



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:59 AM UTC

PDB ID : 1ZQI / pdb_00001zqi
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SEVEN BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF KCL (150 MILLIMOLAR)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-04-12
Resolution : 2.70 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

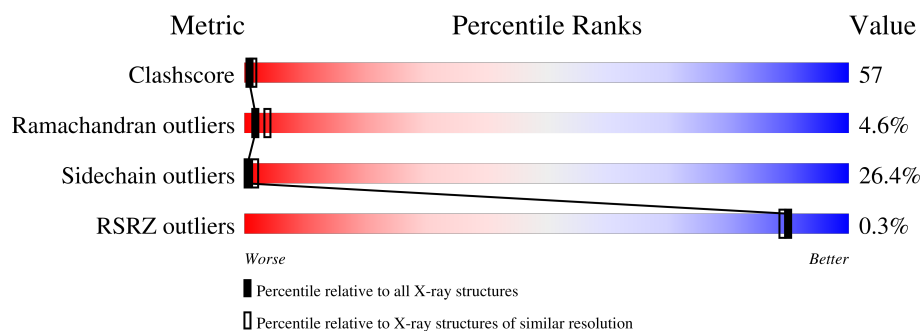
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	
2	P	7	
3	A	335	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3052 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 POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	T	15	Total	O	0	0
			15	15		
5	P	22	Total	O	0	0
			22	22		
5	A	101	Total	O	0	0
			101	101		

3 Residue-property plots [i](#)

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

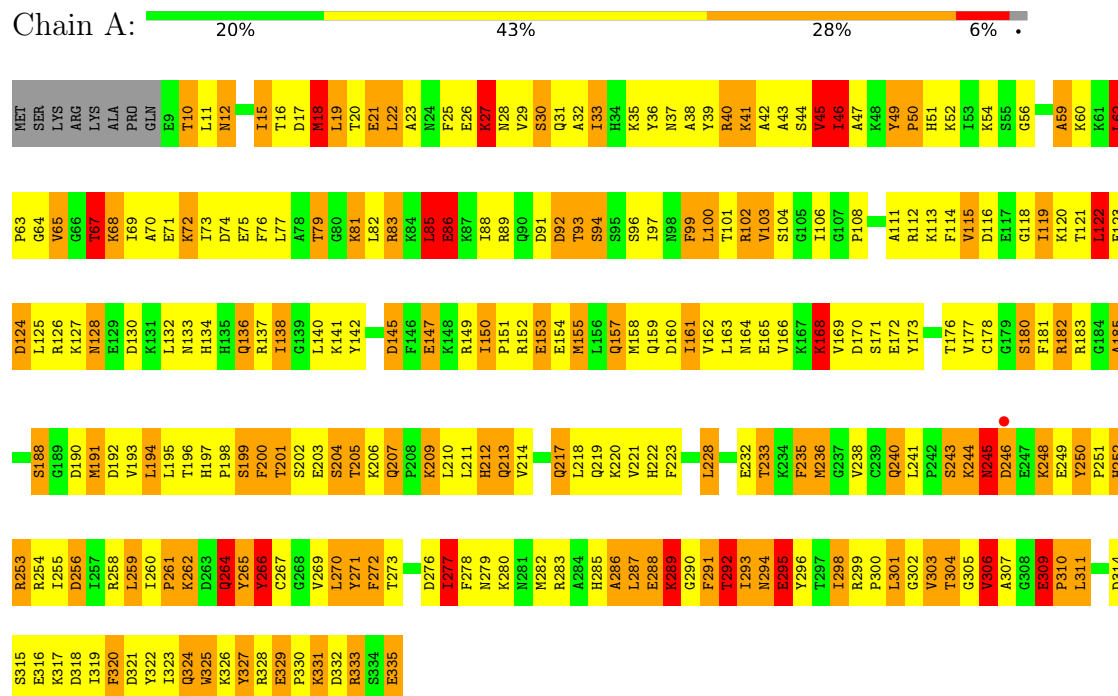
- Molecule 1: DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.50Å 57.81Å 48.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.0 (20.00-2.70) 88.5 (20.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.56Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.179 , (Not available) 0.176 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 179.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3052	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.40% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section:
K

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	1.00	0/162	3.13	11/249 (4.4%)
2	P	1.38	2/160 (1.2%)	4.03	18/243 (7.4%)
3	A	1.65	24/2672 (0.9%)	2.20	115/3590 (3.2%)
All	All	1.60	26/2994 (0.9%)	2.41	144/4082 (3.5%)

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 (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	124	ASP	CA-C	-8.67	1.41	1.52
3	A	270	LEU	CA-C	-7.91	1.42	1.52
3	A	124	ASP	C-O	-7.36	1.15	1.24
2	P	1	DT	OP3-P	7.13	1.62	1.48
3	A	138	ILE	CA-CB	-6.86	1.46	1.54
3	A	103	VAL	CA-CB	-6.42	1.47	1.54
3	A	306	VAL	CA-C	-6.37	1.47	1.52
3	A	103	VAL	C-N	-6.32	1.24	1.33
3	A	140	LEU	CA-C	-6.25	1.45	1.52
2	P	2	DC	C1'-N1	5.97	1.67	1.49
3	A	116	ASP	CA-C	-5.69	1.45	1.52
3	A	321	ASP	CG-OD2	5.67	1.36	1.25
3	A	265	TYR	N-CA	-5.53	1.39	1.46
3	A	15	ILE	CA-C	-5.46	1.46	1.52
3	A	67	THR	N-CA	-5.42	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	70	ALA	C-N	-5.31	1.26	1.33
3	A	122	LEU	CA-C	-5.29	1.46	1.52
3	A	235	PHE	C-O	-5.21	1.17	1.24
3	A	138	ILE	CA-C	-5.20	1.46	1.52
3	A	246	ASP	CG-OD1	5.15	1.35	1.25
3	A	200	PHE	N-CA	5.15	1.52	1.46
3	A	30	SER	C-N	-5.09	1.25	1.33
3	A	162	VAL	CA-C	-5.08	1.46	1.52
3	A	118	GLY	CA-C	5.06	1.58	1.51
3	A	160	ASP	CG-OD2	5.02	1.34	1.25
3	A	71	GLU	CD-OE1	5.01	1.34	1.25

