



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:31 PM UTC

PDB ID : 1ZQN / pdb_00001zqn
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SEVEN BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF BACL2 (15 MILLIMOLAR) AND NACL (15 MILLIMOLAR)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-04-12
Resolution : 3.00 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

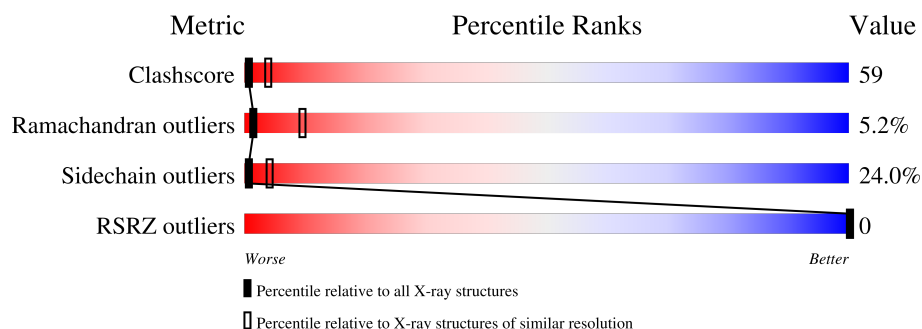
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 3058 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	8	Total	C	N	O	P	0	0	0
			145	69	27	42	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	P	0	0	0
			144	69	24	44	7			

- Molecule 3 is a protein called PROTEIN (DNA POLYMERASE BETA (E.C.2.7.7.7)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	327	Total	C	N	O	S	18	0	0
			2623	1657	458	499	9			

- Molecule 4 is BARIUM ION (CCD ID: BA) (formula: Ba).

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

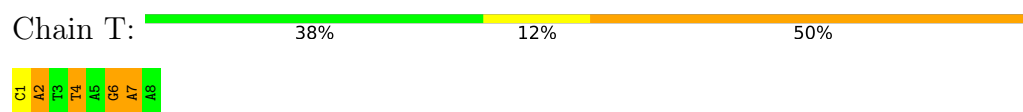
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	T	14	Total	O	0	0
			14	14		
5	P	23	Total	O	0	0
			23	23		
5	A	107	Total	O	0	0
			107	107		

3 Residue-property plots

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

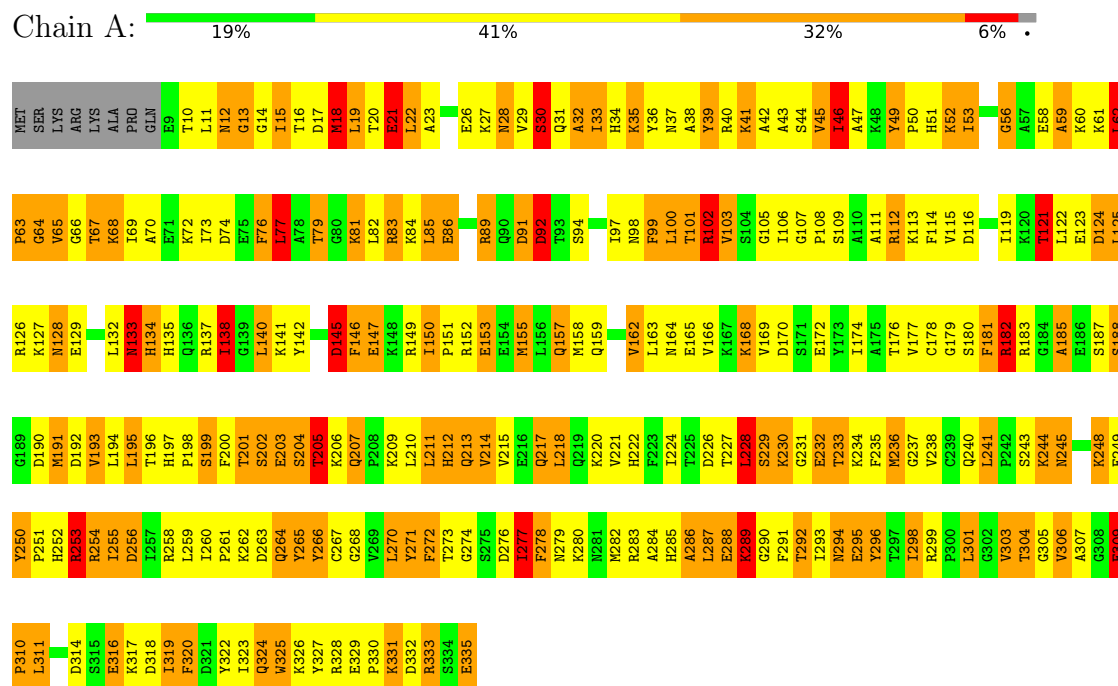
- Molecule 1: DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	177.84Å 57.67Å 47.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.0 (20.00-3.00) 87.5 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.71Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.177 , (Not available) 0.167 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.53 , 315.2	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	3058	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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: BA

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	1.12	0/162	3.28	8/249 (3.2%)
2	P	1.34	1/160 (0.6%)	3.19	11/243 (4.5%)
3	A	1.67	26/2672 (1.0%)	2.27	149/3590 (4.2%)
All	All	1.63	27/2994 (0.9%)	2.41	168/4082 (4.1%)

