



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:37 PM GMT

PDB ID : 1BPZ  
Title : HUMAN DNA POLYMERASE BETA COMPLEXED WITH NICKED DNA  
Authors : Sawaya, M.R.; Prasad, R.; Wilson, S.H.; Kraut, J.; Pelletier, H.  
Deposited on : 1997-04-14  
Resolution : 2.60 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

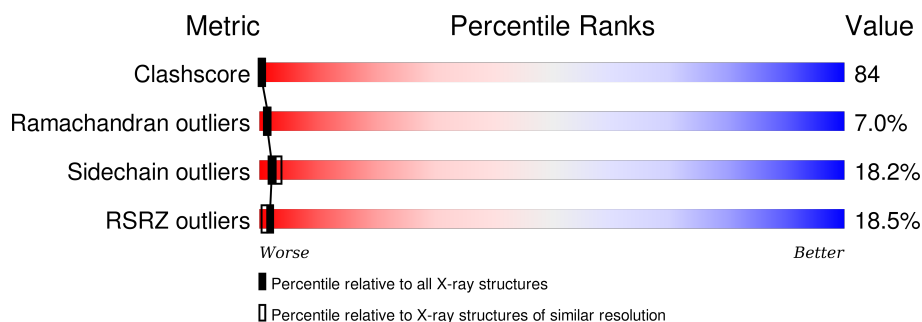
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*




The reported resolution of this entry is 2.60 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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	16	
2	P	11	
3	D	5	
4	A	335	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3333 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\*CP\*GP\*AP\*CP\*CP\*AP\*CP\*GP\*CP\*AP\*TP\*CP\*AP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	16	Total	C	N	O	P	0	0	0
			319	152	61	91	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	11	Total	C	N	O	P	0	0	0
			226	108	42	66	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	5	Total	C	N	O	P	0	0	0
			106	49	20	32	5			

- Molecule 4 is a protein called PROTEIN (DNA POLYMERASE BETA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	331	Total	C	N	O	S	0	0	0
			2653	1676	464	504	9			

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

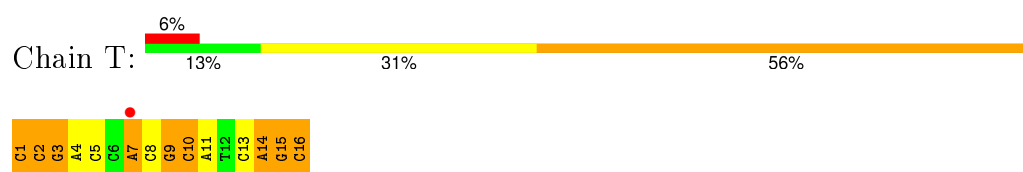
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total 14	O 14	0	0
6	D	1	Total 1	O 1	0	0
6	P	6	Total 6	O 6	0	0
6	T	6	Total 6	O 6	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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\*CP\*GP\*AP\*CP\*CP\*AP\*CP\*GP\*CP\*AP\*TP\*CP\*AP\*GP\*C)-3')



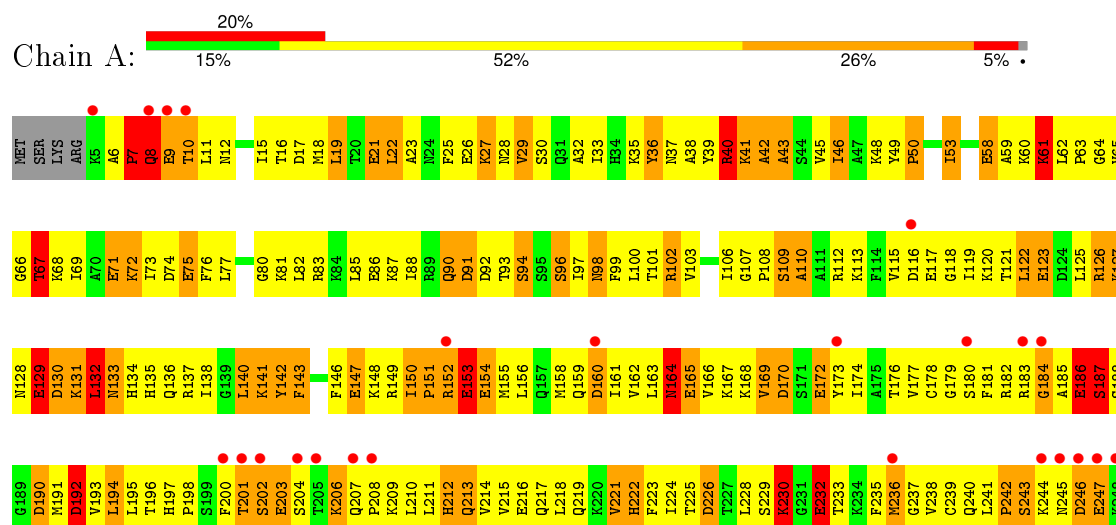
- Molecule 2: DNA (5'-D(\*GP\*CP\*TP\*GP\*AP\*TP\*GP\*CP\*GP\*TP\*G)-3')

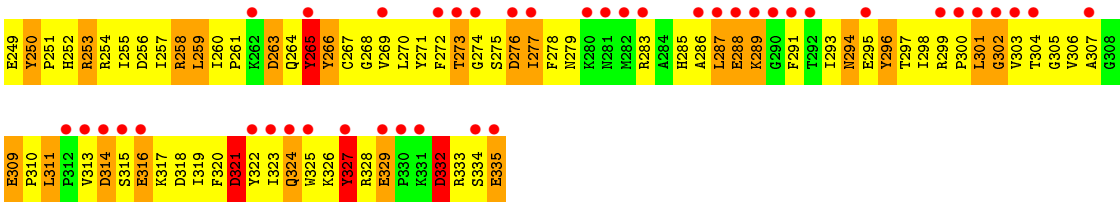


- Molecule 3: DNA (5'-D(\*GP\*TP\*CP\*GP\*G)-3')