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	1	DT	C6-N1-C1'	-24.52	82.58	119.35
2	P	1	DT	C2-N1-C1'	22.41	152.96	119.35
1	T	7	DA	C4-N9-C1'	-19.37	98.00	127.05
1	T	7	DA	C8-N9-C1'	18.05	154.13	127.05
1	T	6	DG	C8-N9-C1'	17.52	153.27	127.00
1	T	6	DG	C4-N9-C1'	-17.23	101.15	127.00
2	P	5	DA	C8-N9-C1'	-16.87	101.74	127.05
2	P	5	DA	C4-N9-C1'	16.19	151.34	127.05
2	P	7	DG	C8-N9-C1'	15.80	150.71	127.00
2	P	7	DG	C4-N9-C1'	-14.95	104.57	127.00
1	T	4	DT	C6-N1-C1'	-14.84	97.09	119.35
2	P	3	DT	C6-N1-C1'	-14.57	97.49	119.35
2	P	3	DT	C2-N1-C1'	14.09	140.49	119.35
2	P	6	DT	C6-N1-C1'	-13.87	98.55	119.35
2	P	2	DC	C2-N1-C1'	13.85	140.48	119.70
2	P	6	DT	C2-N1-C1'	12.87	138.66	119.35
1	T	4	DT	C2-N1-C1'	12.38	137.92	119.35
2	P	2	DC	C6-N1-C1'	-12.05	101.62	119.70
3	A	49	TYR	CA-C-N	11.21	133.85	119.84
3	A	49	TYR	C-N-CA	11.21	133.85	119.84
3	A	49	TYR	O-C-N	10.57	129.72	121.47
3	A	116	ASP	N-CA-CB	10.41	125.45	109.94
3	A	190	ASP	CA-C-N	-9.18	108.97	122.65
3	A	190	ASP	C-N-CA	-9.18	108.97	122.65
3	A	320	PHE	CA-CB-CG	-9.10	104.70	113.80
3	A	168	LYS	N-CA-CB	9.03	123.54	109.82
3	A	28	ASN	CA-CB-CG	-8.95	103.65	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	271	TYR	N-CA-C	8.87	120.64	110.97
3	A	134	HIS	CA-CB-CG	8.87	122.67	113.80
3	A	309	GLU	CA-C-N	8.43	130.37	119.84
3	A	309	GLU	C-N-CA	8.43	130.37	119.84
3	A	243	SER	CB-CA-C	8.14	122.47	110.26
3	A	228	LEU	N-CA-C	-8.05	101.26	112.45
3	A	277	ILE	N-CA-CB	7.95	122.51	110.58
3	A	181	PHE	CB-CA-C	-7.90	98.17	110.81
3	A	212	HIS	CA-CB-CG	-7.84	105.96	113.80
1	T	3	DT	P-O5'-C5'	7.78	131.67	120.00
3	A	318	ASP	CA-CB-CG	-7.67	104.93	112.60
3	A	30	SER	CA-C-N	-7.67	110.29	122.79
3	A	30	SER	C-N-CA	-7.67	110.29	122.79
3	A	119	ILE	CB-CA-C	-7.63	103.98	112.68
3	A	292	THR	CB-CA-C	7.54	121.24	110.24
3	A	116	ASP	CB-CA-C	7.52	122.84	110.81
3	A	193	VAL	N-CA-C	7.44	119.34	107.73
3	A	18	MET	O-C-N	7.42	129.71	122.07
3	A	222	HIS	CA-CB-CG	-7.37	106.44	113.80
3	A	99	PHE	CA-CB-CG	-7.14	106.66	113.80
3	A	83	ARG	N-CA-CB	7.07	120.23	109.91
3	A	223	PHE	N-CA-C	-6.98	103.11	111.69
3	A	35	LYS	CA-C-O	6.96	127.93	120.55
3	A	12	ASN	CB-CA-C	6.79	122.19	110.72
3	A	271	TYR	N-CA-CB	-6.77	100.03	109.91
3	A	193	VAL	N-CA-CB	-6.76	102.99	111.31
3	A	270	LEU	O-C-N	6.74	129.01	122.07
3	A	176	THR	CA-C-N	-6.70	114.15	122.93
3	A	176	THR	C-N-CA	-6.70	114.15	122.93
3	A	164	ASN	N-CA-CB	6.68	119.76	110.07
2	P	7	DG	P-O5'-C5'	-6.66	110.01	120.00
3	A	17	ASP	CB-CA-C	6.60	122.08	110.85
3	A	18	MET	CG-SD-CE	-6.44	86.74	100.90
3	A	86	GLU	N-CA-CB	6.37	119.48	110.12
3	A	252	HIS	O-C-N	6.36	130.48	123.04
3	A	30	SER	O-C-N	-6.30	113.69	122.76
3	A	147	GLU	CA-C-N	6.27	129.77	120.87
3	A	147	GLU	C-N-CA	6.27	129.77	120.87
3	A	85	LEU	N-CA-C	-6.26	104.37	111.07
3	A	18	MET	CA-C-N	6.26	128.58	120.44
3	A	18	MET	C-N-CA	6.26	128.58	120.44
3	A	264	GLN	N-CA-CB	6.25	120.11	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	3	DT	P-O5'-C5'	6.20	129.30	120.00
3	A	40	ARG	N-CA-CB	6.20	119.33	110.16