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	4	0

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	15	ILE	CA-C	-7.94	1.43	1.52
3	A	296	TYR	C-N	-7.68	1.25	1.33
3	A	103	VAL	C-O	-7.55	1.16	1.24
3	A	125	LEU	CA-C	-6.80	1.44	1.52
3	A	125	LEU	C-O	-6.80	1.16	1.24
3	A	116	ASP	CA-C	-6.74	1.44	1.52
3	A	147	GLU	CD-OE2	6.57	1.37	1.25
3	A	220	LYS	C-N	-6.56	1.27	1.34
3	A	65	VAL	C-N	-6.54	1.26	1.33
3	A	62	LEU	C-N	-6.38	1.28	1.33
3	A	15	ILE	CA-CB	-6.30	1.47	1.54
2	P	1	DT	OP3-P	6.16	1.60	1.48
3	A	177	VAL	CA-C	-6.13	1.46	1.52
3	A	237	GLY	C-O	-6.08	1.19	1.24
3	A	271	TYR	N-CA	-6.05	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	85	LEU	C-O	-5.88	1.17	1.24
3	A	63	PRO	C-O	5.67	1.29	1.23
3	A	72	LYS	CA-C	5.62	1.60	1.52
3	A	124	ASP	CA-C	-5.60	1.45	1.52
3	A	138	ILE	CA-CB	-5.43	1.47	1.54
3	A	227	THR	N-CA	-5.26	1.40	1.46
3	A	234	LYS	N-CA	-5.24	1.40	1.46
3	A	241	LEU	CA-C	-5.24	1.47	1.53
3	A	86	GLU	CD-OE1	5.23	1.35	1.25
3	A	65	VAL	CA-C	-5.17	1.47	1.52
3	A	99	PHE	CA-C	5.10	1.59	1.52
3	A	84	LYS	C-N	-5.08	1.27	1.33

