



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:01 PM UTC

PDB ID : 8ICG / pdb_00008icg
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SEVEN BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF DATP (1 MILLIMOLAR) AND MGCL2 (5 MILLIMOLAR)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-04-19
Resolution : 3.30 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

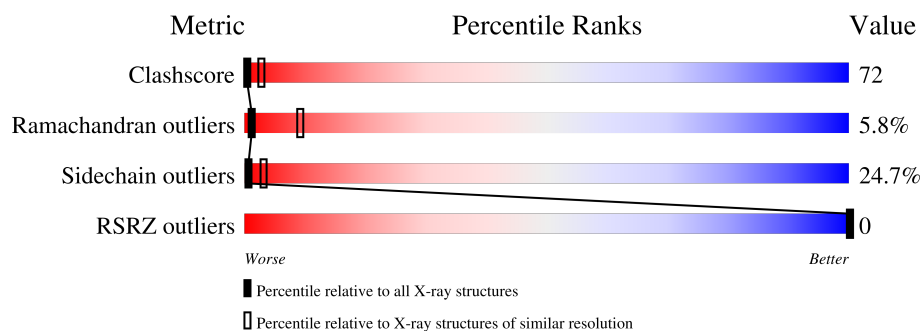
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 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	14	Total	O	0	0
			14	14		
5	P	17	Total	O	0	0
			17	17		
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.

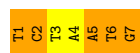
- Molecule 1: DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3')

Chain T: 



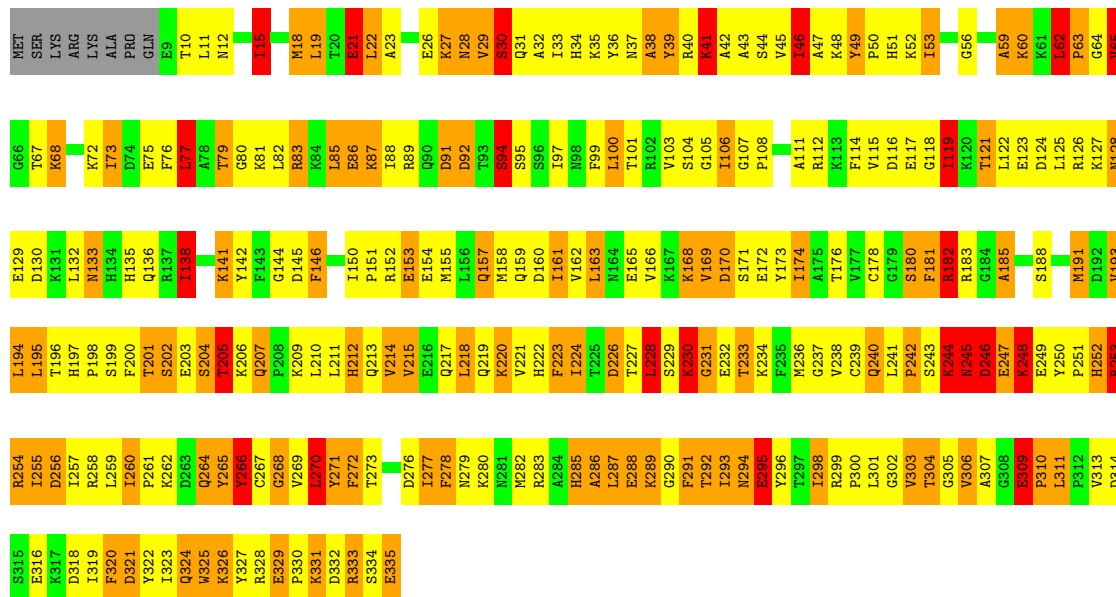
- Molecule 2: DNA (5'-D(*TP*CP*TP*AP*AP*TP*G)-3')

Chain P: 



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

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.80Å 57.73Å 48.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 20.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	93.0 (20.00-3.30) 92.1 (20.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.78Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.141 , (Not available) 0.137 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 352.1	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	0.94	EDS
Total number of atoms	3052	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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	0.97	0/162	3.80	13/249 (5.2%)
2	P	1.15	1/160 (0.6%)	3.02	17/243 (7.0%)
3	A	1.75	35/2672 (1.3%)	2.14	109/3590 (3.0%)
All	All	1.69	36/2994 (1.2%)	2.33	139/4082 (3.4%)

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 (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	247	GLU	C-N	38.72	1.86	1.34
3	A	244	LYS	C-N	9.56	1.47	1.33
3	A	270	LEU	C-N	-6.99	1.25	1.33
3	A	63	PRO	N-CA	-6.66	1.39	1.47
3	A	119	ILE	C-N	-6.64	1.25	1.33
3	A	30	SER	C-N	-6.63	1.25	1.33
3	A	270	LEU	CA-C	-6.38	1.45	1.52
2	P	1	DT	OP3-P	6.34	1.61	1.48
3	A	116	ASP	CA-C	-6.03	1.45	1.52
3	A	220	LYS	CA-C	-5.98	1.44	1.52
3	A	215	VAL	N-CA	-5.96	1.39	1.46
3	A	15	ILE	CA-C	-5.82	1.45	1.52
3	A	72	LYS	C-O	-5.78	1.16	1.24
3	A	182	ARG	NE-CZ	5.70	1.39	1.33
3	A	62	LEU	C-N	-5.69	1.28	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	138	ILE	CA-CB	-5.62	1.46	1.54
3	A	94	SER	N-CA	-5.61	1.39	1.46
3	A	144	GLY	CA-C	5.57	1.58	1.52
3	A	176	THR	CA-C	-5.51	1.45	1.52
3	A	170	ASP	CG-OD2	5.47	1.35	1.25
3	A	65	VAL	C-N	-5.41	1.27	1.33
3	A	224	ILE	CA-CB	-5.35	1.47	1.54
3	A	229	SER	C-N	-5.35	1.26	1.33
3	A	321	ASP	CG-OD2	5.34	1.35	1.25
3	A	125	LEU	C-O	-5.33	1.18	1.24
3	A	326	LYS	CE-NZ	-5.27	1.33	1.49
3	A	269	VAL	N-CA	-5.26	1.39	1.46
3	A	106	ILE	CA-C	-5.26	1.46	1.52
3	A	129	GLU	CD-OE1	5.22	1.35	1.25
3	A	252	HIS	CA-C	-5.14	1.46	1.52
3	A	242	PRO	N-CA	-5.09	1.40	1.47
3	A	254	ARG	C-N	-5.09	1.27	1.33
3	A	116	ASP	N-CA	-5.05	1.40	1.46
3	A	230	LYS	N-CA	-5.04	1.40	1.46
3	A	163	LEU	CA-C	-5.02	1.46	1.52
3	A	29	VAL	CA-CB	-5.00	1.48	1.54