- Molecule 4: PROTEIN (DNA POLYMERASE BETA)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.53 Å   78.66 Å   54.62 Å 90.00°   107.54°   90.00°	Depositor
Resolution (Å)	20.00 – 2.60 29.21 – 2.45	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-2.60) 92.5 (29.21-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.88 (at 2.45 Å)	Xtriage
Refinement program	TNT V. 5-D	Depositor
R, $R_{free}$	0.243 , (Not available) 0.233 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	34.4	Xtriage
Anisotropy	0.796	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 94.3	EDS
Estimated twinning fraction	0.038 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 14690 reflections (0.014%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3333	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	2.49	20/357 (5.6%)	3.01	56/547 (10.2%)
2	P	2.57	14/253 (5.5%)	3.32	46/390 (11.8%)
3	D	3.14	10/118 (8.5%)	3.41	20/179 (11.2%)
4	A	1.16	22/2703 (0.8%)	1.70	64/3632 (1.8%)
All	All	1.59	66/3431 (1.9%)	2.14	186/4748 (3.9%)

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
4	A	1	0

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	15	DG	N3-C4	-11.91	1.27	1.35
2	P	9	DG	N7-C5	11.25	1.46	1.39
4	A	58	GLU	CD-OE1	10.17	1.36	1.25
3	D	1	DG	OP3-P	-10.13	1.49	1.61
2	P	10	DT	C4-C5	-9.89	1.36	1.45
1	T	4	DA	C8-N7	9.24	1.38	1.31
1	T	5	DC	N1-C6	-9.08	1.31	1.37
3	D	1	DG	N7-C5	8.66	1.44	1.39
3	D	4	DG	C8-N7	8.62	1.36	1.30
2	P	1	DG	C5-C6	-8.41	1.33	1.42
2	P	7	DG	C3'-O3'	-8.08	1.33	1.44
2	P	1	DG	N9-C4	-8.08	1.31	1.38
1	T	5	DC	N3-C4	-8.00	1.28	1.33
1	T	4	DA	C6-N6	7.68	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	11	DA	C4'-O4'	-7.58	1.37	1.45
3	D	1	DG	C5-C4	-7.34	1.33	1.38
2	P	5	DA	N7-C5	7.28	1.43	1.39
4	A	129	GLU	CD-OE2	7.26	1.33	1.25
3	D	5	DG	C8-N7	7.24	1.35	1.30
4	A	147	GLU	CD-OE2	7.15	1.33	1.25
4	A	71	GLU	CD-OE2	7.04	1.33	1.25
2	P	1	DG	N7-C5	-7.03	1.35	1.39
4	A	9	GLU	CB-CG	6.86	1.65	1.52
4	A	232	GLU	CD-OE2	6.85	1.33	1.25
3	D	1	DG	C3'-O3'	6.84	1.52	1.44
4	A	154	GLU	CD-OE2	6.84	1.33	1.25
1	T	14	DA	C3'-O3'	-6.81	1.35	1.44
1	T	5	DC	C4-C5	-6.74	1.37	1.43
2	P	9	DG	C2-N3	6.49	1.38	1.32
4	A	172	GLU	CD-OE2	6.44	1.32	1.25
4	A	203	GLU	CD-OE1	6.44	1.32	1.25
2	P	4	DG	N7-C5	6.42	1.43	1.39
1	T	5	DC	O4'-C1'	-6.39	1.34	1.42
1	T	3	DG	N7-C5	6.33	1.43	1.39
4	A	153	GLU	CD-OE2	6.17	1.32	1.25
2	P	5	DA	C5-C6	6.13	1.46	1.41
1	T	16	DC	N3-C4	-6.12	1.29	1.33
4	A	165	GLU	CD-OE2	6.11	1.32	1.25
4	A	21	GLU	CD-OE1	6.08	1.32	1.25
4	A	335	GLU	CD-OE2	6.00	1.32	1.25
4	A	86	GLU	CD-OE1	6.00	1.32	1.25
1	T	15	DG	N9-C4	-5.99	1.33	1.38
4	A	186	GLU	CD-OE1	5.97	1.32	1.25
1	T	4	DA	N9-C4	5.97	1.41	1.37
1	T	15	DG	C8-N7	5.95	1.34	1.30
4	A	249	GLU	CD-OE2	5.86	1.32	1.25
1	T	2	DC	N3-C4	5.72	1.38	1.33
3	D	2	DT	N1-C2	-5.71	1.33	1.38
2	P	7	DG	N1-C2	-5.69	1.33	1.37
1	T	9	DG	N1-C2	-5.67	1.33	1.37
4	A	329	GLU	CD-OE2	5.65	1.31	1.25
1	T	11	DA	C6-N1	5.61	1.39	1.35
4	A	123	GLU	CD-OE2	5.60	1.31	1.25
3	D	3	DC	N1-C6	-5.57	1.33	1.37
4	A	75	GLU	CD-OE1	5.57	1.31	1.25
4	A	316	GLU	CD-OE1	5.45	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	9	DG	C5-C6	-5.37	1.36	1.42
1	T	9	DG	C6-N1	-5.36	1.35	1.39
4	A	247	GLU	CD-OE2	5.32	1.31	1.25
1	T	14	DA	C8-N7	5.29	1.35	1.31
2	P	7	DG	C5-C6	-5.29	1.37	1.42
3	D	4	DG	N7-C5	5.24	1.42	1.39
4	A	288	GLU	CD-OE2	5.12	1.31	1.25
2	P	1	DG	N3-C4	-5.12	1.31	1.35
3	D	2	DT	C4-O4	5.11	1.27	1.23
2	P	9	DG	C5-C6	5.08	1.47	1.42