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	7	DA	C4-N9-C1'	-21.48	94.83	127.05
1	T	7	DA	C8-N9-C1'	21.25	158.93	127.05
1	T	6	DG	C4-N9-C1'	-20.77	95.84	127.00
1	T	6	DG	C8-N9-C1'	19.89	156.83	127.00
2	P	1	DT	C6-N1-C1'	-19.10	90.70	119.35
2	P	7	DG	C8-N9-C1'	18.86	155.30	127.00
2	P	7	DG	C4-N9-C1'	-18.05	99.92	127.00
2	P	1	DT	C2-N1-C1'	17.48	145.57	119.35
1	T	4	DT	C6-N1-C1'	-13.46	99.16	119.35
2	P	5	DA	C4-N9-C1'	12.32	145.53	127.05
2	P	5	DA	C8-N9-C1'	-12.14	108.84	127.05
3	A	49	TYR	CA-C-N	11.78	133.19	120.12
3	A	49	TYR	C-N-CA	11.78	133.19	120.12
1	T	4	DT	C2-N1-C1'	10.85	135.62	119.35
3	A	99	PHE	CA-CB-CG	-10.50	103.30	113.80
3	A	116	ASP	N-CA-CB	10.27	125.22	110.12
3	A	28	ASN	CA-CB-CG	-10.00	102.60	112.60
1	T	2	DA	C4-N9-C1'	-9.86	112.26	127.05
3	A	309	GLU	CA-C-N	9.16	131.29	119.84
3	A	309	GLU	C-N-CA	9.16	131.29	119.84
3	A	157	GLN	N-CA-CB	8.74	122.97	110.12
3	A	49	TYR	O-C-N	8.73	129.07	121.30
3	A	168	LYS	N-CA-CB	8.68	124.48	109.72
3	A	266	TYR	CA-CB-CG	-8.58	98.46	113.90
1	T	2	DA	C8-N9-C1'	8.41	139.67	127.05
3	A	182	ARG	O-C-N	8.40	131.02	122.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	116	ASP	O-C-N	8.29	130.91	122.12
3	A	190	ASP	CA-C-N	-8.23	111.39	123.00
3	A	190	ASP	C-N-CA	-8.23	111.39	123.00
3	A	303	VAL	N-CA-C	8.21	119.98	110.62
3	A	134	HIS	CA-CB-CG	8.07	121.87	113.80
3	A	222	HIS	CA-CB-CG	-7.83	105.97	113.80
3	A	211	LEU	CA-C-N	7.78	131.04	120.54
3	A	211	LEU	C-N-CA	7.78	131.04	120.54
3	A	164	ASN	CA-CB-CG	-7.77	104.83	112.60
3	A	226	ASP	CA-CB-CG	7.50	120.10	112.60
3	A	256	ASP	CA-CB-CG	7.33	119.93	112.60
3	A	151	PRO	N-CA-CB	7.31	109.68	103.25
3	A	146	PHE	CA-CB-CG	-7.30	106.50	113.80
3	A	192	ASP	N-CA-C	7.25	120.75	107.99
3	A	277	ILE	N-CA-CB	7.23	122.64	110.56
3	A	229	SER	CA-C-N	-7.17	112.90	123.00
3	A	229	SER	C-N-CA	-7.17	112.90	123.00
3	A	233	THR	CA-CB-OG1	-7.17	98.85	109.60
3	A	318	ASP	CA-CB-CG	-7.10	105.50	112.60
3	A	67	THR	CA-CB-OG1	7.08	120.22	109.60
3	A	102	ARG	CD-NE-CZ	-7.02	114.57	124.40
3	A	63	PRO	N-CA-CB	7.02	107.93	103.23
3	A	56	GLY	O-C-N	6.91	128.81	122.18
3	A	17	ASP	CB-CA-C	6.85	122.16	110.79
3	A	228	LEU	N-CA-C	-6.80	102.25	112.04
3	A	70	ALA	N-CA-C	-6.80	103.80	111.07
3	A	181	PHE	CA-CB-CG	-6.75	107.05	113.80
3	A	229	SER	N-CA-C	6.68	119.28	108.32
3	A	99	PHE	N-CA-C	6.66	118.33	111.14
3	A	35	LYS	N-CA-C	-6.66	104.02	111.28
3	A	286	ALA	CA-C-N	6.61	129.68	120.29
3	A	286	ALA	C-N-CA	6.61	129.68	120.29
3	A	20	THR	N-CA-CB	6.58	119.90	110.16
3	A	150	ILE	N-CA-CB	6.55	120.39	111.21
3	A	236	MET	CA-C-N	-6.55	115.02	122.42
3	A	236	MET	C-N-CA	-6.55	115.02	122.42
3	A	176	THR	CA-C-N	-6.54	114.84	122.95
3	A	176	THR	C-N-CA	-6.54	114.84	122.95
3	A	229	SER	CA-C-O	6.51	128.08	120.14
3	A	292	THR	CB-CA-C	6.48	120.98	109.65
3	A	193	VAL	N-CA-C	6.47	117.15	107.51
3	A	39	TYR	CA-CB-CG	-6.42	102.35	113.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	76	PHE	CA-CB-CG	6.37	120.17	113.80
2	P	2	DC	C2-N1-C1'	6.37	129.25	119.70
3	A	30	SER	CA-C-N	-6.31	112.58	122.49
3	A	30	SER	C-N-CA	-6.31	112.58	122.49
3	A	18	MET	O-C-N	6.31	128.56	122.07
3	A	65	VAL	CA-C-N	-6.27	116.85	122.43
3	A	65	VAL	C-N-CA	-6.27	116.85	122.43
3	A	205	THR	N-CA-CB	6.25	121.06	110.49
3	A	333	ARG	N-CA-C	-6.22	105.56	113.02
3	A	224	ILE	CA-CB-CG1	-6.21	99.85	110.40
3	A	205	THR	N-CA-C	6.16	123.92	110.80
2	P	6	DT	C6-N1-C1'	-6.16	110.12	119.35
2	P	3	DT	C6-N1-C1'	-6.14	110.14	119.35
3	A	214	VAL	N-CA-C	6.12	116.90	110.72
3	A	40	ARG	N-CA-C	6.10	117.93	111.28
3	A	255	ILE	CA-C-O	-6.05	115.64	121.63
3	A	77	LEU	N-CA-CB	6.02	118.97	110.12
3	A	250	TYR	N-CA-C	5.99	118.17	110.39
3	A	157	GLN	CB-CA-C	5.98	120.72	110.79
3	A	40	ARG	N-CA-CB	5.91	118.81	110.12
3	A	12	ASN	CB-CA-C	5.89	121.03	109.72
3	A	14	GLY	N-CA-C	-5.87	105.54	112.64
3	A	153	GLU	N-CA-CB	5.78	119.28	110.14
3	A	271	TYR	N-CA-C	5.78	117.58	111.28
3	A	68	LYS	N-CA-C	5.78	117.25	111.07
3	A	92	ASP	CA-CB-CG	5.76	118.36	112.60
3	A	253	ARG	N-CA-C	5.75	118.33	109.07
3	A	214	VAL	N-CA-CB	5.75	119.20	110.58
3	A	46	ILE	N-CA-CB	5.74	120.47	110.65
3	A	105	GLY	CA-C-N	5.74	130.91	123.11
3	A	105	GLY	C-N-CA	5.74	130.91	123.11
3	A	229	SER	O-C-N	-5.69	116.94	123.42
3	A	98	ASN	CA-CB-CG	-5.64	106.96	112.60
3	A	215	VAL	O-C-N	5.64	127.34	121.87
3	A	15	ILE	N-CA-C	5.63	116.28	110.36
3	A	116	ASP	CB-CA-C	5.63	120.13	110.79
3	A	20	THR	CA-C-O	-5.62	114.46	120.42
3	A	20	THR	N-CA-C	-5.61	105.25	111.36
3	A	66	GLY	CA-C-N	5.60	127.72	120.44
3	A	66	GLY	C-N-CA	5.60	127.72	120.44
3	A	12	ASN	N-CA-CB	5.57	119.20	110.46
3	A	211	LEU	O-C-N	5.56	128.09	122.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	218	LEU	CA-C-N	5.55	127.98	120.44
3	A	218	LEU	C-N-CA	5.55	127.98	120.44
3	A	21	GLU	N-CA-C	-5.54	104.25	111.02
3	A	121	THR	N-CA-C	5.54	118.66	110.46
3	A	12	ASN	CA-C-N	5.53	132.25	121.41
3	A	12	ASN	C-N-CA	5.53	132.25	121.41
3	A	316	GLU	CA-C-N	5.52	127.94	120.65
3	A	316	GLU	C-N-CA	5.52	127.94	120.65
2	P	2	DC	C6-N1-C1'	-5.47	111.50	119.70
3	A	254	ARG	CA-C-N	-5.46	114.93	122.69
3	A	254	ARG	C-N-CA	-5.46	114.93	122.69
3	A	83	ARG	N-CA-CB	5.44	117.89	110.01
3	A	181	PHE	O-C-N	5.41	127.64	122.07
3	A	296	TYR	CA-C-N	-5.39	112.16	122.08
3	A	296	TYR	C-N-CA	-5.39	112.16	122.08
3	A	84	LYS	CA-C-O	5.39	126.45	120.63
3	A	112	ARG	N-CA-CB	5.39	117.83	110.01
3	A	91	ASP	N-CA-C	5.39	122.28	110.80
3	A	35	LYS	CA-C-O	5.37	126.24	120.55
3	A	162	VAL	N-CA-C	5.36	116.73	110.62
3	A	53	ILE	N-CA-CB	5.35	116.89	110.31
3	A	68	LYS	CB-CA-C	5.34	119.27	110.88
3	A	195	LEU	N-CA-C	5.34	118.10	109.40
3	A	129	GLU	CB-CG-CD	-5.33	103.54	112.60
3	A	12	ASN	N-CA-C	5.32	119.77	113.28
3	A	213	GLN	CB-CA-C	-5.32	102.30	110.81
3	A	133	ASN	CA-C-O	-5.30	115.20	121.66
3	A	278	PHE	CA-CB-CG	-5.29	108.51	113.80
3	A	62	LEU	CA-C-O	5.28	126.68	120.87
3	A	309	GLU	N-CA-C	5.25	121.41	109.81
3	A	145	ASP	O-C-N	-5.23	115.53	122.33
3	A	53	ILE	CB-CA-C	5.21	119.09	111.33
3	A	267	CYS	N-CA-CB	5.19	117.60	110.07
3	A	13	GLY	CA-C-N	5.18	125.85	119.99
3	A	13	GLY	C-N-CA	5.18	125.85	119.99
3	A	17	ASP	CA-CB-CG	-5.18	107.42	112.60
3	A	270	LEU	CA-C-N	5.16	127.19	120.28
3	A	270	LEU	C-N-CA	5.16	127.19	120.28
3	A	319	ILE	CB-CA-C	-5.14	105.20	112.14
3	A	232	GLU	CB-CG-CD	-5.13	103.87	112.60
3	A	15	ILE	N-CA-CB	5.13	116.20	110.51
3	A	181	PHE	CA-C-N	5.12	127.14	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	181	PHE	C-N-CA	5.12	127.14	120.28
3	A	212	HIS	CA-CB-CG	-5.12	108.68	113.80
3	A	74	ASP	N-CA-CB	5.10	117.35	109.91
3	A	107	GLY	N-CA-C	-5.09	101.96	112.34
3	A	77	LEU	O-C-N	5.07	127.50	122.12
2	P	3	DT	C2-N1-C1'	5.07	126.96	119.35
3	A	59	ALA	O-C-N	5.06	127.35	122.09
3	A	320	PHE	N-CA-CB	5.04	117.31	110.01
3	A	66	GLY	O-C-N	5.03	128.19	122.86
3	A	157	GLN	O-C-N	5.03	127.45	122.12
3	A	64	GLY	CA-C-N	-5.03	116.72	122.95
3	A	64	GLY	C-N-CA	-5.03	116.72	122.95
3	A	235	PHE	CA-CB-CG	-5.02	108.78	113.80
3	A	288	GLU	N-CA-C	-5.02	105.27	111.40
3	A	105	GLY	O-C-N	5.02	129.22	122.70
3	A	182	ARG	NE-CZ-NH1	5.01	126.51	121.50

