58	0.42
3:A:244:LYS:H	3:A:244:LYS:HG2	1.69	0.42
3:A:278:PHE:CZ	3:A:320:PHE:CZ	3.02	0.42
3:A:45:VAL:C	3:A:47:ALA:N	2.76	0.42
3:A:145:ASP:HB3	3:A:252:HIS:H	1.85	0.42
3:A:183:ARG:NH1	3:A:275:SER:HB3	2.35	0.42
3:A:210:LEU:HA	3:A:210:LEU:HD23	1.38	0.42
3:A:16:THR:HG22	3:A:43:ALA:O	2.19	0.41
3:A:241:LEU:CB	3:A:250:TYR:CD2	3.01	0.41
3:A:12:ASN:HD21	3:A:53:ILE:H	1.68	0.41
3:A:16:THR:HG22	3:A:43:ALA:HA	2.03	0.41
3:A:131:LYS:H	3:A:131:LYS:HG3	1.48	0.41
3:A:132:LEU:HA	3:A:136:GLN:NE2	2.35	0.41
3:A:22:LEU:HD13	3:A:85:LEU:HD12	2.03	0.41
3:A:112:ARG:HG2	3:A:112:ARG:H	1.55	0.41
3:A:59:ALA:C	3:A:61:LYS:N	2.78	0.41
3:A:125:LEU:HD23	3:A:125:LEU:HA	1.62	0.41
3:A:174:ILE:HD13	3:A:174:ILE:HG21	1.79	0.41
3:A:197:HIS:ND1	3:A:198:PRO:CD	2.79	0.41
2:P:5:DT:O5'	3:A:107:GLY:HA3	2.21	0.41
3:A:56:GLY:O	3:A:59:ALA:HB3	2.21	0.41
3:A:150:ILE:CG1	3:A:253:ARG:HG2	2.51	0.41
3:A:18:MET:HE1	3:A:76:PHE:CB	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:145:ASP:CB	3:A:252:HIS:H	2.34	0.40
3:A:198:PRO:C	3:A:200:PHE:N	2.79	0.40
3:A:62:LEU:CD1	3:A:63:PRO:HD2	2.33	0.40
3:A:79:THR:C	3:A:81:LYS:N	2.79	0.40
3:A:215:VAL:O	3:A:215:VAL:HG12	2.21	0.40
3:A:79:THR:C	3:A:81:LYS:H	2.23	0.40
3:A:292:THR:C	3:A:293:ILE:HG12	2.46	0.40
3:A:330:PRO:HA	3:A:333:ARG:HD2	2.02	0.40
3:A:172:GLU:CG	3:A:198:PRO:HG3	2.51	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]	2.07	0.13

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%)	253 (78%)	53 (16%)	19 (6%)	1 8

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	32	ALA
3	A	185	ALA
3	A	202	SER
3	A	205	THR
3	A	206	LYS
3	A	244	LYS
3	A	247	GLU

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Mol	Chain	Res	Type
3	A	309	GLU
3	A	13	GLY
3	A	204	SER
3	A	289	LYS
3	A	304	THR
3	A	80	GLY
3	A	246	ASP
3	A	30	SER
3	A	178	CYS
3	A	220	LYS
3	A	295	GLU
3	A	207	GLN

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%)	225 (78%)	63 (22%)	1 4

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	11	LEU
3	A	16	THR
3	A	18	MET
3	A	19	LEU
3	A	22	LEU
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	62	LEU
3	A	67	THR
3	A	68	LYS

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Mol	Chain	Res	Type
3	A	72	LYS
3	A	79	THR
3	A	85	LEU
3	A	102	ARG
3	A	112	ARG
3	A	122	LEU
3	A	125	LEU
3	A	131	LYS
3	A	132	LEU
3	A	135	HIS
3	A	138	ILE
3	A	140	LEU
3	A	153	GLU
3	A	158	MET
3	A	168	LYS
3	A	171	SER
3	A	183	ARG
3	A	190	ASP
3	A	194	LEU
3	A	199	SER
3	A	205	THR
3	A	207	GLN
3	A	214	VAL
3	A	218	LEU
3	A	219	GLN
3	A	221	VAL
3	A	226	ASP
3	A	233	THR
3	A	235	PHE
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE
3	A	258	ARG
3	A	264	GLN
3	A	270	LEU
3	A	277	ILE
3	A	287	LEU
3	A	288	GLU
3	A	293	ILE
3	A	294	ASN
3	A	295	GLU

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Mol	Chain	Res	Type
3	A	298	ILE
3	A	301	LEU
3	A	306	VAL
3	A	311	LEU
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 (15) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	28	ASN
3	A	31	GLN
3	A	37	ASN
3	A	90	GLN
3	A	136	GLN
3	A	157	GLN
3	A	159	GLN
3	A	197	HIS
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	222	HIS
3	A	245	ASN
3	A	281	ASN
3	A	294	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	T	7/7 (100%)	-0.66	0 100 100	16, 23, 54, 98	0
2	P	6/6 (100%)	-0.88	0 100 100	12, 20, 30, 31	0
3	A	324/335 (96%)	-0.76	0 100 100	3, 32, 83, 100	0
All	All	337/348 (96%)	-0.76	0 100 100	3, 32, 84, 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	NA	A	342	1/1	0.89	0.10	34,34,34,34	0
4	NA	A	341	1/1	0.94	0.03	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.