3	A	266	TYR	CA-CB-CG	-6.18	102.77	113.90
3	A	270	LEU	CA-C-N	6.17	128.80	120.65
3	A	270	LEU	C-N-CA	6.17	128.80	120.65
3	A	288	GLU	N-CA-C	-6.13	104.22	111.03
3	A	286	ALA	CA-C-N	6.12	128.39	120.44
3	A	286	ALA	C-N-CA	6.12	128.39	120.44
3	A	50	PRO	CA-C-N	-6.07	112.64	122.36
3	A	50	PRO	C-N-CA	-6.07	112.64	122.36
3	A	40	ARG	N-CA-C	6.04	117.95	111.36
3	A	124	ASP	O-C-N	6.03	128.28	122.07
3	A	233	THR	CA-CB-OG1	-6.01	100.59	109.60
3	A	205	THR	N-CA-C	5.98	123.54	110.80
3	A	72	LYS	N-CA-CB	5.98	119.00	110.16
3	A	46	ILE	N-CA-CB	5.93	120.78	110.65
2	P	3	DT	N1-C1'-C2'	5.92	122.38	113.50
3	A	27	LYS	N-CA-CB	-5.92	101.43	110.01
3	A	68	LYS	N-CA-CB	5.89	118.55	110.01
3	A	72	LYS	CB-CA-C	5.85	120.80	110.85
3	A	115	VAL	CB-CA-C	-5.83	104.17	112.22
3	A	245	ASN	CB-CA-C	5.78	118.86	111.40
3	A	164	ASN	CA-C-N	-5.77	111.54	120.31
3	A	164	ASN	C-N-CA	-5.77	111.54	120.31
2	P	5	DA	P-O3'-C3'	5.77	128.85	120.20
3	A	157	GLN	N-CA-CB	5.74	119.14	110.30
3	A	251	PRO	CB-CA-C	-5.68	103.95	111.23
1	T	5	DA	P-O5'-C5'	-5.68	111.47	120.00
3	A	219	GLN	CB-CA-C	-5.67	101.94	110.90
3	A	209	LYS	O-C-N	5.63	128.09	122.12
3	A	291	PHE	N-CA-C	5.63	116.80	108.86
3	A	102	ARG	CD-NE-CZ	-5.62	116.53	124.40
3	A	150	ILE	N-CA-CB	5.59	118.44	111.39
3	A	103	VAL	CA-CB-CG1	-5.56	100.95	110.40
3	A	303	VAL	N-CA-C	5.54	120.86	109.34
2	P	3	DT	O5'-C5'-C4'	-5.52	102.52	110.80
3	A	17	ASP	N-CA-C	5.51	117.37	111.36
2	P	2	DC	P-O5'-C5'	-5.49	111.76	120.00
3	A	250	TYR	N-CA-C	5.49	117.52	110.39
3	A	261	PRO	CA-C-O	-5.49	115.51	121.27
3	A	261	PRO	CB-CA-C	-5.42	104.66	111.71
3	A	277	ILE	N-CA-C	5.42	116.19	110.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	246	ASP	CA-CB-CG	-5.40	107.20	112.60
3	A	256	ASP	CA-CB-CG	5.40	118.00	112.60
3	A	240	GLN	CB-CA-C	-5.33	100.73	109.80
3	A	102	ARG	CA-CB-CG	-5.33	103.44	114.10
3	A	190	ASP	O-C-N	-5.33	117.97	123.29
3	A	333	ARG	N-CA-C	-5.30	106.66	113.02
3	A	27	LYS	CB-CA-C	5.29	119.19	110.88
1	T	5	DA	O3'-P-O5'	-5.28	96.08	104.00
3	A	153	GLU	N-CA-CB	5.27	118.34	110.22
3	A	192	ASP	N-CA-C	5.26	118.03	107.41
1	T	3	DT	O5'-C5'-C4'	-5.24	102.95	110.80
3	A	205	THR	N-CA-CB	5.23	119.32	110.49
3	A	12	ASN	CA-C-O	5.21	125.74	119.59
3	A	180	SER	CA-CB-OG	-5.19	100.71	111.10
3	A	264	GLN	CB-CA-C	5.19	119.02	109.99
3	A	45	VAL	O-C-N	5.15	127.13	121.83
3	A	193	VAL	O-C-N	-5.14	116.40	122.77
3	A	136	GLN	N-CA-C	5.14	116.88	111.28
3	A	50	PRO	CB-CA-C	-5.12	103.11	111.56
3	A	74	ASP	N-CA-CB	5.12	117.57	109.94
3	A	155	MET	CA-C-N	5.12	127.14	120.28
3	A	155	MET	C-N-CA	5.12	127.14	120.28
3	A	246	ASP	N-CA-C	5.12	121.71	110.80
3	A	252	HIS	CA-CB-CG	-5.10	108.70	113.80
3	A	103	VAL	CA-C-N	-5.09	114.33	121.72
3	A	103	VAL	C-N-CA	-5.09	114.33	121.72
3	A	320	PHE	N-CA-CB	5.08	117.55	109.82
1	T	5	DA	O5'-C5'-C4'	5.08	118.42	110.80
3	A	96	SER	CA-C-N	-5.06	114.08	120.56
3	A	96	SER	C-N-CA	-5.06	114.08	120.56
3	A	65	VAL	N-CA-C	5.05	114.88	107.15
3	A	62	LEU	C-N-CD	-5.04	104.36	125.00
3	A	59	ALA	O-C-N	5.02	127.24	122.07