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	12	ASN	CA
3	A	116	ASP	CA
3	A	168	LYS	CA
3	A	205	THR	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4	0
2	P	144	0	81	20	0
3	A	2623	0	2641	313	0
4	A	2	0	0	0	0
5	A	107	0	0	16	0
5	P	23	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	T	14	0	0	0	0
All	All	3058	0	2802	333	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 59.

All (333) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:5:DA:H2''	2:P:6:DT:H5''	1.23	1.11
2:P:6:DT:H2''	2:P:7:DG:H5''	1.26	1.10
3:A:270:LEU:HD21	3:A:282:MET:HE1	1.38	1.04
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.24	1.01
3:A:245:ASN:HD22	3:A:245:ASN:N	1.52	1.00
2:P:5:DA:H2''	2:P:6:DT:C5'	1.94	0.97
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.47	0.96
3:A:245:ASN:H	3:A:245:ASN:ND2	1.63	0.95
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.49	0.94
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.52	0.91
1:T:6:DG:H2''	1:T:7:DA:C8	2.06	0.91
3:A:155:MET:HA	3:A:158:MET:HE3	1.52	0.89
2:P:6:DT:C2'	2:P:7:DG:H5''	2.02	0.89
3:A:243:SER:HB3	3:A:249:GLU:HA	1.55	0.88
3:A:60:LYS:HA	3:A:65:VAL:HG12	1.57	0.86
3:A:201:THR:HA	3:A:261:PRO:HB3	1.57	0.86
3:A:15:ILE:HB	3:A:46:ILE:HD11	1.58	0.85
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.16	0.85
3:A:155:MET:HE2	3:A:188:SER:HB2	1.58	0.84
3:A:270:LEU:HD21	3:A:282:MET:CE	2.08	0.83
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.77	0.83
3:A:330:PRO:HA	3:A:333:ARG:CG	2.08	0.82
3:A:12:ASN:HD21	3:A:53:ILE:H	1.24	0.82
3:A:49:TYR:CE2	3:A:51:HIS:HB2	2.14	0.82
3:A:201:THR:HA	3:A:261:PRO:CB	2.10	0.80
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.28	0.80
3:A:29:VAL:HA	3:A:97:ILE:HD12	1.65	0.78
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.13	0.77
3:A:53:ILE:HG21	3:A:59:ALA:HB2	1.65	0.77
3:A:286:ALA:HB2	3:A:323:ILE:HG21	1.66	0.77
3:A:306:VAL:HG22	5:A:632:HOH:O	1.83	0.77
3:A:82:LEU:HD23	3:A:85:LEU:HB2	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:217:GLN:NE2	3:A:217:GLN:HA	2.00	0.76
3:A:11:LEU:HD23	3:A:11:LEU:H	1.51	0.76
3:A:229:SER:HB3	5:A:513:HOH:O	1.85	0.75
3:A:323:ILE:O	3:A:324:GLN:HG2	1.86	0.75
2:P:6:DT:H2''	2:P:7:DG:C5'	2.11	0.75
3:A:133:ASN:ND2	3:A:135:HIS:H	1.85	0.75
3:A:121:THR:HG23	3:A:124:ASP:OD1	1.87	0.75
3:A:282:MET:HB2	3:A:325:TRP:CZ3	2.24	0.72
3:A:330:PRO:HA	3:A:333:ARG:HG2	1.70	0.72
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.72	0.71
3:A:99:PHE:O	3:A:102:ARG:HG3	1.90	0.71
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.25	0.70
3:A:180:SER:HB3	3:A:183:ARG:NH2	2.08	0.69
3:A:18:MET:HE2	3:A:82:LEU:HD22	1.75	0.69
3:A:180:SER:HB2	3:A:185:ALA:HB2	1.72	0.69
3:A:121:THR:HG23	3:A:124:ASP:CG	2.18	0.69
3:A:217:GLN:HA	3:A:217:GLN:HE21	1.57	0.68
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.20	0.68
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.23	0.68
3:A:76:PHE:HD1	3:A:77:LEU:HD12	1.58	0.68
3:A:254:ARG:HB3	3:A:254:ARG:NH1	2.08	0.68
3:A:294:ASN:O	3:A:296:TYR:N	2.27	0.68
3:A:207:GLN:HB3	3:A:210:LEU:HG	1.74	0.68
3:A:60:LYS:HA	3:A:65:VAL:CG1	2.23	0.68
3:A:41:LYS:HE2	3:A:64:GLY:HA3	1.75	0.68
3:A:125:LEU:HD22	3:A:132:LEU:HD21	1.76	0.68
3:A:141:LYS:HE2	3:A:142:TYR:CZ	2.29	0.67
3:A:41:LYS:O	3:A:45:VAL:HG13	1.95	0.67
3:A:59:ALA:O	3:A:62:LEU:HB2	1.94	0.67
3:A:174:ILE:O	3:A:195:LEU:HD12	1.94	0.67
3:A:201:THR:CA	3:A:261:PRO:HB3	2.25	0.67
3:A:204:SER:O	3:A:206:LYS:N	2.27	0.67
3:A:23:ALA:HB2	3:A:39:TYR:HB2	1.77	0.67
3:A:282:MET:HE3	5:A:550:HOH:O	1.95	0.67
3:A:331:LYS:HG2	3:A:332:ASP:N	2.03	0.67
3:A:18:MET:CE	3:A:82:LEU:HD13	2.25	0.66
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.77	0.66
3:A:245:ASN:HD22	3:A:245:ASN:H	0.78	0.66
3:A:58:GLU:O	3:A:61:LYS:HG3	1.96	0.66
3:A:127:LYS:HB2	3:A:128:ASN:ND2	2.10	0.66