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	7	DA	C4-N9-C1'	-31.84	79.29	127.05
1	T	7	DA	C8-N9-C1'	30.67	173.06	127.05
2	P	6	DT	C2-N1-C1'	20.75	150.48	119.35
2	P	6	DT	C6-N1-C1'	-20.61	88.43	119.35
1	T	4	DT	C6-N1-C1'	-19.37	90.29	119.35
1	T	4	DT	C2-N1-C1'	18.46	147.04	119.35
2	P	1	DT	C6-N1-C1'	-11.72	101.77	119.35
3	A	247	GLU	O-C-N	-11.44	107.38	122.59
2	P	2	DC	C2-N1-C1'	11.24	136.57	119.70
2	P	1	DT	C2-N1-C1'	10.95	135.78	119.35
3	A	49	TYR	CA-C-N	10.41	132.85	119.84
3	A	49	TYR	C-N-CA	10.41	132.85	119.84
3	A	320	PHE	CA-CB-CG	-10.05	103.75	113.80
2	P	2	DC	C6-N1-C1'	-9.15	105.97	119.70
2	P	7	DG	C4-N9-C1'	-9.10	113.34	127.00
3	A	272	PHE	CA-CB-CG	-9.08	104.72	113.80
3	A	244	LYS	O-C-N	-9.00	110.62	122.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	7	DG	C8-N9-C1'	8.86	140.29	127.00
3	A	157	GLN	N-CA-CB	8.63	122.58	110.07
3	A	88	ILE	CB-CA-C	-8.50	100.66	112.14
3	A	168	LYS	N-CA-CB	8.22	121.92	110.01
3	A	318	ASP	CA-CB-CG	-7.99	104.61	112.60
3	A	181	PHE	CA-C-N	7.93	132.36	120.31
3	A	181	PHE	C-N-CA	7.93	132.36	120.31
3	A	15	ILE	N-CA-CB	7.90	119.79	110.55
3	A	28	ASN	CA-CB-CG	-7.85	104.75	112.60
3	A	286	ALA	CA-C-N	7.80	130.73	120.28
3	A	286	ALA	C-N-CA	7.80	130.73	120.28
3	A	285	HIS	CA-CB-CG	-7.79	106.01	113.80
3	A	181	PHE	CA-CB-CG	-7.70	106.10	113.80
3	A	30	SER	CA-C-N	-7.70	112.57	123.20
3	A	30	SER	C-N-CA	-7.70	112.57	123.20
1	T	1	DC	P-O3'-C3'	7.61	131.61	120.20
3	A	291	PHE	N-CA-C	7.50	119.09	108.74
3	A	271	TYR	N-CA-C	7.50	120.10	111.11
3	A	52	LYS	CA-C-N	-7.40	110.92	120.98
3	A	52	LYS	C-N-CA	-7.40	110.92	120.98
3	A	68	LYS	N-CA-CB	7.37	120.67	109.91
1	T	6	DG	C4-N9-C1'	-7.31	116.04	127.00
3	A	266	TYR	CA-CB-CG	-7.26	100.83	113.90
2	P	3	DT	C2-N1-C1'	7.17	130.11	119.35
3	A	195	LEU	N-CA-C	6.97	120.88	109.72
2	P	5	DA	C4-N9-C1'	6.95	137.47	127.05
3	A	83	ARG	N-CA-CB	6.90	120.35	110.13
3	A	264	GLN	CB-CA-C	6.84	122.53	110.35
3	A	116	ASP	CB-CA-C	6.77	122.02	110.79
1	T	6	DG	C8-N9-C1'	6.71	137.06	127.00
3	A	309	GLU	CA-C-N	6.66	128.17	119.84
3	A	309	GLU	C-N-CA	6.66	128.17	119.84
3	A	240	GLN	N-CA-C	6.62	119.27	108.55
3	A	39	TYR	CA-CB-CG	-6.61	102.00	113.90
3	A	271	TYR	CA-CB-CG	-6.59	102.04	113.90
3	A	334	SER	N-CA-C	6.57	120.16	111.75
3	A	49	TYR	O-C-N	6.57	128.88	121.32
3	A	260	ILE	O-C-N	6.55	125.82	121.69
3	A	311	LEU	CA-C-N	6.53	127.55	119.98
3	A	311	LEU	C-N-CA	6.53	127.55	119.98
3	A	40	ARG	N-CA-CB	6.50	119.89	110.20
2	P	3	DT	C6-N1-C1'	-6.47	109.64	119.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	253	ARG	N-CA-C	6.42	120.00	109.72
2	P	5	DA	C8-N9-C1'	-6.36	117.51	127.05
3	A	87	LYS	CA-C-N	6.32	129.12	120.46
3	A	87	LYS	C-N-CA	6.32	129.12	120.46
3	A	288	GLU	N-CA-C	-6.31	103.70	111.40
3	A	65	VAL	CA-C-N	-6.30	116.82	122.43
3	A	65	VAL	C-N-CA	-6.30	116.82	122.43
3	A	38	ALA	CA-C-N	6.25	128.94	120.38
3	A	38	ALA	C-N-CA	6.25	128.94	120.38
1	T	4	DT	C1'-O4'-C4'	-6.24	100.34	109.70
3	A	224	ILE	CA-CB-CG1	-6.24	99.80	110.40
3	A	291	PHE	CA-CB-CG	-6.17	107.63	113.80
3	A	15	ILE	O-C-N	6.16	127.95	121.91
3	A	41	LYS	N-CA-CB	6.15	118.98	110.07
3	A	333	ARG	N-CA-C	-6.13	104.97	112.88
3	A	292	THR	CB-CA-C	6.12	120.20	109.80
3	A	214	VAL	CB-CA-C	-5.99	103.95	112.22
3	A	34	HIS	CA-CB-CG	-5.95	107.85	113.80
3	A	28	ASN	N-CA-C	5.95	120.26	111.04
3	A	68	LYS	O-C-N	5.92	128.19	122.03
3	A	313	VAL	N-CA-C	5.91	116.98	108.48
3	A	320	PHE	O-C-N	5.90	128.39	122.08
3	A	129	GLU	CB-CG-CD	-5.89	102.58	112.60
3	A	68	LYS	N-CA-C	5.89	117.39	110.97
3	A	309	GLU	N-CA-C	5.88	122.81	109.81
3	A	193	VAL	N-CA-C	5.88	115.81	106.88
2	P	4	DA	C4-N9-C1'	-5.87	118.25	127.05
3	A	233	THR	O-C-N	5.84	127.86	121.85
3	A	53	ILE	N-CA-CB	5.83	117.49	110.31
3	A	77	LEU	N-CA-CB	5.82	118.51	110.07
3	A	86	GLU	N-CA-CB	5.78	118.61	110.12
3	A	27	LYS	N-CA-CB	-5.77	101.64	110.01
2	P	1	DT	P-O5'-C5'	-5.75	111.38	120.00
3	A	68	LYS	CB-CA-C	5.74	119.80	110.96
3	A	185	ALA	N-CA-C	5.74	118.65	110.10
3	A	157	GLN	CB-CA-C	5.73	119.95	110.90
3	A	32	ALA	N-CA-C	5.71	116.58	108.54
1	T	5	DA	O3'-P-O5'	-5.70	95.45	104.00
3	A	214	VAL	N-CA-C	5.70	116.47	110.72
3	A	117	GLU	N-CA-C	-5.69	105.59	112.54
1	T	3	DT	C6-N1-C1'	5.69	127.89	119.35
3	A	229	SER	CA-C-O	5.69	127.15	120.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	276	ASP	N-CA-CB	5.69	118.60	110.06
3	A	92	ASP	N-CA-CB	5.60	118.09	109.91
3	A	219	GLN	O-C-N	5.58	129.49	122.23
3	A	256	ASP	CA-CB-CG	5.58	118.17	112.60
3	A	59	ALA	O-C-N	5.57	127.82	122.03
3	A	320	PHE	CA-C-N	5.56	128.05	120.54
3	A	320	PHE	C-N-CA	5.56	128.05	120.54
1	T	4	DT	P-O3'-C3'	-5.56	111.87	120.20
3	A	181	PHE	O-C-N	5.55	128.49	122.11
3	A	248	LYS	N-CA-C	5.53	116.60	107.20
3	A	205	THR	N-CA-C	5.53	122.57	110.80
3	A	303	VAL	N-CA-C	5.52	120.83	109.34
2	P	3	DT	N1-C1'-C2'	5.49	121.73	113.50
2	P	4	DA	C8-N9-C1'	5.48	135.27	127.05
3	A	309	GLU	CB-CA-C	5.46	120.92	110.17
3	A	212	HIS	CA-CB-CG	-5.42	108.38	113.80
3	A	231	GLY	N-CA-C	-5.41	103.74	111.42
3	A	91	ASP	N-CA-CB	5.39	119.61	110.49
3	A	146	PHE	CA-CB-CG	-5.37	108.43	113.80
2	P	3	DT	C4'-C3'-O3'	-5.35	101.97	110.00
3	A	226	ASP	O-C-N	5.32	129.44	123.48
3	A	278	PHE	CA-CB-CG	-5.27	108.53	113.80
3	A	223	PHE	N-CA-C	-5.26	105.14	112.45
3	A	92	ASP	CA-CB-CG	5.25	117.85	112.60
3	A	87	LYS	CB-CA-C	5.25	119.19	110.90
3	A	116	ASP	CA-CB-CG	-5.24	107.36	112.60
3	A	21	GLU	CA-C-N	5.16	127.95	120.79
3	A	21	GLU	C-N-CA	5.16	127.95	120.79
3	A	246	ASP	CA-CB-CG	5.15	117.75	112.60
3	A	73	ILE	N-CA-CB	5.13	116.55	110.55
3	A	228	LEU	N-CA-C	-5.12	104.66	112.04
1	T	3	DT	O4'-C1'-N1	5.10	116.05	108.40
3	A	268	GLY	N-CA-C	-5.08	106.61	112.50
3	A	53	ILE	CB-CA-C	5.08	118.89	111.33
3	A	46	ILE	N-CA-CB	5.04	119.55	111.23
3	A	62	LEU	CA-C-O	5.04	126.71	120.87
3	A	95	SER	CB-CA-C	-5.02	102.46	110.79
1	T	7	DA	N9-C1'-C2'	-5.02	105.97	113.50