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	116	ASP	CA
3	A	205	THR	CA
3	A	264	GLN	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	145	0	80	7	0
2	P	144	0	81	16	0
3	A	2623	0	2641	299	0
4	A	2	0	0	0	0
5	A	101	0	0	18	0
5	P	22	0	0	3	0
5	T	15	0	0	1	0
All	All	3052	0	2802	321	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 57.

All (321) 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:270:LEU:HD21	3:A:282:MET:HE1	1.43	0.99
3:A:245:ASN:HD22	3:A:245:ASN:N	1.55	0.98
3:A:243:SER:HB3	3:A:249:GLU:HA	1.46	0.96
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.48	0.95
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.47	0.95
3:A:245:ASN:H	3:A:245:ASN:ND2	1.68	0.90
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.12	0.90
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.53	0.90
2:P:1:DT:H2''	2:P:2:DC:H5'	1.55	0.88
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.05	0.86
3:A:11:LEU:HD23	3:A:11:LEU:H	1.39	0.86
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.06	0.86
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.40	0.86
3:A:155:MET:HA	3:A:158:MET:HE3	1.60	0.84
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.79	0.80
3:A:245:ASN:HD22	3:A:245:ASN:H	0.84	0.80
3:A:155:MET:HE2	3:A:188:SER:HB2	1.62	0.80
3:A:41:LYS:HE2	3:A:64:GLY:HA3	1.62	0.79
2:P:5:DA:H2''	2:P:6:DT:H5''	1.64	0.79
3:A:16:THR:O	3:A:20:THR:HG23	1.82	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:323:ILE:O	3:A:324:GLN:HG2	1.85	0.77
3:A:243:SER:CB	3:A:249:GLU:HA	2.14	0.77
3:A:289:LYS:HD3	3:A:289:LYS:N	1.99	0.76
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.64	0.76
3:A:111:ALA:O	3:A:115:VAL:HG23	1.84	0.76
3:A:277:ILE:HD11	3:A:335:GLU:HB3	1.68	0.74
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.71	0.73
3:A:270:LEU:HD21	3:A:282:MET:CE	2.17	0.73
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.34	0.73
2:P:6:DT:H2''	2:P:7:DG:H5''	1.72	0.71
3:A:18:MET:CE	3:A:76:PHE:HB2	2.22	0.70
3:A:200:PHE:HB2	5:A:625:HOH:O	1.90	0.70
3:A:26:GLU:HA	3:A:30:SER:OG	1.92	0.70
3:A:155:MET:HA	3:A:158:MET:CE	2.22	0.69
3:A:180:SER:HB3	3:A:183:ARG:HH21	1.57	0.69
3:A:277:ILE:CG1	3:A:335:GLU:HB2	2.22	0.69
3:A:286:ALA:HB2	3:A:323:ILE:HG21	1.72	0.69
2:P:6:DT:H2''	2:P:7:DG:C8	2.28	0.69
3:A:82:LEU:HD23	3:A:85:LEU:HB2	1.73	0.68
1:T:6:DG:H2''	1:T:7:DA:C8	2.28	0.68
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.22	0.68
3:A:159:GLN:O	3:A:163:LEU:HG	1.93	0.68
3:A:180:SER:CA	3:A:183:ARG:HH21	2.07	0.68
3:A:210:LEU:HB3	3:A:259:LEU:HD21	1.76	0.68
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.75	0.67
3:A:277:ILE:HD11	3:A:335:GLU:CB	2.23	0.67
2:P:1:DT:H2''	2:P:2:DC:C5'	2.24	0.67
3:A:262:LYS:O	3:A:262:LYS:HG3	1.91	0.67
1:T:1:DC:H2''	1:T:2:DA:OP2	1.94	0.67
3:A:127:LYS:HB2	3:A:128:ASN:ND2	2.09	0.67
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.76	0.66
3:A:278:PHE:HB2	3:A:333:ARG:O	1.95	0.66
3:A:295:GLU:N	3:A:295:GLU:OE1	2.28	0.66
3:A:31:GLN:N	5:A:641:HOH:O	2.28	0.66
2:P:5:DA:H2''	2:P:6:DT:C5'	2.26	0.66
3:A:292:THR:O	3:A:298:ILE:HA	1.96	0.66
3:A:294:ASN:O	3:A:296:TYR:N	2.29	0.65
3:A:41:LYS:O	3:A:45:VAL:HG13	1.97	0.65
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.31	0.65
3:A:59:ALA:O	3:A:62:LEU:HB2	1.96	0.65
2:P:4:DA:N7	5:P:664:HOH:O	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:165:GLU:CB	3:A:217:GLN:HG3	2.24	0.65
3:A:191:MET:HG3	3:A:255:ILE:HG13	1.79	0.65
3:A:286:ALA:O	3:A:291:PHE:N	2.30	0.65
3:A:15:ILE:O	3:A:19:LEU:HB2	1.97	0.65
3:A:152:ARG:HA	3:A:155:MET:HB2	1.77	0.65
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.32	0.64
3:A:114:PHE:CZ	3:A:132:LEU:HD23	2.32	0.64
3:A:287:LEU:HD13	3:A:291:PHE:O	1.97	0.64