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	DG	C8-N9-C4	15.11	112.44	106.40
2	P	10	DT	C4-C5-C7	-14.50	110.30	119.00
3	D	1	DG	N7-C8-N9	-12.95	106.62	113.10
2	P	10	DT	O5'-P-OP1	-12.12	94.79	105.70
2	P	10	DT	C6-C5-C7	11.97	130.08	122.90
1	T	10	DC	N3-C4-C5	11.94	126.68	121.90
1	T	14	DA	O4'-C1'-N9	-11.63	99.86	108.00
2	P	10	DT	C5-C4-O4	-11.45	116.89	124.90
1	T	2	DC	P-O3'-C3'	10.94	132.82	119.70
3	D	5	DG	C8-N9-C4	10.61	110.64	106.40
2	P	7	DG	O4'-C1'-N9	-10.44	100.69	108.00
1	T	9	DG	O4'-C1'-N9	-10.33	100.77	108.00
4	A	258	ARG	NE-CZ-NH1	10.30	125.45	120.30
2	P	9	DG	C8-N9-C4	10.26	110.50	106.40
3	D	2	DT	P-O5'-C5'	-10.15	104.67	120.90
1	T	11	DA	C8-N9-C4	10.11	109.84	105.80
2	P	4	DG	C8-N9-C4	9.93	110.37	106.40
1	T	16	DC	N3-C4-N4	-9.34	111.47	118.00
1	T	5	DC	C6-N1-C2	-9.28	116.59	120.30
4	A	126	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	T	1	DC	O4'-C1'-N1	-9.11	101.62	108.00
2	P	1	DG	C2-N3-C4	-9.04	107.38	111.90
1	T	14	DA	C8-N9-C4	8.91	109.36	105.80
4	A	8	GLN	N-CA-C	8.86	134.93	111.00
4	A	39	TYR	CB-CG-CD2	8.86	126.32	121.00
2	P	6	DT	N1-C1'-C2'	8.78	129.28	112.60
3	D	1	DG	O4'-C1'-N9	-8.78	101.86	108.00
4	A	17	ASP	CB-CG-OD2	-8.71	110.46	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5	DG	N7-C8-N9	-8.52	108.84	113.10
4	A	102	ARG	NE-CZ-NH2	-8.51	116.05	120.30
4	A	74	ASP	CB-CG-OD2	-8.43	110.71	118.30
4	A	170	ASP	CB-CG-OD2	-8.37	110.77	118.30
3	D	2	DT	C4-C5-C7	8.31	123.99	119.00
4	A	83	ARG	NE-CZ-NH1	8.30	124.45	120.30
4	A	126	ARG	NE-CZ-NH1	8.27	124.43	120.30
2	P	10	DT	N3-C4-O4	8.23	124.84	119.90
2	P	10	DT	P-O5'-C5'	-8.21	107.77	120.90
4	A	83	ARG	NE-CZ-NH2	-8.19	116.21	120.30
4	A	170	ASP	CB-CG-OD1	8.14	125.63	118.30
3	D	5	DG	C2-N3-C4	-7.96	107.92	111.90
4	A	39	TYR	CB-CG-CD1	-7.88	116.27	121.00
4	A	109	SER	N-CA-CB	7.84	122.25	110.50
2	P	1	DG	O4'-C1'-N9	-7.81	102.53	108.00
2	P	9	DG	O5'-P-OP2	7.72	119.96	110.70
1	T	5	DC	O4'-C1'-N1	7.70	113.39	108.00
1	T	7	DA	C8-N9-C4	7.70	108.88	105.80
4	A	314	ASP	CB-CG-OD1	-7.63	111.43	118.30
4	A	160	ASP	CB-CG-OD2	-7.61	111.45	118.30
3	D	2	DT	C6-C5-C7	-7.56	118.36	122.90
1	T	5	DC	N1-C2-O2	-7.47	114.42	118.90
2	P	5	DA	C8-N9-C4	7.46	108.78	105.80
1	T	2	DC	N3-C4-C5	-7.40	118.94	121.90
4	A	130	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	T	13	DC	N1-C1'-C2'	7.39	126.64	112.60
1	T	9	DG	N9-C4-C5	-7.38	102.45	105.40
1	T	2	DC	C4'-C3'-C2'	7.36	109.73	103.10
2	P	6	DT	O4'-C1'-C2'	7.36	111.79	105.90
1	T	4	DA	C5-C6-N1	-7.35	114.03	117.70
1	T	3	DG	O4'-C1'-N9	7.28	113.10	108.00
4	A	17	ASP	CB-CG-OD1	7.27	124.84	118.30
4	A	258	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	T	11	DA	O4'-C1'-N9	-7.21	102.95	108.00
1	T	11	DA	N7-C8-N9	-7.19	110.20	113.80