All (2) chirality outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
-----	-------	-----	------	------

Mol	Chain	Res	Type	Atom
3	A	264	GLN	CA
3	A	309	GLU	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	11	0
2	P	144	0	81	17	0
3	A	2623	0	2640	382	0
4	A	2	0	0	0	0
5	A	107	0	0	17	0
5	P	17	0	0	1	0
5	T	14	0	0	4	0
All	All	3052	0	2801	404	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 72.

All (404) 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'	1.26	1.09
3:A:151:PRO:HG2	3:A:154:GLU:HG3	1.35	1.09
2:P:1:DT:H2''	2:P:2:DC:H5'	1.39	1.04
2:P:6:DT:H2''	2:P:7:DG:H5''	1.40	1.01
3:A:245:ASN:H	3:A:245:ASN:ND2	1.40	0.99
3:A:155:MET:HE2	3:A:188:SER:HB2	1.41	0.99
3:A:18:MET:HE2	3:A:82:LEU:HD22	1.44	0.99
3:A:245:ASN:N	3:A:245:ASN:HD22	1.54	0.98
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.47	0.97
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.45	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:12:ASN:HD21	3:A:53:ILE:H	1.14	0.94
3:A:277:ILE:HG12	3:A:335:GLU:HA	1.53	0.91
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.51	0.91
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.52	0.90
3:A:245:ASN:H	3:A:245:ASN:HD22	0.94	0.90
3:A:60:LYS:HA	3:A:65:VAL:HG23	1.53	0.89
3:A:243:SER:HB3	3:A:249:GLU:HA	1.51	0.89
3:A:29:VAL:HG21	3:A:94:SER:HB2	1.54	0.88
3:A:300:PRO:HD3	3:A:311:LEU:HD13	1.51	0.88
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.04	0.88
3:A:155:MET:HA	3:A:158:MET:HE3	1.55	0.86
1:T:6:DG:H2''	1:T:7:DA:C8	2.11	0.84
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.42	0.84
3:A:180:SER:HB3	3:A:183:ARG:HH21	1.43	0.83
3:A:121:THR:HG23	3:A:124:ASP:CG	2.04	0.83
3:A:41:LYS:HE2	3:A:64:GLY:HA3	1.62	0.82
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.64	0.80
2:P:6:DT:H2''	2:P:7:DG:C5'	2.15	0.77
3:A:191:MET:HG2	3:A:255:ILE:HG12	1.64	0.77
3:A:254:ARG:NH1	3:A:255:ILE:H	1.82	0.77
2:P:6:DT:C2'	2:P:7:DG:H5''	2.14	0.77
3:A:306:VAL:HG22	5:A:650:HOH:O	1.83	0.77
3:A:323:ILE:O	3:A:324:GLN:HG2	1.85	0.77
3:A:331:LYS:HG2	3:A:332:ASP:N	1.99	0.77
3:A:151:PRO:HG2	3:A:154:GLU:CG	2.14	0.76
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.67	0.76
3:A:128:ASN:N	3:A:128:ASN:ND2	2.34	0.76
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.16	0.75
3:A:172:GLU:HB3	3:A:197:HIS:NE2	2.02	0.75
3:A:214:VAL:O	3:A:218:LEU:HD22	1.87	0.74
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.85	0.74
3:A:128:ASN:N	3:A:128:ASN:HD22	1.85	0.74
3:A:181:PHE:HA	5:A:530:HOH:O	1.87	0.74
3:A:59:ALA:O	3:A:65:VAL:HG21	1.87	0.74
3:A:97:ILE:HG23	3:A:111:ALA:HB1	1.70	0.73
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.70	0.73
3:A:291:PHE:CD1	3:A:300:PRO:HA	2.24	0.73
3:A:180:SER:CB	3:A:183:ARG:HH21	2.01	0.72
3:A:300:PRO:CD	3:A:311:LEU:HD13	2.19	0.72
3:A:108:PRO:O	3:A:112:ARG:HG3	1.89	0.72
3:A:155:MET:HE2	3:A:188:SER:CB	2.20	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:194:LEU:HD11	3:A:258:ARG:HD3	1.73	0.71
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.72	0.71
2:P:5:DA:H2''	2:P:6:DT:C5'	2.12	0.71
3:A:18:MET:O	3:A:21:GLU:HB2	1.89	0.71
3:A:59:ALA:O	3:A:62:LEU:HB2	1.91	0.71
3:A:27:LYS:HB2	3:A:36:TYR:CD1	2.26	0.71
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.71	0.70
3:A:15:ILE:CD1	3:A:73:ILE:HG23	2.21	0.70
3:A:180:SER:HB3	3:A:183:ARG:NH2	2.05	0.69
3:A:245:ASN:O	3:A:246:ASP:O	2.10	0.69
3:A:292:THR:O	3:A:293:ILE:HD13	1.91	0.69
3:A:79:THR:O	3:A:81:LYS:N	2.25	0.69
3:A:121:THR:O	3:A:124:ASP:HB2	1.92	0.69
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.24	0.68
3:A:243:SER:OG	3:A:249:GLU:HG3	1.92	0.68
3:A:293:ILE:HD12	3:A:298:ILE:HG13	1.74	0.68
3:A:292:THR:C	3:A:293:ILE:HD13	2.18	0.68