3:A:180:SER:HB3	3:A:183:ARG:NH2	2.11	0.64
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.33	0.64
3:A:150:ILE:HD11	3:A:253:ARG:HG2	1.78	0.64
2:P:1:DT:C2'	2:P:2:DC:H5'	2.28	0.63
3:A:27:LYS:HB2	3:A:36:TYR:CD1	2.33	0.63
3:A:282:MET:HE3	5:A:555:HOH:O	1.98	0.63
3:A:323:ILE:C	3:A:324:GLN:HG2	2.22	0.63
3:A:163:LEU:HD23	3:A:163:LEU:N	2.13	0.63
3:A:92:ASP:HB3	5:A:647:HOH:O	1.97	0.63
3:A:180:SER:CB	3:A:183:ARG:HH21	2.11	0.62
2:P:4:DA:H5'	5:P:569:HOH:O	1.99	0.62
3:A:330:PRO:HA	3:A:333:ARG:CG	2.25	0.62
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.15	0.61
3:A:123:GLU:O	3:A:127:LYS:HG2	2.01	0.61
1:T:6:DG:N7	5:T:652:HOH:O	2.30	0.61
3:A:248:LYS:O	3:A:248:LYS:HG2	2.00	0.61
3:A:264:GLN:NE2	3:A:296:TYR:HB3	2.16	0.61
3:A:165:GLU:HB3	3:A:217:GLN:CG	2.29	0.60
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.37	0.60
3:A:93:THR:HG22	3:A:94:SER:N	2.14	0.60
3:A:217:GLN:NE2	3:A:217:GLN:HA	2.16	0.60
3:A:306:VAL:HG22	5:A:650:HOH:O	2.02	0.60
3:A:200:PHE:O	3:A:262:LYS:N	2.33	0.59
3:A:62:LEU:HD12	3:A:63:PRO:HD2	1.85	0.59
3:A:142:TYR:CE2	3:A:238:VAL:HG11	2.37	0.59
3:A:76:PHE:HD2	3:A:77:LEU:HD12	1.68	0.59
3:A:123:GLU:HG3	5:A:623:HOH:O	2.03	0.59
3:A:11:LEU:HD23	3:A:11:LEU:N	2.09	0.59
3:A:194:LEU:HD12	3:A:258:ARG:HD3	1.84	0.59
3:A:180:SER:HA	3:A:183:ARG:HE	1.67	0.59
3:A:292:THR:HG23	5:A:580:HOH:O	2.03	0.58
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.33	0.58
3:A:253:ARG:HG3	3:A:253:ARG:HH11	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:83:ARG:O	3:A:86:GLU:N	2.36	0.58
3:A:327:TYR:HD1	3:A:328:ARG:N	2.02	0.58
3:A:23:ALA:HB2	3:A:39:TYR:HB2	1.85	0.58
3:A:141:LYS:HE2	3:A:142:TYR:CZ	2.38	0.57
3:A:149:ARG:NH2	3:A:188:SER:HA	2.19	0.57
3:A:196:THR:OG1	3:A:197:HIS:N	2.33	0.57
3:A:191:MET:CG	3:A:255:ILE:HG13	2.33	0.57
3:A:157:GLN:HE22	3:A:244:LYS:NZ	2.01	0.57
3:A:328:ARG:O	3:A:333:ARG:NE	2.34	0.57
2:P:5:DA:C2'	2:P:6:DT:H5''	2.32	0.57
3:A:166:VAL:O	3:A:169:VAL:HG12	2.04	0.57
3:A:172:GLU:HB3	3:A:197:HIS:NE2	2.20	0.56
3:A:293:ILE:HD13	3:A:298:ILE:CG1	2.30	0.56
3:A:288:GLU:C	3:A:290:GLY:H	2.13	0.56
3:A:18:MET:O	3:A:21:GLU:HB2	2.05	0.56
3:A:298:ILE:HA	5:A:593:HOH:O	2.04	0.56
3:A:298:ILE:N	5:A:578:HOH:O	2.30	0.56
3:A:326:LYS:O	3:A:328:ARG:HG2	2.06	0.56
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.35	0.56
3:A:245:ASN:N	3:A:245:ASN:ND2	2.31	0.56
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.88	0.55
3:A:286:ALA:HB1	3:A:291:PHE:HB2	1.88	0.55
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.42	0.55
3:A:240:GLN:NE2	3:A:250:TYR:O	2.29	0.55
3:A:41:LYS:HE2	3:A:64:GLY:HA2	1.89	0.55
3:A:60:LYS:HA	3:A:65:VAL:HG12	1.88	0.55
3:A:329:GLU:O	3:A:333:ARG:HG2	2.06	0.55
3:A:259:LEU:HD12	3:A:260:ILE:H	1.72	0.55
3:A:39:TYR:OH	3:A:72:LYS:HE3	2.07	0.55
3:A:212:HIS:HB3	5:A:541:HOH:O	2.07	0.55
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.90	0.54
3:A:120:LYS:N	3:A:124:ASP:OD2	2.40	0.54
1:T:2:DA:H2''	1:T:3:DT:OP2	2.07	0.54
3:A:125:LEU:CD2	3:A:132:LEU:HD21	2.36	0.54
3:A:316:GLU:O	3:A:320:PHE:HD2	1.91	0.54
3:A:204:SER:O	3:A:206:LYS:N	2.41	0.54
3:A:128:ASN:N	3:A:128:ASN:HD22	2.05	0.54
3:A:41:LYS:O	3:A:44:SER:HB3	2.08	0.54
3:A:41:LYS:NZ	3:A:64:GLY:O	2.30	0.53
3:A:326:LYS:O	3:A:326:LYS:HG3	2.08	0.53
3:A:29:VAL:HA	3:A:97:ILE:HD12	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:38:ALA:O	3:A:41:LYS:HD3	2.09	0.53
3:A:81:LYS:NZ	3:A:86:GLU:HB2	2.24	0.53
3:A:310:PRO:HB3	5:A:626:HOH:O	2.08	0.53
3:A:12:ASN:HA	5:A:553:HOH:O	2.09	0.53
3:A:177:VAL:HG11	3:A:191:MET:HE2	1.91	0.53
3:A:18:MET:HE1	3:A:76:PHE:CB	2.39	0.53
3:A:254:ARG:NH2	5:A:657:HOH:O	2.42	0.52
3:A:169:VAL:HG13	3:A:170:ASP:N	2.25	0.52