4	A	74	ASP	CB-CG-OD1	7.14	124.73	118.30
4	A	92	ASP	CB-CG-OD1	-7.11	111.90	118.30
3	D	4	DG	C8-N9-C4	7.07	109.23	106.40
1	T	10	DC	C2-N3-C4	-7.06	116.37	119.90
3	D	2	DT	O5'-P-OP1	-7.05	99.36	105.70
1	T	5	DC	N1-C2-N3	7.01	124.11	119.20
2	P	1	DG	C8-N9-C4	6.99	109.20	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	332	ASP	CB-CG-OD1	-6.97	112.03	118.30
2	P	5	DA	P-O5'-C5'	-6.94	109.80	120.90
4	A	132	LEU	CB-CA-C	-6.90	97.08	110.20
4	A	246	ASP	CB-CG-OD2	-6.86	112.13	118.30
2	P	8	DC	N1-C2-O2	-6.78	114.83	118.90
3	D	4	DG	O4'-C1'-N9	6.72	112.71	108.00
2	P	1	DG	N3-C4-C5	6.70	131.95	128.60
1	T	16	DC	C5-C4-N4	6.66	124.86	120.20
4	A	67	THR	CA-CB-CG2	-6.60	103.16	112.40
4	A	91	ASP	CB-CG-OD1	-6.55	112.40	118.30
2	P	3	DT	O4'-C1'-N1	6.52	112.57	108.00
3	D	1	DG	N9-C4-C5	-6.51	102.80	105.40
4	A	246	ASP	CB-CG-OD1	6.49	124.14	118.30
2	P	6	DT	C4'-C3'-C2'	6.48	108.93	103.10
4	A	130	ASP	CB-CG-OD1	6.43	124.08	118.30
1	T	16	DC	C6-N1-C2	6.37	122.85	120.30
4	A	321	ASP	CB-CG-OD1	6.34	124.01	118.30
4	A	40	ARG	N-CA-CB	6.33	122.00	110.60
4	A	190	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	T	11	DA	N9-C4-C5	-6.30	103.28	105.80
4	A	110	ALA	N-CA-CB	-6.29	101.30	110.10
4	A	148	LYS	CB-CA-C	-6.25	97.90	110.40
1	T	10	DC	P-O3'-C3'	6.24	127.19	119.70
3	D	4	DG	N3-C4-N9	-6.23	122.26	126.00
4	A	101	THR	CA-CB-OG1	-6.23	95.92	109.00
4	A	318	ASP	CB-CG-OD2	-6.22	112.70	118.30
4	A	276	ASP	CB-CG-OD1	-6.21	112.71	118.30
1	T	16	DC	P-O5'-C5'	-6.21	110.97	120.90
2	P	5	DA	N1-C6-N6	-6.20	114.88	118.60
1	T	5	DC	N1-C1'-C2'	6.19	124.36	112.60
4	A	164	ASN	N-CA-CB	6.18	121.72	110.60
4	A	321	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	T	1	DC	C6-N1-C2	6.15	122.76	120.30
2	P	5	DA	N9-C1'-C2'	6.15	124.29	112.60
4	A	258	ARG	CD-NE-CZ	6.15	132.21	123.60
3	D	5	DG	N3-C4-C5	6.14	131.67	128.60
1	T	4	DA	C2-N3-C4	-6.11	107.55	110.60
1	T	9	DG	C6-C5-N7	-6.11	126.73	130.40
1	T	14	DA	N7-C8-N9	-6.09	110.76	113.80
2	P	6	DT	C2-N3-C4	-6.05	123.57	127.20
1	T	9	DG	N3-C4-N9	6.00	129.60	126.00
4	A	263	ASP	CB-CG-OD1	-5.99	112.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	160	ASP	CB-CG-OD1	5.98	123.69	118.30
1	T	9	DG	C8-N9-C4	5.97	108.79	106.40
3	D	5	DG	O4'-C1'-N9	-5.97	103.82	108.00
4	A	164	ASN	CB-CA-C	5.95	122.29	110.40
3	D	4	DG	N3-C4-C5	5.93	131.56	128.60
2	P	5	DA	O5'-P-OP1	-5.91	100.38	105.70
2	P	5	DA	N7-C8-N9	-5.90	110.85	113.80
2	P	9	DG	N7-C8-N9	-5.86	110.17	113.10
4	A	7	PRO	C-N-CA	5.84	136.29	121.70
4	A	259	LEU	CA-CB-CG	-5.83	101.88	115.30
1	T	16	DC	O4'-C1'-C2'	5.82	110.56	105.90
2	P	4	DG	O4'-C1'-N9	5.82	112.07	108.00
3	D	4	DG	C4-N9-C1'	-5.80	118.96	126.50
2	P	1	DG	O4'-C1'-C2'	5.79	110.53	105.90
1	T	1	DC	C5-C6-N1	-5.77	118.11	121.00
1	T	9	DG	C2-N3-C4	-5.76	109.02	111.90