2:P:5:DA:C2'	2:P:6:DT:H5''	2.12	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:327:TYR:HD1	3:A:328:ARG:N	1.94	0.65
3:A:298:ILE:N	5:A:569:HOH:O	2.29	0.65
3:A:11:LEU:HA	3:A:52:LYS:HZ1	1.62	0.65
3:A:182:ARG:HG2	3:A:182:ARG:NH1	1.98	0.65
3:A:255:ILE:HG12	3:A:256:ASP:N	2.10	0.65
3:A:157:GLN:HE22	3:A:244:LYS:NZ	1.95	0.65
3:A:295:GLU:N	3:A:295:GLU:OE1	2.29	0.64
3:A:211:LEU:HD12	3:A:211:LEU:O	1.98	0.64
3:A:73:ILE:O	3:A:77:LEU:HD13	1.98	0.63
3:A:270:LEU:HD22	3:A:319:ILE:HD13	1.79	0.63
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.14	0.63
3:A:276:ASP:O	3:A:280:LYS:HG3	1.99	0.62
3:A:180:SER:HB3	3:A:183:ARG:HH21	1.64	0.62
3:A:323:ILE:C	3:A:324:GLN:HG2	2.23	0.62
3:A:209:LYS:HA	3:A:212:HIS:HB2	1.80	0.62
3:A:18:MET:HE2	3:A:82:LEU:HD13	1.82	0.62
3:A:277:ILE:CG1	3:A:335:GLU:HB2	2.29	0.62
3:A:111:ALA:O	3:A:115:VAL:HG23	1.99	0.62
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.82	0.62
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.81	0.62
3:A:26:GLU:HA	3:A:30:SER:OG	2.00	0.61
3:A:92:ASP:HB3	5:A:629:HOH:O	2.00	0.61
3:A:253:ARG:NH1	5:A:503:HOH:O	2.34	0.61
3:A:289:LYS:HD3	3:A:289:LYS:N	2.08	0.61
3:A:254:ARG:HB3	3:A:254:ARG:CZ	2.31	0.61
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.16	0.61
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.48	0.61
3:A:188:SER:HB3	5:A:522:HOH:O	2.01	0.61
3:A:254:ARG:NH2	5:A:639:HOH:O	2.33	0.60
3:A:248:LYS:O	3:A:248:LYS:HG2	2.01	0.60
3:A:245:ASN:N	3:A:245:ASN:ND2	2.28	0.60
3:A:123:GLU:O	3:A:127:LYS:HG2	2.02	0.60
3:A:259:LEU:O	3:A:260:ILE:HD13	2.02	0.60
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.34	0.60
3:A:236:MET:HG3	3:A:256:ASP:OD1	2.01	0.60
3:A:180:SER:HB2	3:A:185:ALA:CB	2.32	0.60
2:P:6:DT:H2'	2:P:7:DG:C8	2.37	0.59
3:A:114:PHE:CZ	3:A:132:LEU:HD23	2.37	0.59
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.31	0.59
1:T:1:DC:H2''	1:T:2:DA:OP2	2.01	0.59
3:A:286:ALA:O	3:A:291:PHE:N	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:326:LYS:HG3	3:A:326:LYS:O	2.02	0.59
3:A:292:THR:O	3:A:298:ILE:HA	2.02	0.59
3:A:11:LEU:H	3:A:11:LEU:CD2	2.15	0.59
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.37	0.59
2:P:6:DT:H6	2:P:6:DT:H5'	1.69	0.58
3:A:277:ILE:HD11	3:A:335:GLU:HB3	1.86	0.58
3:A:31:GLN:N	5:A:623:HOH:O	2.26	0.57
3:A:180:SER:CA	3:A:183:ARG:HH21	2.18	0.57
3:A:299:ARG:CD	3:A:310:PRO:HD3	2.33	0.57
3:A:33:ILE:HG23	3:A:34:HIS:H	1.69	0.57
3:A:326:LYS:O	3:A:328:ARG:HG2	2.04	0.57
3:A:11:LEU:HD23	3:A:11:LEU:N	2.14	0.56
3:A:169:VAL:HG13	3:A:170:ASP:H	1.71	0.56
3:A:262:LYS:O	3:A:262:LYS:HG3	2.02	0.56
3:A:277:ILE:HG13	3:A:335:GLU:HB2	1.87	0.56
3:A:102:ARG:NE	3:A:147:GLU:OE2	2.38	0.56
3:A:133:ASN:O	3:A:137:ARG:HG3	2.06	0.56
3:A:201:THR:HA	3:A:261:PRO:CA	2.35	0.56
3:A:299:ARG:HG2	3:A:310:PRO:HD3	1.88	0.56
3:A:157:GLN:HE22	3:A:244:LYS:HZ1	1.53	0.56
3:A:180:SER:CB	3:A:183:ARG:HH21	2.19	0.56
3:A:159:GLN:O	3:A:163:LEU:HG	2.05	0.56
3:A:243:SER:CB	3:A:249:GLU:HA	2.34	0.56
3:A:282:MET:HB2	3:A:325:TRP:HZ3	1.71	0.55
3:A:288:GLU:C	3:A:290:GLY:H	2.15	0.55
3:A:182:ARG:HH11	3:A:273:THR:CG2	2.20	0.55
3:A:182:ARG:HH11	3:A:273:THR:HG21	1.70	0.54
3:A:180:SER:HA	3:A:183:ARG:HE	1.72	0.54
3:A:253:ARG:HH11	3:A:253:ARG:CG	2.20	0.54
3:A:298:ILE:HA	5:A:581:HOH:O	2.07	0.54
3:A:207:GLN:OE1	3:A:210:LEU:HD21	2.07	0.54
3:A:295:GLU:HA	5:A:580:HOH:O	2.07	0.54
3:A:328:ARG:O	3:A:333:ARG:NE	2.29	0.54
3:A:309:GLU:N	3:A:309:GLU:OE1	2.41	0.54
3:A:29:VAL:HG21	3:A:94:SER:OG	2.08	0.54
3:A:124:ASP:O	3:A:128:ASN:ND2	2.42	0.54
3:A:182:ARG:O	3:A:182:ARG:HG3	2.08	0.54
3:A:330:PRO:CA	3:A:333:ARG:HG2	2.37	0.53
3:A:15:ILE:O	3:A:19:LEU:HB2	2.08	0.53
3:A:278:PHE:HB2	3:A:333:ARG:O	2.08	0.53
3:A:27:LYS:HB2	3:A:36:TYR:CD1	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:207:GLN:HB3	3:A:210:LEU:CG	2.39	0.53
3:A:303:VAL:O	3:A:305:GLY:N	2.42	0.53
3:A:197:HIS:CE1	3:A:199:SER:HB3	2.44	0.53