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.24	0.52
3:A:155:MET:HE2	3:A:188:SER:CB	2.39	0.51
3:A:180:SER:HA	3:A:183:ARG:NE	2.25	0.51
3:A:11:LEU:H	3:A:11:LEU:CD2	2.16	0.51
3:A:271:TYR:CE1	3:A:283:ARG:NH2	2.78	0.51
3:A:103:VAL:HG12	3:A:104:SER:N	2.23	0.51
3:A:182:ARG:HG2	3:A:182:ARG:NH1	2.10	0.51
3:A:309:GLU:N	3:A:309:GLU:OE1	2.43	0.51
3:A:180:SER:HB2	3:A:185:ALA:HB2	1.91	0.51
3:A:133:ASN:O	3:A:137:ARG:HG3	2.11	0.51
3:A:151:PRO:HG2	3:A:154:GLU:HG3	1.93	0.51
3:A:200:PHE:CE2	3:A:261:PRO:HD3	2.46	0.51
3:A:188:SER:HB3	5:A:522:HOH:O	2.11	0.51
3:A:200:PHE:CE2	3:A:261:PRO:N	2.79	0.51
3:A:212:HIS:N	3:A:212:HIS:CD2	2.77	0.51
3:A:150:ILE:HD13	3:A:253:ARG:HG2	1.90	0.51
3:A:207:GLN:HB3	3:A:210:LEU:HG	1.93	0.50
3:A:198:PRO:C	3:A:200:PHE:H	2.19	0.50
3:A:258:ARG:NH2	3:A:272:PHE:CZ	2.80	0.50
3:A:76:PHE:CD2	3:A:77:LEU:HD12	2.47	0.50
3:A:41:LYS:HD3	3:A:42:ALA:N	2.27	0.50
3:A:180:SER:HA	3:A:183:ARG:HH21	1.76	0.50
3:A:207:GLN:O	3:A:210:LEU:HB2	2.12	0.50
3:A:15:ILE:CG2	3:A:46:ILE:HD11	2.42	0.50
3:A:260:ILE:HG22	3:A:261:PRO:N	2.27	0.50
3:A:197:HIS:ND1	3:A:199:SER:HB3	2.27	0.50
3:A:210:LEU:CB	3:A:259:LEU:HD21	2.41	0.49
3:A:12:ASN:OD1	3:A:51:HIS:O	2.30	0.49
3:A:41:LYS:HD3	3:A:42:ALA:H	1.77	0.49
3:A:157:GLN:O	3:A:161:ILE:HG13	2.12	0.49
3:A:76:PHE:HD2	3:A:77:LEU:CD1	2.26	0.49
3:A:79:THR:C	3:A:81:LYS:H	2.21	0.49
3:A:108:PRO:O	3:A:112:ARG:HG3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:201:THR:HA	3:A:261:PRO:HB3	1.94	0.49
3:A:232:GLU:C	3:A:233:THR:HG23	2.39	0.48
3:A:128:ASN:ND2	3:A:128:ASN:N	2.61	0.48
3:A:259:LEU:O	3:A:260:ILE:HD13	2.13	0.48
3:A:292:THR:O	3:A:298:ILE:HG13	2.13	0.48
3:A:315:SER:OG	3:A:316:GLU:N	2.46	0.48
3:A:169:VAL:HG13	3:A:170:ASP:H	1.78	0.48
3:A:277:ILE:HG13	3:A:335:GLU:HB2	1.92	0.48
3:A:25:PHE:CG	3:A:88:ILE:HD13	2.48	0.48
3:A:197:HIS:CE1	3:A:199:SER:HB3	2.49	0.48
3:A:12:ASN:ND2	5:A:642:HOH:O	2.47	0.48
3:A:69:ILE:O	3:A:72:LYS:N	2.47	0.48
3:A:122:LEU:CD2	3:A:126:ARG:NH2	2.77	0.47
3:A:81:LYS:NZ	3:A:86:GLU:CB	2.77	0.47
3:A:122:LEU:HD23	3:A:126:ARG:CZ	2.44	0.47
3:A:209:LYS:HD3	3:A:209:LYS:HA	1.81	0.47
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.44	0.47
2:P:1:DT:H2'	2:P:2:DC:C6	2.49	0.47
2:P:6:DT:C2'	2:P:7:DG:C8	2.97	0.47
3:A:259:LEU:HD12	3:A:260:ILE:N	2.29	0.47
3:A:293:ILE:HA	5:A:593:HOH:O	2.14	0.47
3:A:127:LYS:HB2	3:A:128:ASN:HD22	1.80	0.47
3:A:154:GLU:C	3:A:158:MET:HE2	2.40	0.47
3:A:217:GLN:HA	3:A:217:GLN:HE21	1.79	0.47
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.50	0.47
3:A:15:ILE:HG21	3:A:46:ILE:CD1	2.45	0.47
3:A:29:VAL:HG21	3:A:94:SER:HB2	1.97	0.46
3:A:173:TYR:OH	3:A:213:GLN:NE2	2.48	0.46
1:T:7:DA:H61	2:P:1:DT:H3	1.62	0.46
3:A:54:LYS:HA	3:A:54:LYS:HD2	1.73	0.46
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.35	0.46
3:A:303:VAL:C	3:A:305:GLY:H	2.23	0.46
3:A:306:VAL:HG23	3:A:307:ALA:N	2.26	0.46
3:A:29:VAL:HG22	3:A:94:SER:HA	1.97	0.45
3:A:319:ILE:O	3:A:322:TYR:HB2	2.17	0.45
3:A:56:GLY:O	3:A:59:ALA:HB3	2.15	0.45
3:A:149:ARG:NH2	3:A:188:SER:CA	2.79	0.45
3:A:264:GLN:HB3	3:A:296:TYR:O	2.17	0.45
3:A:73:ILE:HG22	3:A:77:LEU:HD22	1.98	0.45
3:A:276:ASP:O	3:A:280:LYS:HG3	2.16	0.45
3:A:180:SER:HA	3:A:183:ARG:NH2	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:331:LYS:HG2	3:A:332:ASP:N	2.16	0.45
3:A:77:LEU:CD1	3:A:77:LEU:N	2.79	0.45
3:A:207:GLN:O	3:A:210:LEU:N	2.49	0.45
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.81	0.45
3:A:16:THR:HG21	3:A:47:ALA:HB2	1.98	0.45
3:A:200:PHE:O	3:A:261:PRO:HA	2.16	0.45
3:A:211:LEU:HD12	3:A:211:LEU:O	2.17	0.45
3:A:27:LYS:HB2	3:A:36:TYR:CG	2.52	0.45
3:A:27:LYS:CB	3:A:36:TYR:CD1	3.00	0.45
3:A:285:HIS:NE2	5:A:583:HOH:O	2.36	0.45
3:A:125:LEU:HD22	3:A:132:LEU:HD21	1.98	0.44