2	P	4	DG	N7-C8-N9	-5.76	110.22	113.10
1	T	5	DC	C2-N3-C4	-5.74	117.03	119.90
1	T	10	DC	C6-N1-C2	5.73	122.59	120.30
4	A	332	ASP	CB-CG-OD2	5.70	123.43	118.30
2	P	1	DG	N1-C6-O6	5.68	123.31	119.90
4	A	92	ASP	CB-CG-OD2	5.66	123.39	118.30
1	T	9	DG	N3-C2-N2	5.62	123.83	119.90
2	P	5	DA	C6-C5-N7	5.59	136.21	132.30
2	P	8	DC	C2-N3-C4	-5.57	117.11	119.90
4	A	53	ILE	CA-CB-CG1	-5.55	100.45	111.00
4	A	314	ASP	CB-CG-OD2	5.54	123.28	118.30
2	P	1	DG	C4'-C3'-C2'	5.50	108.05	103.10
2	P	7	DG	C8-N9-C4	5.49	108.60	106.40
4	A	212	HIS	CA-CB-CG	-5.48	104.28	113.60
2	P	6	DT	C5-C6-N1	-5.47	120.42	123.70
1	T	9	DG	N1-C2-N2	-5.43	111.31	116.20
4	A	86	GLU	CB-CA-C	5.43	121.26	110.40
3	D	4	DG	C2-N3-C4	-5.43	109.19	111.90
1	T	11	DA	C5-C6-N6	-5.42	119.37	123.70
1	T	15	DG	N3-C4-N9	-5.41	122.75	126.00
1	T	2	DC	O3'-P-O5'	5.41	114.27	104.00
2	P	1	DG	N7-C8-N9	-5.40	110.40	113.10
1	T	10	DC	N3-C4-N4	-5.39	114.22	118.00
2	P	9	DG	N1-C6-O6	-5.37	116.68	119.90
2	P	7	DG	C2-N3-C4	-5.36	109.22	111.90
4	A	36	TYR	CB-CG-CD2	-5.32	117.81	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	5	DC	C4-C5-C6	5.30	120.05	117.40
4	A	150	ILE	C-N-CD	-5.27	109.00	120.60
4	A	43	ALA	N-CA-CB	-5.27	102.72	110.10
1	T	9	DG	C4-C5-N7	5.25	112.90	110.80
1	T	16	DC	C2-N1-C1'	-5.25	113.03	118.80
4	A	243	SER	N-CA-CB	5.25	118.37	110.50
4	A	29	VAL	N-CA-CB	-5.24	99.97	111.50
4	A	72	LYS	CB-CA-C	5.23	120.86	110.40
2	P	10	DT	O4'-C1'-N1	5.21	111.65	108.00
3	D	3	DC	C4'-C3'-C2'	5.21	107.79	103.10
4	A	36	TYR	CB-CG-CD1	5.20	124.12	121.00
1	T	14	DA	C4'-C3'-C2'	5.20	107.78	103.10
4	A	9	GLU	N-CA-CB	5.20	119.95	110.60
1	T	10	DC	O4'-C4'-C3'	5.19	109.12	106.00
2	P	7	DG	N9-C4-C5	-5.19	103.32	105.40
4	A	230	LYS	CB-CA-C	5.19	120.79	110.40
1	T	13	DC	C2-N1-C1'	-5.15	113.13	118.80
4	A	192	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	T	5	DC	C5-C4-N4	5.14	123.80	120.20
4	A	86	GLU	N-CA-CB	5.13	119.84	110.60
1	T	14	DA	N9-C1'-C2'	5.12	122.33	112.60
2	P	1	DG	P-O3'-C3'	-5.12	113.56	119.70
2	P	10	DT	N3-C4-C5	5.10	118.26	115.20
2	P	2	DC	P-O3'-C3'	5.09	125.81	119.70
4	A	61	LYS	CB-CG-CD	5.08	124.81	111.60
1	T	15	DG	C5'-C4'-C3'	5.07	123.22	114.10
4	A	318	ASP	CB-CG-OD1	5.06	122.86	118.30
2	P	3	DT	C2-N3-C4	5.04	130.23	127.20
2	P	10	DT	C5-C6-N1	-5.04	120.68	123.70
4	A	19	LEU	CB-CG-CD1	-5.04	102.44	111.00
1	T	13	DC	C6-N1-C1'	5.01	126.81	120.80
1	T	4	DA	P-O5'-C5'	5.01	128.91	120.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	164	ASN	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	319	0	179	15	0
2	P	226	0	126	18	0
3	D	106	0	57	7	0
4	A	2653	0	2674	507	0
5	A	2	0	0	0	0
6	A	14	0	0	0	0
6	D	1	0	0	0	0
6	P	6	0	0	1	0
6	T	6	0	0	1	0
All	All	3333	0	3036	534	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 84.