3:A:41:LYS:HZ3	3:A:42:ALA:HB2	1.59	0.68
3:A:327:TYR:HD1	3:A:328:ARG:N	1.92	0.68
3:A:114:PHE:CZ	3:A:132:LEU:HD23	2.29	0.67
3:A:73:ILE:HG22	3:A:77:LEU:HD22	1.75	0.67
2:P:1:DT:H2''	2:P:2:DC:C5'	2.19	0.67
3:A:38:ALA:O	3:A:41:LYS:HD3	1.94	0.67
3:A:155:MET:HA	3:A:158:MET:CE	2.25	0.67
3:A:209:LYS:HA	3:A:212:HIS:HB2	1.75	0.67
3:A:294:ASN:HB2	3:A:295:GLU:OE1	1.93	0.67
3:A:259:LEU:O	3:A:260:ILE:HD13	1.95	0.67
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.30	0.67
3:A:56:GLY:O	3:A:59:ALA:HB3	1.95	0.67
3:A:254:ARG:NH1	3:A:255:ILE:N	2.42	0.67
3:A:123:GLU:HG3	5:A:623:HOH:O	1.95	0.66
3:A:286:ALA:O	3:A:291:PHE:N	2.29	0.65
3:A:211:LEU:O	3:A:214:VAL:HG22	1.96	0.65
3:A:240:GLN:NE2	3:A:250:TYR:O	2.29	0.65
3:A:75:GLU:O	3:A:75:GLU:HG2	1.96	0.64
3:A:243:SER:CB	3:A:249:GLU:HA	2.24	0.64
3:A:18:MET:HE1	3:A:76:PHE:CB	2.27	0.64
3:A:277:ILE:HG13	3:A:335:GLU:CB	2.27	0.64
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.79	0.64
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.12	0.64
3:A:282:MET:HB2	3:A:325:TRP:HZ3	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:282:MET:HE3	5:A:555:HOH:O	1.97	0.63
1:T:6:DG:N7	5:T:652:HOH:O	2.30	0.63
1:T:2:DA:N6	2:P:5:DA:N6	2.46	0.63
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.96	0.63
3:A:62:LEU:HD12	3:A:63:PRO:HD2	1.81	0.63
3:A:97:ILE:HG23	3:A:111:ALA:CB	2.29	0.63
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.47	0.62
3:A:228:LEU:HB2	3:A:236:MET:O	1.98	0.62
3:A:170:ASP:HB3	3:A:173:TYR:CE2	2.34	0.62
3:A:330:PRO:HA	3:A:333:ARG:CG	2.25	0.62
3:A:253:ARG:HG2	3:A:253:ARG:HH11	1.64	0.62
3:A:124:ASP:O	3:A:128:ASN:ND2	2.33	0.62
3:A:18:MET:HG2	3:A:19:LEU:N	2.08	0.62
5:T:617:HOH:O	3:A:234:LYS:HD3	1.99	0.62
3:A:279:ASN:O	3:A:283:ARG:HG3	2.00	0.62
2:P:5:DA:P	3:A:107:GLY:HA3	2.40	0.61
3:A:150:ILE:N	3:A:188:SER:O	2.32	0.61
3:A:152:ARG:HA	3:A:155:MET:HB2	1.81	0.61
3:A:214:VAL:HG23	3:A:215:VAL:N	2.16	0.61
3:A:180:SER:CA	3:A:183:ARG:HH21	2.12	0.61
3:A:41:LYS:O	3:A:44:SER:HB3	1.99	0.61
3:A:253:ARG:HH11	3:A:253:ARG:CG	2.13	0.61
3:A:287:LEU:HD13	3:A:291:PHE:O	2.01	0.61
3:A:329:GLU:O	3:A:333:ARG:HG2	2.00	0.61
3:A:201:THR:HA	3:A:261:PRO:CB	2.30	0.61
3:A:277:ILE:HG13	3:A:335:GLU:HB2	1.82	0.61
3:A:237:GLY:O	3:A:254:ARG:NH1	2.33	0.60
3:A:277:ILE:HD13	3:A:277:ILE:H	1.65	0.60
3:A:254:ARG:NH1	3:A:254:ARG:HB3	2.15	0.60
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.47	0.60
3:A:122:LEU:C	3:A:122:LEU:HD23	2.26	0.60
3:A:180:SER:HA	3:A:183:ARG:HE	1.67	0.60
3:A:285:HIS:CD2	3:A:323:ILE:HD12	2.37	0.60
3:A:288:GLU:C	3:A:290:GLY:H	2.10	0.59
3:A:248:LYS:O	3:A:248:LYS:HG2	2.02	0.59
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.37	0.59
3:A:309:GLU:N	3:A:309:GLU:OE1	2.35	0.59
3:A:254:ARG:HB3	3:A:254:ARG:CZ	2.33	0.59
3:A:133:ASN:HD22	3:A:135:HIS:H	1.51	0.59
1:T:7:DA:H61	2:P:1:DT:H3	1.51	0.59
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:182:ARG:HH11	3:A:182:ARG:CG	2.16	0.59
3:A:194:LEU:HD21	3:A:272:PHE:CD2	2.37	0.58
3:A:299:ARG:HD2	3:A:310:PRO:HD3	1.84	0.58
2:P:1:DT:H2'	2:P:2:DC:C6	2.38	0.58
3:A:291:PHE:CE1	3:A:300:PRO:HA	2.38	0.58
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.36	0.58
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.32	0.58
3:A:29:VAL:HG21	3:A:94:SER:CB	2.30	0.58
3:A:204:SER:O	3:A:206:LYS:N	2.36	0.58
3:A:115:VAL:O	3:A:118:GLY:N	2.36	0.58
3:A:270:LEU:HD23	3:A:319:ILE:HD13	1.86	0.57
3:A:60:LYS:HA	3:A:65:VAL:CG2	2.31	0.57
3:A:249:GLU:CG	3:A:250:TYR:H	2.17	0.57
3:A:122:LEU:HD21	3:A:126:ARG:CZ	2.33	0.57
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.87	0.57
3:A:60:LYS:CA	3:A:65:VAL:HG23	2.30	0.57
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.34	0.57
3:A:194:LEU:CD1	3:A:258:ARG:HD3	2.34	0.56