2:P:6:DT:C4	2:P:7:DG:C6	3.05	0.44
3:A:197:HIS:CG	3:A:198:PRO:CD	2.99	0.44
3:A:29:VAL:HG21	3:A:94:SER:CB	2.47	0.44
3:A:155:MET:SD	3:A:158:MET:HE1	2.58	0.44
3:A:195:LEU:HA	3:A:195:LEU:HD12	1.41	0.44
3:A:26:GLU:HB3	3:A:32:ALA:HB3	2.00	0.44
3:A:103:VAL:CG1	3:A:104:SER:N	2.79	0.44
3:A:271:TYR:CD1	3:A:283:ARG:NH2	2.85	0.44
3:A:60:LYS:HA	3:A:65:VAL:CG1	2.47	0.44
3:A:197:HIS:CD2	3:A:198:PRO:CD	3.00	0.44
3:A:18:MET:O	3:A:22:LEU:HD22	2.18	0.44
3:A:201:THR:HA	3:A:261:PRO:CB	2.48	0.44
3:A:15:ILE:HB	3:A:46:ILE:HD11	1.99	0.44
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.58	0.44
3:A:315:SER:C	3:A:317:LYS:N	2.76	0.43
3:A:145:ASP:HB3	3:A:252:HIS:O	2.18	0.43
3:A:11:LEU:HA	3:A:52:LYS:HZ2	1.82	0.43
3:A:75:GLU:O	3:A:79:THR:HG23	2.17	0.43
3:A:241:LEU:HD23	3:A:241:LEU:HA	1.88	0.43
3:A:18:MET:HE2	3:A:82:LEU:HD22	1.99	0.43
3:A:150:ILE:N	3:A:188:SER:O	2.44	0.43
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.51	0.43
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.34	0.43
3:A:236:MET:HG3	3:A:256:ASP:OD1	2.17	0.43
3:A:327:TYR:C	3:A:327:TYR:CD1	2.96	0.43
3:A:282:MET:HB2	3:A:325:TRP:CZ3	2.53	0.43
1:T:4:DT:H2"	1:T:5:DA:C8	2.54	0.43
3:A:82:LEU:CD2	3:A:85:LEU:HD22	2.48	0.43
3:A:150:ILE:CG1	3:A:253:ARG:HG2	2.49	0.43
3:A:302:GLY:N	3:A:307:ALA:HB2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:40:ARG:HE	3:A:40:ARG:HB2	1.54	0.42
3:A:15:ILE:CG2	3:A:46:ILE:CD1	2.97	0.42
3:A:19:LEU:HD23	3:A:43:ALA:HA	2.01	0.42
3:A:200:PHE:HE2	3:A:261:PRO:N	2.17	0.42
3:A:288:GLU:O	3:A:290:GLY:N	2.52	0.42
3:A:287:LEU:HD13	3:A:287:LEU:HA	1.40	0.42
3:A:12:ASN:HB3	3:A:46:ILE:HD12	2.01	0.42
3:A:79:THR:HG23	3:A:79:THR:H	1.53	0.42
3:A:102:ARG:NE	3:A:147:GLU:OE2	2.53	0.42
3:A:259:LEU:HD12	3:A:259:LEU:HA	1.42	0.42
3:A:303:VAL:C	3:A:305:GLY:N	2.77	0.42
3:A:12:ASN:HA	3:A:12:ASN:HD22	1.77	0.42
3:A:31:GLN:HE21	3:A:112:ARG:NH1	2.07	0.42
3:A:249:GLU:HG3	3:A:250:TYR:N	2.35	0.42
3:A:301:LEU:HD12	3:A:301:LEU:HA	1.59	0.42
3:A:23:ALA:HB2	3:A:39:TYR:HB3	2.00	0.42
3:A:299:ARG:HA	3:A:300:PRO:HD3	1.94	0.42
3:A:171:SER:O	3:A:171:SER:OG	2.29	0.42
3:A:235:PHE:CD2	3:A:235:PHE:C	2.98	0.42
3:A:33:ILE:H	3:A:33:ILE:HG22	1.61	0.42
3:A:270:LEU:CD2	3:A:282:MET:HE1	2.33	0.42
1:T:1:DC:H6	1:T:1:DC:H2'	1.54	0.41
3:A:73:ILE:O	3:A:77:LEU:HD13	2.20	0.41
3:A:99:PHE:HD2	3:A:100:LEU:HD13	1.85	0.41
3:A:246:ASP:C	3:A:248:LYS:H	2.28	0.41
3:A:299:ARG:HE	3:A:299:ARG:HB2	1.71	0.41
3:A:200:PHE:HE2	3:A:261:PRO:HD3	1.84	0.41
3:A:155:MET:SD	3:A:158:MET:CE	3.09	0.41
3:A:191:MET:HE2	3:A:191:MET:HB2	1.45	0.41
3:A:200:PHE:CE2	3:A:261:PRO:CD	3.03	0.41
3:A:327:TYR:HD1	3:A:327:TYR:C	2.28	0.41
3:A:79:THR:O	3:A:81:LYS:N	2.53	0.41
3:A:133:ASN:H	3:A:136:GLN:HE21	1.67	0.41
3:A:282:MET:HA	3:A:325:TRP:CH2	2.56	0.41
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.61	0.41
3:A:60:LYS:HZ2	3:A:67:THR:HB	1.86	0.41
3:A:180:SER:HB2	3:A:185:ALA:CB	2.51	0.41
3:A:267:CYS:N	5:A:508:HOH:O	2.27	0.41
3:A:285:HIS:CE1	3:A:289:LYS:HG2	2.56	0.41
3:A:122:LEU:CD2	3:A:126:ARG:CZ	2.98	0.41
2:P:6:DT:C2'	2:P:7:DG:H5''	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:18:MET:HE2	3:A:82:LEU:HD13	2.02	0.41
3:A:29:VAL:CG2	3:A:94:SER:HA	2.51	0.41
3:A:11:LEU:N	3:A:11:LEU:CD2	2.80	0.41
3:A:157:GLN:HE22	3:A:244:LYS:HZ3	1.69	0.41
3:A:217:GLN:O	3:A:220:LYS:HB3	2.21	0.41
3:A:302:GLY:N	3:A:307:ALA:CB	2.83	0.41
3:A:266:TYR:HA	3:A:269:VAL:HB	2.03	0.41
3:A:303:VAL:O	3:A:305:GLY:N	2.53	0.41
3:A:194:LEU:CD1	3:A:258:ARG:HD3	2.49	0.40
3:A:195:LEU:HG	3:A:196:THR:N	2.36	0.40
3:A:287:LEU:HB3	3:A:288:GLU:OE2	2.21	0.40
2:P:6:DT:H5'	5:P:567:HOH:O	2.20	0.40
3:A:130:ASP:HA	3:A:137:ARG:HH21	1.85	0.40
3:A:177:VAL:CG1	3:A:191:MET:HE2	2.52	0.40