3:A:207:GLN:HB3	3:A:210:LEU:CD1	2.39	0.53
3:A:240:GLN:NE2	3:A:252:HIS:CE1	2.77	0.53
3:A:128:ASN:ND2	3:A:128:ASN:N	2.56	0.52
3:A:19:LEU:HD23	3:A:43:ALA:HA	1.92	0.52
3:A:207:GLN:O	3:A:210:LEU:N	2.39	0.52
3:A:149:ARG:NH2	3:A:187:SER:O	2.43	0.52
3:A:169:VAL:HG13	3:A:170:ASP:N	2.23	0.52
3:A:128:ASN:N	3:A:128:ASN:HD22	2.07	0.52
3:A:15:ILE:HB	3:A:46:ILE:CD1	2.37	0.52
3:A:271:TYR:CD1	3:A:283:ARG:NH2	2.78	0.52
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.45	0.52
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.92	0.52
3:A:15:ILE:CB	3:A:46:ILE:HD11	2.37	0.51
3:A:140:LEU:HD12	3:A:140:LEU:O	2.10	0.51
3:A:292:THR:C	3:A:293:ILE:HD13	2.35	0.51
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.91	0.51
2:P:1:DT:H2'	2:P:2:DC:C6	2.45	0.51
3:A:41:LYS:HD3	3:A:42:ALA:H	1.76	0.51
3:A:271:TYR:CE1	3:A:283:ARG:NH2	2.78	0.51
3:A:103:VAL:CB	3:A:106:ILE:HD12	2.41	0.51
3:A:232:GLU:O	3:A:233:THR:HG23	2.11	0.51
3:A:138:ILE:HD12	3:A:228:LEU:CD1	2.40	0.51
3:A:18:MET:O	3:A:21:GLU:HB2	2.10	0.51
3:A:198:PRO:C	3:A:200:PHE:H	2.19	0.51
3:A:142:TYR:CE1	3:A:252:HIS:CG	3.00	0.50
3:A:253:ARG:HH11	3:A:253:ARG:HG3	1.76	0.50
3:A:152:ARG:HA	3:A:155:MET:HB2	1.93	0.50
3:A:319:ILE:O	3:A:322:TYR:HB2	2.12	0.50
1:T:7:DA:H61	2:P:1:DT:H3	1.60	0.50
2:P:6:DT:C5'	2:P:6:DT:H6	2.25	0.50
3:A:19:LEU:HB3	3:A:43:ALA:HB2	1.94	0.49
3:A:202:SER:N	3:A:261:PRO:HB3	2.26	0.49
3:A:140:LEU:HD12	3:A:140:LEU:C	2.37	0.49
3:A:284:ALA:O	3:A:287:LEU:HB2	2.13	0.49
3:A:33:ILE:HG23	3:A:34:HIS:N	2.27	0.49
3:A:133:ASN:HD22	3:A:134:HIS:N	2.10	0.49
3:A:150:ILE:N	3:A:188:SER:O	2.40	0.49
3:A:201:THR:C	3:A:261:PRO:HB3	2.38	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.41	0.49
3:A:146:PHE:HZ	3:A:238:VAL:HG22	1.79	0.48
1:T:4:DT:OP1	3:A:231:GLY:HA3	2.12	0.48
3:A:292:THR:O	3:A:298:ILE:HG13	2.14	0.48
3:A:31:GLN:HE21	3:A:112:ARG:NH1	2.06	0.48
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.96	0.48
3:A:264:GLN:NE2	3:A:296:TYR:HB3	2.29	0.48
3:A:183:ARG:HD3	3:A:273:THR:O	2.14	0.47
3:A:243:SER:OG	3:A:249:GLU:HG3	2.14	0.47
3:A:271:TYR:HB2	5:A:580:HOH:O	2.14	0.47
3:A:81:LYS:NZ	3:A:86:GLU:CB	2.77	0.47
3:A:191:MET:O	3:A:191:MET:HG3	2.10	0.47
2:P:6:DT:H5'	5:P:561:HOH:O	2.14	0.47
3:A:149:ARG:HH21	3:A:187:SER:C	2.22	0.47
3:A:83:ARG:O	3:A:86:GLU:N	2.47	0.47
2:P:5:DA:H2'	2:P:6:DT:H71	1.97	0.47
3:A:56:GLY:O	3:A:59:ALA:HB3	2.14	0.47
3:A:179:GLY:O	3:A:182:ARG:HB3	2.15	0.47
3:A:197:HIS:ND1	3:A:199:SER:HB3	2.30	0.47
3:A:265:TYR:O	3:A:268:GLY:N	2.47	0.47
3:A:155:MET:HE2	3:A:188:SER:CB	2.38	0.47
3:A:317:LYS:O	3:A:320:PHE:N	2.48	0.47
3:A:138:ILE:HD12	3:A:228:LEU:HD12	1.96	0.46
3:A:162:VAL:O	3:A:166:VAL:HG23	2.16	0.46
3:A:12:ASN:ND2	3:A:53:ILE:H	2.04	0.46
3:A:114:PHE:CZ	3:A:132:LEU:CD2	2.98	0.46
3:A:183:ARG:NH2	5:A:615:HOH:O	2.49	0.46
3:A:194:LEU:HD21	3:A:272:PHE:HD2	1.80	0.46
2:P:5:DA:P	3:A:109:SER:HB3	2.56	0.46
3:A:38:ALA:O	3:A:41:LYS:HD3	2.16	0.46
3:A:207:GLN:HB2	5:A:610:HOH:O	2.16	0.46
3:A:230:LYS:HB3	3:A:230:LYS:HE2	1.75	0.46
3:A:299:ARG:CG	3:A:310:PRO:HD3	2.45	0.46
2:P:1:DT:C2'	2:P:2:DC:C6	2.99	0.46
2:P:6:DT:C4	2:P:7:DG:C6	3.04	0.46
3:A:81:LYS:NZ	3:A:86:GLU:HB2	2.31	0.46
3:A:211:LEU:HD23	3:A:231:GLY:O	2.16	0.46
3:A:125:LEU:CD2	3:A:132:LEU:HD21	2.45	0.45
3:A:303:VAL:C	3:A:305:GLY:H	2.23	0.45
3:A:200:PHE:C	3:A:201:THR:HG22	2.41	0.45
3:A:241:LEU:HB2	3:A:250:TYR:CD2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:85:LEU:HD12	3:A:85:LEU:HA	1.54	0.45
3:A:182:ARG:HG2	3:A:273:THR:CG2	2.47	0.45
3:A:254:ARG:NH1	3:A:255:ILE:O	2.45	0.45
3:A:329:GLU:O	3:A:333:ARG:HG2	2.17	0.45
3:A:89:ARG:HD3	3:A:89:ARG:C	2.42	0.45
3:A:259:LEU:HD12	3:A:259:LEU:HA	1.39	0.45
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.51	0.45
3:A:21:GLU:OE1	3:A:85:LEU:HG	2.17	0.45
3:A:62:LEU:HD12	3:A:62:LEU:HA	1.78	0.45
3:A:165:GLU:HB3	3:A:217:GLN:CG	2.36	0.45
3:A:174:ILE:HB	3:A:196:THR:HG22	1.98	0.45