3:A:323:ILE:C	3:A:324:GLN:HG2	2.29	0.56
3:A:35:LYS:O	3:A:38:ALA:HB3	2.05	0.56
3:A:265:TYR:O	3:A:268:GLY:N	2.38	0.56
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.53	0.56
3:A:212:HIS:HB3	5:A:541:HOH:O	2.04	0.56
3:A:207:GLN:O	3:A:210:LEU:HB2	2.06	0.56
3:A:31:GLN:HB2	3:A:112:ARG:NH1	2.20	0.56
3:A:194:LEU:HD21	3:A:272:PHE:HD2	1.71	0.56
3:A:316:GLU:O	3:A:320:PHE:HD2	1.89	0.56
3:A:15:ILE:HB	3:A:46:ILE:CD1	2.36	0.55
3:A:127:LYS:HB2	3:A:128:ASN:ND2	2.21	0.55
3:A:298:ILE:HA	5:A:593:HOH:O	2.05	0.55
3:A:121:THR:HG23	3:A:124:ASP:OD2	2.06	0.55
3:A:320:PHE:CE1	3:A:328:ARG:HG3	2.41	0.55
3:A:133:ASN:ND2	3:A:135:HIS:H	2.02	0.55
3:A:15:ILE:HD13	3:A:73:ILE:HG23	1.89	0.55
3:A:45:VAL:HG23	3:A:46:ILE:N	2.21	0.55
3:A:277:ILE:CG1	3:A:335:GLU:HA	2.31	0.55
3:A:286:ALA:HB1	3:A:291:PHE:HB2	1.89	0.55
3:A:165:GLU:O	3:A:169:VAL:HG12	2.07	0.55
3:A:180:SER:HA	3:A:183:ARG:HH21	1.72	0.55
2:P:5:DA:H2'	2:P:6:DT:H71	1.89	0.54
3:A:182:ARG:HH11	3:A:273:THR:HG21	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:111:ALA:O	3:A:115:VAL:HG23	2.06	0.54
3:A:81:LYS:NZ	3:A:86:GLU:HB2	2.22	0.54
3:A:217:GLN:NE2	3:A:217:GLN:HA	2.23	0.54
3:A:165:GLU:O	3:A:168:LYS:N	2.40	0.54
3:A:282:MET:HA	3:A:325:TRP:CH2	2.43	0.54
3:A:254:ARG:HH11	3:A:255:ILE:H	1.53	0.54
3:A:196:THR:OG1	3:A:197:HIS:N	2.40	0.54
3:A:151:PRO:HB2	3:A:153:GLU:HG2	1.89	0.54
3:A:257:ILE:HG22	3:A:258:ARG:N	2.21	0.54
3:A:326:LYS:O	3:A:328:ARG:HG2	2.07	0.54
3:A:238:VAL:HA	3:A:253:ARG:O	2.07	0.54
3:A:260:ILE:HG22	3:A:261:PRO:O	2.08	0.53
3:A:15:ILE:CD1	3:A:77:LEU:HD11	2.33	0.53
3:A:174:ILE:O	3:A:195:LEU:HD12	2.09	0.53
3:A:21:GLU:OE1	3:A:85:LEU:HG	2.07	0.53
3:A:103:VAL:HB	3:A:106:ILE:CD1	2.28	0.53
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.89	0.53
3:A:270:LEU:C	3:A:270:LEU:HD12	2.34	0.53
3:A:15:ILE:HB	3:A:46:ILE:HD11	1.91	0.53
3:A:201:THR:HA	3:A:261:PRO:HB3	1.91	0.53
3:A:19:LEU:HD23	3:A:43:ALA:HA	1.91	0.53
3:A:152:ARG:NH2	3:A:181:PHE:O	2.30	0.53
3:A:326:LYS:O	3:A:326:LYS:HG3	2.09	0.53
3:A:115:VAL:C	3:A:118:GLY:H	2.16	0.52
3:A:165:GLU:HB2	3:A:218:LEU:CD1	2.40	0.52
3:A:293:ILE:HA	5:A:593:HOH:O	2.08	0.52
2:P:5:DA:O5'	3:A:107:GLY:HA3	2.08	0.52
3:A:18:MET:CE	3:A:76:PHE:HB2	2.39	0.52
3:A:31:GLN:HB2	3:A:112:ARG:HH12	1.74	0.52
3:A:178:CYS:SG	3:A:194:LEU:HB2	2.49	0.52
3:A:188:SER:HB3	5:A:522:HOH:O	2.09	0.52
3:A:218:LEU:HB2	3:A:224:ILE:CD1	2.39	0.52
3:A:157:GLN:O	3:A:161:ILE:HG13	2.10	0.52
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.45	0.52
3:A:79:THR:O	3:A:79:THR:OG1	2.28	0.52
3:A:240:GLN:NE2	3:A:252:HIS:CE1	2.78	0.52
3:A:278:PHE:CZ	3:A:282:MET:HE2	2.44	0.52
3:A:285:HIS:HD2	3:A:323:ILE:HD12	1.75	0.52
3:A:26:GLU:HA	3:A:30:SER:OG	2.10	0.51
3:A:174:ILE:HG22	3:A:265:TYR:CE2	2.45	0.51
3:A:155:MET:CE	3:A:188:SER:HB2	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:5:DA:C2'	2:P:6:DT:H71	2.41	0.51
3:A:212:HIS:N	3:A:212:HIS:CD2	2.77	0.51
3:A:240:GLN:O	3:A:242:PRO:HD3	2.10	0.51
3:A:279:ASN:O	3:A:283:ARG:N	2.41	0.51
3:A:282:MET:CB	3:A:325:TRP:HZ3	2.24	0.51
3:A:321:ASP:O	3:A:324:GLN:N	2.37	0.51
1:T:4:DT:H2''	1:T:5:DA:C8	2.46	0.51
3:A:270:LEU:HD12	5:A:584:HOH:O	2.10	0.51
3:A:152:ARG:O	3:A:155:MET:HB2	2.11	0.51
3:A:299:ARG:HG2	3:A:310:PRO:HA	1.92	0.51
3:A:165:GLU:HB3	3:A:217:GLN:CG	2.40	0.51
3:A:200:PHE:C	3:A:201:THR:HG22	2.36	0.51
3:A:236:MET:HG3	3:A:256:ASP:OD1	2.11	0.50
3:A:172:GLU:HB3	3:A:197:HIS:CD2	2.46	0.50
3:A:332:ASP:OD1	3:A:332:ASP:O	2.30	0.50
3:A:243:SER:O	3:A:244:LYS:O	2.30	0.50
1:T:1:DC:H2''	1:T:2:DA:OP2	2.11	0.50
3:A:182:ARG:NH2	3:A:316:GLU:OE1	2.34	0.50
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.39	0.50
3:A:45:VAL:O	3:A:48:LYS:N	2.41	0.50
3:A:260:ILE:HG23	3:A:261:PRO:CD	2.39	0.50