All (534) 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)
4:A:133:ASN:ND2	4:A:136:GLN:H	1.48	1.10
4:A:313:VAL:HG11	4:A:319:ILE:HG13	1.40	1.02
4:A:277:ILE:HG13	4:A:335:GLU:HB3	1.39	1.02
4:A:194:LEU:HD12	4:A:265:TYR:HE1	1.23	1.01
4:A:182:ARG:HE	4:A:273:THR:HG21	1.25	1.00
4:A:152:ARG:HA	4:A:155:MET:HB2	1.41	0.98
4:A:194:LEU:HD11	4:A:260:ILE:HD12	1.42	0.98
4:A:133:ASN:HD21	4:A:136:GLN:H	1.13	0.96
4:A:169:VAL:HG11	4:A:214:VAL:HG12	1.48	0.94
4:A:134:HIS:CE1	4:A:138:ILE:HD11	2.03	0.93
4:A:251:PRO:HG2	4:A:253:ARG:NH2	1.85	0.91
4:A:294:ASN:HD21	4:A:297:THR:H	1.12	0.89
4:A:251:PRO:HG2	4:A:253:ARG:HH21	1.36	0.89
4:A:194:LEU:HD11	4:A:260:ILE:CD1	2.01	0.89
4:A:27:LYS:HE3	4:A:28:ASN:HD21	1.36	0.89
4:A:277:ILE:CG1	4:A:335:GLU:HB3	2.03	0.87
4:A:36:TYR:CE2	4:A:40:ARG:HD2	2.09	0.87
1:T:2:DC:H2"	1:T:3:DG:C8	2.11	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:138:ILE:H	4:A:138:ILE:HD12	1.41	0.85
4:A:135:HIS:CD2	4:A:228:LEU:HB3	2.12	0.85
4:A:150:ILE:CD1	4:A:253:ARG:HD3	2.05	0.85
4:A:195:LEU:HG	4:A:196:THR:N	1.91	0.85
4:A:18:MET:HE1	4:A:82:LEU:HD13	1.59	0.84
4:A:301:LEU:HD12	4:A:302:GLY:N	1.92	0.84
4:A:207:GLN:HB2	4:A:209:LYS:HD3	1.57	0.84
4:A:133:ASN:ND2	4:A:136:GLN:HG3	1.93	0.83
4:A:295:GLU:HG2	4:A:296:TYR:CE1	2.14	0.83
4:A:122:LEU:HD21	4:A:140:LEU:HD11	1.58	0.83
4:A:194:LEU:HD12	4:A:265:TYR:CE1	2.13	0.82
4:A:150:ILE:HD13	4:A:253:ARG:HD3	1.60	0.81
4:A:207:GLN:HB2	4:A:209:LYS:CD	2.10	0.81
3:D:4:DG:H2"	3:D:5:DG:C8	2.15	0.81
4:A:161:ILE:HG22	4:A:165:GLU:HG2	1.62	0.81
4:A:125:LEU:HB3	4:A:140:LEU:HD22	1.63	0.80
4:A:33:ILE:H	4:A:33:ILE:HD12	1.46	0.79
4:A:133:ASN:ND2	4:A:136:GLN:N	2.30	0.79
4:A:150:ILE:HD11	4:A:253:ARG:HB3	1.65	0.79
1:T:8:DC:H5"	4:A:296:TYR:OH	1.83	0.78
4:A:294:ASN:ND2	4:A:297:THR:H	1.81	0.78
4:A:155:MET:CE	4:A:188:SER:HB2	2.14	0.78
4:A:18:MET:CE	4:A:82:LEU:HD22	2.14	0.78
4:A:37:ASN:HA	4:A:40:ARG:HG3	1.66	0.78
4:A:27:LYS:HE3	4:A:28:ASN:ND2	1.98	0.78
4:A:18:MET:CE	4:A:82:LEU:HD13	2.13	0.77
4:A:41:LYS:O	4:A:45:VAL:HG13	1.83	0.77
4:A:133:ASN:CG	4:A:136:GLN:HG3	2.05	0.77
4:A:313:VAL:HG11	4:A:319:ILE:CG1	2.15	0.77
4:A:278:PHE:CE2	4:A:333:ARG:HG2	2.19	0.77
4:A:208:PRO:HD2	4:A:209:LYS:HD2	1.65	0.77
4:A:90:GLN:NE2	4:A:91:ASP:N	2.32	0.77
4:A:122:LEU:CD2	4:A:140:LEU:HD11	2.14	0.77
4:A:317:LYS:HD3	4:A:327:TYR:HB2	1.68	0.76
4:A:169:VAL:HG22	4:A:173:TYR:HE2	1.49	0.76
4:A:174:ILE:C	4:A:195:LEU:HD12	2.05	0.76
4:A:146:PHE:CE1	4:A:254:ARG:HG2	2.21	0.76
4:A:67:THR:O	4:A:71:GLU:HG3	1.86	0.75
4:A:241:LEU:HD22	4:A:242:PRO:HD2	1.69	0.75
4:A:230:LYS:HB3	4:A:230:LYS:NZ	2.02	0.75
4:A:200:PHE:CE2	4:A:259:LEU:HG	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:196:THR:HG23	4:A:265:TYR:CE1	2.23	0.74
4:A:169:VAL:CG2	4:A:213:GLN:HE21	2.00	0.74
4:A:162:VAL:O	4:A:166:VAL:HG13	1.88	0.73
4:A:270:LEU:CD2	4:A:319:ILE:HG21	2.18	0.73
4:A:182:ARG:HE	4:A:273:THR:CG2	1.99	0.73
4:A:38:ALA:O	4:A:41:LYS:HE2	1.88	0.73
4:A:211:LEU:O	4:A:215:VAL:HG23	1.88	0.73
4:A:196:THR:CG2	4:A:260:ILE:HB	2.18	0.73
4:A:287:LEU:HD22	4:A:291:PHE:O	1.89	0.73