There are no symmetry-related clashes.

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%)	278 (86%)	32 (10%)	15 (5%)	2 4

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	185	ALA
3	A	202	SER
3	A	205	THR
3	A	244	LYS
3	A	265	TYR
3	A	295	GLU
3	A	204	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	266	TYR
3	A	289	LYS
3	A	304	THR
3	A	91	ASP
3	A	10	THR
3	A	309	GLU
3	A	207	GLN
3	A	310	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%)	212 (74%)	76 (26%)	0 2

All (76) 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	21	GLU
3	A	22	LEU
3	A	27	LYS
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
3	A	79	THR
3	A	81	LYS
3	A	85	LEU
3	A	86	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	89	ARG
3	A	92	ASP
3	A	93	THR
3	A	94	SER
3	A	100	LEU
3	A	101	THR
3	A	113	LYS
3	A	119	ILE
3	A	121	THR
3	A	122	LEU
3	A	128	ASN
3	A	138	ILE
3	A	145	ASP
3	A	153	GLU
3	A	161	ILE
3	A	168	LYS
3	A	182	ARG
3	A	188	SER
3	A	191	MET
3	A	194	LEU
3	A	199	SER
3	A	201	THR
3	A	203	GLU
3	A	213	GLN
3	A	214	VAL
3	A	217	GLN
3	A	218	LEU
3	A	221	VAL
3	A	228	LEU
3	A	236	MET
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	259	LEU
3	A	262	LYS
3	A	264	GLN
3	A	272	PHE
3	A	277	ILE
3	A	279	ASN
3	A	287	LEU
3	A	289	LYS
3	A	292	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	293	ILE
3	A	294	ASN
3	A	295	GLU
3	A	298	ILE
3	A	301	LEU
3	A	304	THR
3	A	306	VAL
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	324	GLN
3	A	325	TRP
3	A	327	TYR
3	A	329	GLU
3	A	331	LYS
3	A	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) 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	128	ASN
3	A	133	ASN
3	A	136	GLN
3	A	157	GLN
3	A	213	GLN
3	A	217	GLN
3	A	245	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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%)	-0.41	0	100 100	19, 38, 98, 99	0
2	P	7/7 (100%)	-0.88	0	100 100	17, 28, 47, 75	0
3	A	325/335 (97%)	-0.77	1 (0%)	90 89	7, 36, 84, 100	0
All	All	340/350 (97%)	-0.76	1 (0%)	90 89	7, 36, 86, 100	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	246	ASP	2.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	K	A	342	1/1	0.94	0.13	65,65,65,65	0
4	K	A	341	1/1	0.99	0.05	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.