3:A:295:GLU:HA	5:A:592:HOH:O	2.11	0.50
3:A:270:LEU:HD23	3:A:319:ILE:HG21	1.93	0.50
3:A:145:ASP:HB3	3:A:252:HIS:O	2.12	0.49
3:A:182:ARG:HH11	3:A:273:THR:CG2	2.24	0.49
3:A:266:TYR:O	3:A:270:LEU:N	2.44	0.49
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.77	0.49
2:P:5:DA:H1'	5:P:565:HOH:O	2.11	0.49
3:A:44:SER:O	3:A:47:ALA:HB3	2.13	0.49
3:A:128:ASN:HD22	3:A:128:ASN:H	1.60	0.49
3:A:245:ASN:ND2	3:A:245:ASN:N	2.17	0.49
3:A:299:ARG:CD	3:A:310:PRO:HD3	2.43	0.49
3:A:22:LEU:HD22	3:A:85:LEU:HD13	1.94	0.49
3:A:195:LEU:O	3:A:260:ILE:N	2.45	0.49
3:A:282:MET:HG2	5:A:555:HOH:O	2.13	0.49
3:A:62:LEU:HD12	3:A:63:PRO:CD	2.42	0.49
3:A:22:LEU:HD13	3:A:22:LEU:HA	1.49	0.48
3:A:271:TYR:HB2	5:A:592:HOH:O	2.12	0.48
3:A:22:LEU:HD22	3:A:85:LEU:CD1	2.43	0.48
3:A:146:PHE:N	3:A:146:PHE:CD1	2.80	0.48
3:A:170:ASP:OD1	3:A:171:SER:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:121:THR:HG23	3:A:124:ASP:OD1	2.14	0.48
3:A:294:ASN:N	3:A:294:ASN:HD22	2.12	0.48
3:A:223:PHE:O	3:A:239:CYS:HA	2.14	0.48
3:A:28:ASN:HD22	3:A:28:ASN:HA	1.29	0.48
3:A:30:SER:HB3	5:A:561:HOH:O	2.14	0.48
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.55	0.48
3:A:162:VAL:O	3:A:166:VAL:HG23	2.14	0.48
3:A:287:LEU:HD13	3:A:287:LEU:HA	1.37	0.48
3:A:45:VAL:CG2	3:A:46:ILE:N	2.77	0.47
3:A:172:GLU:HG3	3:A:198:PRO:HG2	1.95	0.47
2:P:5:DA:C2'	2:P:6:DT:H5'	2.20	0.47
3:A:265:TYR:O	3:A:267:CYS:N	2.47	0.47
3:A:241:LEU:HB2	3:A:250:TYR:CG	2.50	0.47
3:A:254:ARG:HH11	3:A:254:ARG:HA	1.80	0.47
3:A:29:VAL:CG2	3:A:94:SER:HB2	2.36	0.47
3:A:251:PRO:HG2	3:A:253:ARG:NH2	2.29	0.47
3:A:254:ARG:HH11	3:A:254:ARG:CA	2.27	0.47
3:A:328:ARG:O	3:A:333:ARG:NE	2.29	0.47
3:A:154:GLU:C	3:A:158:MET:HE2	2.39	0.47
3:A:278:PHE:CE1	3:A:328:ARG:HD3	2.49	0.47
1:T:7:DA:H1'	5:T:634:HOH:O	2.15	0.47
3:A:180:SER:HB2	3:A:185:ALA:HB3	1.96	0.47
3:A:100:LEU:HD21	3:A:119:ILE:O	2.15	0.47
2:P:1:DT:C2'	2:P:2:DC:H5'	2.28	0.47
3:A:270:LEU:CD2	3:A:319:ILE:HD13	2.45	0.47
3:A:29:VAL:HA	3:A:97:ILE:HD12	1.95	0.47
3:A:73:ILE:CG2	3:A:77:LEU:HD22	2.42	0.47
3:A:249:GLU:HG3	3:A:250:TYR:H	1.80	0.47
3:A:300:PRO:HG3	3:A:311:LEU:CD1	2.45	0.46
3:A:105:GLY:O	3:A:136:GLN:OE1	2.34	0.46
3:A:11:LEU:HD23	3:A:11:LEU:H	1.80	0.46
3:A:166:VAL:O	3:A:169:VAL:HG13	2.15	0.46
3:A:218:LEU:N	3:A:218:LEU:HD13	2.30	0.46
3:A:302:GLY:N	3:A:307:ALA:CB	2.79	0.46
3:A:53:ILE:HG21	3:A:59:ALA:HB2	1.98	0.46
3:A:62:LEU:HD12	3:A:62:LEU:HA	1.63	0.46
3:A:182:ARG:NH1	3:A:273:THR:CG2	2.78	0.46
1:T:4:DT:H1'	5:T:527:HOH:O	2.15	0.46
3:A:191:MET:HG2	3:A:255:ILE:CG1	2.40	0.46
3:A:200:PHE:CE2	3:A:261:PRO:N	2.84	0.46
3:A:294:ASN:O	3:A:296:TYR:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:198:PRO:C	3:A:200:PHE:H	2.24	0.46
3:A:302:GLY:N	3:A:307:ALA:HB3	2.31	0.46
3:A:76:PHE:HD1	3:A:77:LEU:CD1	2.29	0.46
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.51	0.46
3:A:214:VAL:HG23	3:A:215:VAL:HG23	1.98	0.46
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.30	0.46
3:A:122:LEU:CD2	3:A:126:ARG:NH1	2.79	0.46
3:A:278:PHE:CZ	3:A:282:MET:CE	2.99	0.46
3:A:302:GLY:HA3	3:A:307:ALA:HB2	1.98	0.45
3:A:174:ILE:CG2	3:A:265:TYR:CE2	2.99	0.45
3:A:282:MET:CB	3:A:325:TRP:CZ3	3.00	0.45
3:A:114:PHE:HB3	3:A:119:ILE:HB	1.98	0.45
3:A:288:GLU:OE1	3:A:288:GLU:HA	2.15	0.45
3:A:259:LEU:HD12	3:A:259:LEU:HA	1.73	0.45
3:A:270:LEU:HD13	3:A:270:LEU:HA	1.80	0.45
3:A:59:ALA:C	3:A:65:VAL:HG21	2.42	0.45
3:A:83:ARG:O	3:A:83:ARG:HG3	2.12	0.45
3:A:250:TYR:HB3	5:A:577:HOH:O	2.17	0.45
3:A:155:MET:HB3	3:A:181:PHE:CE1	2.52	0.45
3:A:170:ASP:HB3	3:A:173:TYR:CD2	2.52	0.45
3:A:260:ILE:CG2	3:A:261:PRO:N	2.80	0.45
3:A:114:PHE:CZ	3:A:132:LEU:CD2	2.98	0.45
3:A:282:MET:HB2	3:A:325:TRP:CZ3	2.48	0.45
3:A:286:ALA:O	3:A:291:PHE:HB2	2.17	0.45