3:A:182:ARG:NH1	3:A:273:THR:CG2	2.78	0.45
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.98	0.45
3:A:299:ARG:HG2	3:A:310:PRO:CD	2.47	0.45
3:A:194:LEU:N	3:A:194:LEU:CD1	2.79	0.45
3:A:11:LEU:CD2	3:A:11:LEU:N	2.78	0.45
3:A:101:THR:HA	3:A:106:ILE:HG22	1.99	0.45
3:A:194:LEU:N	3:A:194:LEU:HD12	2.32	0.45
3:A:22:LEU:HD21	3:A:82:LEU:HD21	1.99	0.44
3:A:150:ILE:HG21	3:A:158:MET:CE	2.44	0.44
2:P:1:DT:H2''	2:P:2:DC:C5'	2.47	0.44
3:A:260:ILE:HG22	3:A:261:PRO:N	2.32	0.44
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.82	0.44
3:A:82:LEU:HD23	3:A:85:LEU:HD22	1.99	0.44
3:A:62:LEU:HD12	3:A:63:PRO:HD2	1.99	0.44
3:A:126:ARG:C	3:A:128:ASN:N	2.74	0.44
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.47	0.44
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.82	0.44
3:A:150:ILE:HG12	3:A:253:ARG:HG2	2.00	0.44
3:A:22:LEU:HD13	3:A:22:LEU:HA	1.72	0.43
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.53	0.43
3:A:212:HIS:N	3:A:212:HIS:CD2	2.84	0.43
3:A:155:MET:SD	3:A:158:MET:CE	3.07	0.43
3:A:172:GLU:HB3	3:A:197:HIS:NE2	2.34	0.43
3:A:287:LEU:HD13	3:A:287:LEU:HA	1.44	0.43
2:P:1:DT:H2'	2:P:2:DC:C5	2.53	0.43
3:A:34:HIS:O	3:A:38:ALA:N	2.43	0.43
3:A:82:LEU:CD2	3:A:85:LEU:HD22	2.49	0.43
3:A:306:VAL:HG23	3:A:307:ALA:N	2.31	0.43
3:A:155:MET:CA	3:A:158:MET:HE3	2.37	0.43
3:A:26:GLU:HB3	3:A:32:ALA:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.34	0.42
3:A:102:ARG:HH11	3:A:102:ARG:HD3	1.59	0.42
3:A:303:VAL:C	3:A:305:GLY:N	2.77	0.42
3:A:28:ASN:HD22	3:A:28:ASN:HA	1.41	0.42
3:A:255:ILE:CG1	3:A:256:ASP:N	2.81	0.42
3:A:200:PHE:O	3:A:262:LYS:N	2.43	0.42
3:A:288:GLU:O	3:A:290:GLY:N	2.53	0.42
3:A:274:GLY:O	3:A:278:PHE:HD2	2.02	0.42
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.54	0.42
3:A:16:THR:HG21	3:A:47:ALA:HB2	2.00	0.42
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.23	0.42
3:A:163:LEU:N	3:A:163:LEU:HD23	2.34	0.42
3:A:33:ILE:O	3:A:36:TYR:HB3	2.19	0.42
3:A:60:LYS:C	3:A:62:LEU:N	2.77	0.42
3:A:270:LEU:HA	3:A:316:GLU:OE2	2.20	0.42
3:A:273:THR:O	3:A:273:THR:HG22	2.19	0.42
3:A:293:ILE:HA	5:A:581:HOH:O	2.18	0.42
2:P:5:DA:OP2	3:A:109:SER:HB3	2.20	0.41
3:A:108:PRO:O	3:A:112:ARG:HG3	2.20	0.41
3:A:165:GLU:HA	3:A:168:LYS:CG	2.37	0.41
3:A:76:PHE:O	3:A:79:THR:O	2.38	0.41
3:A:77:LEU:N	3:A:77:LEU:CD1	2.83	0.41
3:A:134:HIS:O	3:A:138:ILE:HG13	2.20	0.41
3:A:277:ILE:HD11	3:A:335:GLU:CB	2.49	0.41
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.47	0.41
3:A:100:LEU:O	3:A:103:VAL:HB	2.20	0.41
3:A:250:TYR:HB3	5:A:568:HOH:O	2.20	0.41
3:A:19:LEU:HD11	3:A:69:ILE:HG23	2.02	0.41
3:A:81:LYS:NZ	3:A:86:GLU:HB3	2.35	0.41
3:A:133:ASN:C	3:A:137:ARG:HG3	2.44	0.41
3:A:211:LEU:HD12	3:A:211:LEU:C	2.42	0.41
3:A:286:ALA:O	3:A:291:PHE:HB2	2.20	0.41
3:A:49:TYR:CZ	3:A:51:HIS:HB2	2.55	0.41
3:A:194:LEU:CD1	3:A:258:ARG:HD3	2.51	0.41
3:A:327:TYR:C	3:A:327:TYR:CD1	2.99	0.41
2:P:4:DA:H5'	5:P:563:HOH:O	2.21	0.41
3:A:69:ILE:O	3:A:73:ILE:HG13	2.21	0.41
3:A:289:LYS:HD3	3:A:289:LYS:HA	1.49	0.41
3:A:32:ALA:HB1	3:A:35:LYS:HB2	2.03	0.41
3:A:145:ASP:OD1	3:A:145:ASP:N	2.54	0.41
3:A:198:PRO:C	3:A:200:PHE:N	2.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:203:GLU:O	3:A:205:THR:N	2.54	0.41
3:A:301:LEU:HA	3:A:301:LEU:HD12	1.52	0.41
3:A:179:GLY:C	3:A:181:PHE:N	2.78	0.41
3:A:254:ARG:NH1	3:A:255:ILE:N	2.69	0.41
3:A:260:ILE:HG23	3:A:260:ILE:HD12	1.68	0.41
3:A:279:ASN:HD22	3:A:279:ASN:HA	1.59	0.40
3:A:196:THR:OG1	3:A:262:LYS:HA	2.22	0.40
3:A:282:MET:HA	3:A:325:TRP:CH2	2.57	0.40
3:A:316:GLU:O	3:A:320:PHE:HD2	2.04	0.40
3:A:18:MET:CE	3:A:76:PHE:HB2	2.51	0.40
3:A:121:THR:H	3:A:124:ASP:CG	2.30	0.40
3:A:155:MET:SD	3:A:158:MET:HE1	2.62	0.40
3:A:250:TYR:HA	3:A:251:PRO:HD3	1.90	0.40
3:A:253:ARG:NH1	3:A:253:ARG:CG	2.83	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%)	276 (85%)	32 (10%)	17 (5%)	1 9