4:A:150:ILE:HB	4:A:155:MET:HE3	1.71	0.73
4:A:241:LEU:CD2	4:A:242:PRO:HD2	2.19	0.73
4:A:218:LEU:HD22	4:A:223:PHE:CD2	2.24	0.73
4:A:285:HIS:HD2	4:A:323:ILE:HD12	1.53	0.72
4:A:207:GLN:HB2	4:A:209:LYS:NZ	2.04	0.72
4:A:174:ILE:O	4:A:195:LEU:HD12	1.90	0.72
4:A:22:LEU:CD1	4:A:85:LEU:HD13	2.20	0.72
4:A:197:HIS:CG	4:A:198:PRO:HD2	2.26	0.71
4:A:138:ILE:N	4:A:138:ILE:HD12	2.02	0.71
4:A:26:GLU:OE1	4:A:35:LYS:HD2	1.89	0.71
4:A:156:LEU:O	4:A:159:GLN:HG2	1.91	0.71
4:A:169:VAL:HG23	4:A:213:GLN:HE21	1.56	0.71
2:P:2:DC:H2''	2:P:3:DT:O5'	1.90	0.71
4:A:317:LYS:HD3	4:A:327:TYR:CD2	2.25	0.71
4:A:201:THR:HG22	4:A:204:SER:HB3	1.74	0.70
2:P:11:DG:H4'	4:A:258:ARG:NH1	2.06	0.70
4:A:210:LEU:O	4:A:214:VAL:HG22	1.91	0.70
4:A:236:MET:HA	4:A:256:ASP:OD1	1.91	0.69
4:A:154:GLU:O	4:A:158:MET:HG3	1.92	0.69
4:A:19:LEU:HD12	4:A:43:ALA:CA	2.22	0.69
4:A:228:LEU:CD2	4:A:237:GLY:HA2	2.23	0.69
4:A:123:GLU:O	4:A:126:ARG:HB2	1.91	0.69
4:A:270:LEU:HD22	4:A:319:ILE:HG21	1.73	0.69
4:A:196:THR:HG22	4:A:260:ILE:HB	1.75	0.69
4:A:152:ARG:O	4:A:156:LEU:HG	1.93	0.69
4:A:207:GLN:HB2	4:A:209:LYS:CE	2.22	0.69
4:A:266:TYR:HA	4:A:269:VAL:HB	1.72	0.69
4:A:158:MET:HE3	4:A:253:ARG:HD2	1.75	0.68
4:A:236:MET:HG2	4:A:256:ASP:OD1	1.93	0.68
4:A:32:ALA:HB1	4:A:35:LYS:HB2	1.76	0.68
4:A:93:THR:O	4:A:97:ILE:HG13	1.93	0.68
2:P:11:DG:H4'	4:A:258:ARG:HH12	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:174:ILE:O	4:A:195:LEU:HA	1.94	0.68
4:A:158:MET:CE	4:A:253:ARG:HD2	2.24	0.68
2:P:11:DG:H5''	4:A:192:ASP:OD2	1.92	0.68
4:A:194:LEU:HD22	4:A:258:ARG:HB2	1.75	0.68
4:A:36:TYR:CZ	4:A:40:ARG:HD2	2.28	0.68
4:A:286:ALA:CB	4:A:323:ILE:HG21	2.23	0.68
4:A:59:ALA:HA	4:A:62:LEU:HD23	1.75	0.68
4:A:194:LEU:HD13	4:A:195:LEU:H	1.58	0.68
4:A:218:LEU:HD22	4:A:223:PHE:HD2	1.58	0.68
1:T:1:DC:H6	1:T:1:DC:HO5'	1.42	0.67
4:A:301:LEU:HD12	4:A:302:GLY:H	1.58	0.67
4:A:152:ARG:NH2	4:A:184:GLY:HA2	2.09	0.67
4:A:138:ILE:O	4:A:141:LYS:HB3	1.94	0.67
4:A:293:ILE:HG22	4:A:294:ASN:N	2.09	0.67
4:A:122:LEU:HD21	4:A:140:LEU:CD1	2.24	0.67
4:A:15:ILE:CG2	4:A:46:ILE:HD13	2.24	0.67
4:A:293:ILE:HG22	4:A:294:ASN:H	1.58	0.67
4:A:226:ASP:N	4:A:226:ASP:OD1	2.28	0.67
4:A:69:ILE:O	4:A:73:ILE:HG13	1.95	0.66
4:A:271:TYR:CD2	4:A:295:GLU:HB3	2.29	0.66
4:A:313:VAL:CG1	4:A:319:ILE:HG13	2.20	0.66
4:A:122:LEU:HA	4:A:125:LEU:HD12	1.78	0.66
4:A:169:VAL:HG22	4:A:173:TYR:CE2	2.31	0.66
4:A:294:ASN:HD21	4:A:297:THR:N	1.91	0.66
4:A:170:ASP:HB3	4:A:173:TYR:CD2	2.31	0.66
4:A:18:MET:HE2	4:A:82:LEU:HD22	1.77	0.66
4:A:42:ALA:O	4:A:45:VAL:HG22	1.95	0.66
4:A:265:TYR:O	4:A:268:GLY:N	2.29	0.66
4:A:110:ALA:HA	4:A:113:LYS:HE2	1.79	0.65
4:A:159:GLN:O	4:A:163:LEU:HD23	1.95	0.65
4:A:270:LEU:HD22	4:A:319:ILE:HD13	1.78	0.65
4:A:152:ARG:CA	4:A:155:MET:HB2	2.20	0.65
4:A:224:ILE:HG23	4:A:238:VAL:O	1.96	0.65
2:P:7:DG:H2''	2:P:8:DC:O5'	1.95	0.65
4:A:270:LEU:CD2	4:A:319:ILE:HD13	2.26	0.65
4:A:201:THR:C	4:A:261:PRO:HB3	2.17	0.65
4:A:125:LEU:HB3	4:A:140:LEU:CD2	2.26	0.65
4:A:150:ILE:CG2	4:A:155:MET:HG2	2.26	0.65
4:A:228:LEU:HD22	4:A:228:LEU:N	2.12	0.65
4:A:132:LEU:HD13	4:A:136:GLN:CB	2.27	0.64