3:A:291:PHE:HD1	3:A:300:PRO:HA	1.78	0.45
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.51	0.45
3:A:99:PHE:CD1	3:A:99:PHE:C	2.95	0.45
3:A:300:PRO:HD2	3:A:309:GLU:O	2.17	0.45
3:A:49:TYR:CE2	3:A:51:HIS:HB2	2.53	0.44
3:A:178:CYS:SG	3:A:194:LEU:CD2	3.06	0.44
3:A:195:LEU:HD12	3:A:195:LEU:HA	1.74	0.44
1:T:4:DT:H2"	1:T:5:DA:H8	1.81	0.44
3:A:41:LYS:HD3	3:A:42:ALA:H	1.83	0.44
3:A:65:VAL:HG23	3:A:65:VAL:O	2.16	0.44
3:A:158:MET:HE3	3:A:158:MET:HB2	1.72	0.44
3:A:292:THR:O	3:A:298:ILE:HA	2.18	0.44
3:A:81:LYS:HZ2	3:A:86:GLU:HB2	1.82	0.44
3:A:212:HIS:CD2	3:A:212:HIS:H	2.35	0.44
3:A:320:PHE:O	3:A:323:ILE:HG13	2.18	0.44
3:A:62:LEU:CD1	3:A:63:PRO:HD2	2.47	0.44
3:A:214:VAL:CG2	3:A:215:VAL:N	2.79	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:62:LEU:CG	3:A:63:PRO:HD2	2.47	0.44
3:A:249:GLU:CG	3:A:250:TYR:N	2.80	0.44
3:A:218:LEU:HB2	3:A:224:ILE:HD12	2.00	0.44
3:A:295:GLU:H	3:A:295:GLU:CD	2.25	0.44
3:A:322:TYR:N	3:A:322:TYR:CD1	2.85	0.44
3:A:191:MET:CG	3:A:255:ILE:HG12	2.41	0.43
3:A:201:THR:OG1	3:A:202:SER:N	2.51	0.43
3:A:154:GLU:HB3	5:A:521:HOH:O	2.17	0.43
3:A:199:SER:OG	3:A:207:GLN:OE1	2.33	0.43
3:A:211:LEU:O	3:A:211:LEU:HD12	2.19	0.43
3:A:254:ARG:HH12	3:A:255:ILE:H	1.63	0.43
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.52	0.43
3:A:254:ARG:NH1	3:A:254:ARG:CB	2.80	0.43
3:A:62:LEU:C	3:A:65:VAL:HG22	2.44	0.43
3:A:260:ILE:HG22	3:A:261:PRO:N	2.33	0.43
3:A:304:THR:H	3:A:304:THR:HG23	1.41	0.43
3:A:19:LEU:HB3	3:A:43:ALA:HB2	1.99	0.43
3:A:166:VAL:HG13	3:A:173:TYR:HB3	2.01	0.43
3:A:278:PHE:CE2	3:A:282:MET:HE2	2.53	0.43
3:A:311:LEU:HB3	3:A:322:TYR:HE2	1.84	0.43
3:A:182:ARG:NH1	3:A:182:ARG:CG	2.79	0.42
3:A:227:THR:HG21	3:A:230:LYS:HB2	2.00	0.42
3:A:327:TYR:CD1	3:A:328:ARG:N	2.80	0.42
3:A:36:TYR:CD2	3:A:36:TYR:C	2.96	0.42
3:A:272:PHE:HA	5:A:532:HOH:O	2.18	0.42
3:A:270:LEU:HD12	3:A:270:LEU:O	2.20	0.42
3:A:280:LYS:O	3:A:283:ARG:HB2	2.18	0.42
3:A:303:VAL:O	3:A:305:GLY:N	2.52	0.42
3:A:127:LYS:HB2	3:A:128:ASN:HD21	1.82	0.42
3:A:133:ASN:ND2	3:A:133:ASN:C	2.77	0.42
3:A:157:GLN:HE22	3:A:244:LYS:NZ	2.18	0.42
3:A:60:LYS:O	3:A:60:LYS:HG3	2.18	0.42
3:A:119:ILE:HG23	3:A:119:ILE:HD13	1.67	0.42
3:A:207:GLN:HB2	5:A:625:HOH:O	2.19	0.42
3:A:183:ARG:HE	3:A:183:ARG:HB2	1.44	0.42
3:A:12:ASN:ND2	3:A:53:ILE:H	1.97	0.42
3:A:15:ILE:HG22	3:A:19:LEU:HD22	2.01	0.42
3:A:128:ASN:C	3:A:130:ASP:N	2.78	0.42
3:A:163:LEU:HA	3:A:163:LEU:HD23	1.19	0.42
3:A:200:PHE:CE2	3:A:260:ILE:C	2.98	0.42
1:T:4:DT:OP1	3:A:233:THR:OG1	2.37	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:62:LEU:HB2	3:A:65:VAL:HG21	2.02	0.41
3:A:85:LEU:HD12	3:A:85:LEU:HA	1.72	0.41
3:A:159:GLN:HG2	3:A:160:ASP:N	2.36	0.41
3:A:165:GLU:HB2	3:A:218:LEU:HD11	2.01	0.41
3:A:327:TYR:CD1	3:A:327:TYR:C	2.99	0.41
3:A:260:ILE:CG2	3:A:261:PRO:CD	2.98	0.41
3:A:288:GLU:C	3:A:290:GLY:N	2.78	0.41
3:A:138:ILE:O	3:A:138:ILE:HG22	2.20	0.41
3:A:217:GLN:O	3:A:221:VAL:HG22	2.21	0.41
1:T:4:DT:O5'	3:A:231:GLY:HA3	2.20	0.41
3:A:133:ASN:HD22	3:A:133:ASN:C	2.28	0.41
3:A:262:LYS:O	3:A:262:LYS:HG3	2.17	0.41
3:A:43:ALA:O	3:A:47:ALA:HB2	2.21	0.41
3:A:119:ILE:HG21	3:A:119:ILE:HD12	1.78	0.41
3:A:261:PRO:HG2	3:A:264:GLN:HG3	2.02	0.41
3:A:288:GLU:O	3:A:290:GLY:N	2.54	0.41
3:A:306:VAL:HG23	3:A:307:ALA:N	2.36	0.41
3:A:97:ILE:O	3:A:97:ILE:HG22	2.21	0.41
3:A:141:LYS:HE2	3:A:142:TYR:CZ	2.56	0.41
3:A:241:LEU:HD23	3:A:241:LEU:HA	1.92	0.40
3:A:73:ILE:O	3:A:77:LEU:HD13	2.21	0.40
3:A:142:TYR:CE1	3:A:252:HIS:CG	3.09	0.40
3:A:277:ILE:CG1	3:A:335:GLU:CB	2.97	0.40
3:A:300:PRO:HG3	3:A:311:LEU:HD11	2.03	0.40
3:A:254:ARG:HH11	3:A:255:ILE:N	2.15	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	325/335 (97%)	263 (81%)	43 (13%)	19 (6%)	1 9