All (17) Ramachandran outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	304	THR
3	A	13	GLY
3	A	32	ALA
3	A	289	LYS
3	A	91	ASP
3	A	266	TYR
3	A	207	GLN
3	A	298	ILE
3	A	309	GLU
3	A	310	PRO

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%)	219 (76%)	69 (24%)	1 4

All (69) 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	30	SER
3	A	33	ILE
3	A	37	ASN
3	A	41	LYS
3	A	44	SER
3	A	45	VAL
3	A	46	ILE
3	A	52	LYS
3	A	62	LEU
3	A	67	THR
3	A	68	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	77	LEU
3	A	79	THR
3	A	81	LYS
3	A	89	ARG
3	A	92	ASP
3	A	100	LEU
3	A	101	THR
3	A	102	ARG
3	A	113	LYS
3	A	119	ILE
3	A	121	THR
3	A	122	LEU
3	A	128	ASN
3	A	133	ASN
3	A	138	ILE
3	A	140	LEU
3	A	145	ASP
3	A	153	GLU
3	A	155	MET
3	A	182	ARG
3	A	188	SER
3	A	191	MET
3	A	193	VAL
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	230	LYS
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	263	ASP
3	A	264	GLN
3	A	272	PHE
3	A	277	ILE
3	A	287	LEU
3	A	289	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	294	ASN
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	331	LYS
3	A	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	28	ASN
3	A	31	GLN
3	A	37	ASN
3	A	128	ASN
3	A	133	ASN
3	A	134	HIS
3	A	136	GLN
3	A	157	GLN
3	A	213	GLN
3	A	217	GLN
3	A	240	GLN
3	A	245	ASN
3	A	252	HIS
3	A	264	GLN
3	A	279	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%)	-0.21	0 100 100	16, 34, 84, 100	0
2	P	7/7 (100%)	-0.78	0 100 100	9, 23, 32, 48	0
3	A	325/335 (97%)	-0.73	0 100 100	5, 31, 83, 100	0
All	All	340/350 (97%)	-0.72	0 100 100	5, 31, 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	BA	A	341	1/1	0.99	0.03	59,59,59,59	0
4	BA	A	342	1/1	0.99	0.03	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.