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	202	SER
3	A	205	THR
3	A	222	HIS
3	A	244	LYS
3	A	246	ASP
3	A	247	GLU
3	A	265	TYR
3	A	295	GLU
3	A	80	GLY
3	A	204	SER
3	A	266	TYR
3	A	289	LYS
3	A	304	THR
3	A	91	ASP
3	A	245	ASN
3	A	310	PRO
3	A	220	LYS
3	A	309	GLU
3	A	207	GLN

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%)	217 (75%)	71 (25%)	1 3

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	THR
3	A	15	ILE
3	A	18	MET
3	A	19	LEU
3	A	21	GLU
3	A	22	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	30	SER
3	A	33	ILE
3	A	37	ASN
3	A	41	LYS
3	A	46	ILE
3	A	60	LYS
3	A	62	LEU
3	A	65	VAL
3	A	67	THR
3	A	68	LYS
3	A	77	LEU
3	A	79	THR
3	A	85	LEU
3	A	87	LYS
3	A	89	ARG
3	A	92	ASP
3	A	94	SER
3	A	100	LEU
3	A	101	THR
3	A	104	SER
3	A	119	ILE
3	A	121	THR
3	A	128	ASN
3	A	133	ASN
3	A	138	ILE
3	A	141	LYS
3	A	153	GLU
3	A	161	ILE
3	A	169	VAL
3	A	174	ILE
3	A	180	SER
3	A	182	ARG
3	A	191	MET
3	A	193	VAL
3	A	194	LEU
3	A	201	THR
3	A	203	GLU
3	A	205	THR
3	A	213	GLN
3	A	218	LEU
3	A	226	ASP
3	A	228	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	230	LYS
3	A	232	GLU
3	A	245	ASN
3	A	246	ASP
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE
3	A	270	LEU
3	A	277	ILE
3	A	287	LEU
3	A	293	ILE
3	A	294	ASN
3	A	295	GLU
3	A	298	ILE
3	A	301	LEU
3	A	306	VAL
3	A	309	GLU
3	A	314	ASP
3	A	324	GLN
3	A	325	TRP
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 (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	136	GLN
3	A	157	GLN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	222	HIS
3	A	240	GLN
3	A	245	ASN
3	A	252	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	264	GLN
3	A	294	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	247:GLU	C	248:LYS	N	1.86

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%)	-0.88	0 100 100	16, 37, 97, 99	0
2	P	7/7 (100%)	-1.21	0 100 100	14, 24, 37, 75	0
3	A	325/335 (97%)	-1.08	0 100 100	1, 30, 84, 100	0
All	All	340/350 (97%)	-1.08	0 100 100	1, 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	NA	A	342	1/1	0.96	0.11	51,51,51,51	0
4	NA	A	341	1/1	0.99	0.02	1,1,1,1	0

6.5 Other polymers [i](#)

There are no such residues in this entry.