4:A:28:ASN:O	4:A:108:PRO:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:244:LYS:HB3	4:A:247:GLU:HB2	1.79	0.64
4:A:286:ALA:HA	4:A:323:ILE:CG2	2.27	0.64
4:A:201:THR:HG22	4:A:204:SER:CB	2.26	0.64
4:A:196:THR:HA	4:A:259:LEU:CD1	2.27	0.64
4:A:153:GLU:O	4:A:156:LEU:HB2	1.98	0.64
4:A:317:LYS:HB2	4:A:327:TYR:CD2	2.32	0.64
4:A:326:LYS:O	4:A:326:LYS:HG3	1.98	0.64
4:A:207:GLN:CB	4:A:209:LYS:HD3	2.28	0.63
4:A:216:GLU:HA	4:A:219:GLN:OE1	1.98	0.63
4:A:173:TYR:OH	4:A:210:LEU:HA	1.97	0.63
1:T:2:DC:H2"	1:T:3:DG:H8	1.63	0.63
4:A:132:LEU:HD13	4:A:136:GLN:HB2	1.79	0.63
4:A:154:GLU:OE1	4:A:253:ARG:NH1	2.32	0.63
4:A:255:ILE:HG12	4:A:256:ASP:N	2.14	0.63
4:A:278:PHE:HB2	4:A:333:ARG:O	1.99	0.63
4:A:285:HIS:HE1	4:A:289:LYS:NZ	1.96	0.63
4:A:133:ASN:HD21	4:A:136:GLN:N	1.91	0.62
4:A:323:ILE:C	4:A:324:GLN:HG2	2.18	0.62
4:A:87:LYS:O	4:A:90:GLN:NE2	2.30	0.62
4:A:317:LYS:HB2	4:A:327:TYR:CE2	2.34	0.62
4:A:155:MET:HE3	4:A:188:SER:HB2	1.80	0.62
4:A:238:VAL:HG12	4:A:239:CYS:N	2.15	0.62
1:T:14:DA:H2"	1:T:15:DG:O5'	1.99	0.62
4:A:59:ALA:O	4:A:62:LEU:N	2.29	0.62
4:A:169:VAL:CG2	4:A:173:TYR:HE2	2.13	0.61
4:A:317:LYS:CD	4:A:327:TYR:HB2	2.28	0.61
4:A:283:ARG:NH2	4:A:294:ASN:HA	2.14	0.61
4:A:87:LYS:HA	4:A:90:GLN:HG3	1.81	0.61
4:A:90:GLN:HE21	4:A:91:ASP:N	1.97	0.61
4:A:91:ASP:OD2	4:A:94:SER:HB3	2.00	0.61
4:A:7:PRO:O	4:A:8:GLN:HG2	1.99	0.61
4:A:190:ASP:OD1	4:A:190:ASP:N	2.29	0.61
4:A:152:ARG:O	4:A:156:LEU:N	2.29	0.61
4:A:317:LYS:HD3	4:A:327:TYR:HD2	1.65	0.61
4:A:172:GLU:HB3	4:A:198:PRO:CG	2.29	0.61
2:P:1:DG:H2"	2:P:2:DC:O5'	2.00	0.61
4:A:194:LEU:CD1	4:A:265:TYR:HE1	2.07	0.61
4:A:332:ASP:OD1	4:A:332:ASP:N	2.29	0.60
4:A:285:HIS:NE2	4:A:323:ILE:O	2.35	0.60
4:A:278:PHE:HA	4:A:335:GLU:HA	1.83	0.60
4:A:250:TYR:HB3	4:A:251:PRO:CD	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:102:ARG:NH2	4:A:147:GLU:OE1	2.29	0.60
4:A:172:GLU:HB3	4:A:198:PRO:HG2	1.82	0.60
4:A:300:PRO:HD3	4:A:311:LEU:HD13	1.83	0.60
4:A:186:GLU:N	4:A:186:GLU:OE1	2.29	0.60
4:A:7:PRO:C	4:A:8:GLN:HG2	2.22	0.60
4:A:309:GLU:OE1	4:A:309:GLU:HA	2.02	0.60
4:A:177:VAL:HG12	4:A:178:CYS:N	2.17	0.60
4:A:192:ASP:HB3	4:A:258:ARG:NH2	2.17	0.60
4:A:200:PHE:HE2	4:A:259:LEU:HG	1.63	0.60
4:A:18:MET:HE1	4:A:82:LEU:CD1	2.31	0.60
4:A:122:LEU:HD22	4:A:126:ARG:CZ	2.32	0.59
4:A:161:ILE:CG2	4:A:165:GLU:HG2	2.29	0.59
4:A:270:LEU:HD22	4:A:319:ILE:CD1	2.31	0.59
4:A:180:SER:O	4:A:183:ARG:N	2.35	0.59
2:P:11:DG:N2	4:A:271:TYR:OH	2.29	0.59
4:A:15:ILE:O	4:A:18:MET:HG2	2.02	0.59
4:A:65:VAL:HG12	4:A:66:GLY:N	2.18	0.59
4:A:48:LYS:O	4:A:50:PRO:HD3	2.03	0.59
4:A:150:ILE:HG22	4:A:155:MET:HG2	1.85	0.59
4:A:21:GLU:CG	4:A:85:LEU:HD21	2.32	0.59
4:A:207:GLN:OE1	4:A:209:LYS:HE2	2.03	0.58
4:A:209:LYS:O	4:A:213:GLN:HB3	2.02	0.58
4:A:110:ALA:O	4:A:113:LYS:HB3	2.03	0.58
4:A:298:ILE:HG23	4:A:311:LEU:HB2	1.85	0.58
4:A:192:ASP:HB3	4:A:258:ARG:HH22	1.68	0.58
4:A:196:THR:HG22	4:A:260:ILE:H	1.68	0.58
4:A:135:HIS:HD2	4:A:228:LEU:HB3	1.66	0.58
4:A:150:ILE:HG23	4:A:253:ARG:HH11	1.69	0.58
4:A:228:LEU:HB2	4:A:236:MET:O	2.04	0.58
4:A:150:ILE:O	4:A:187:SER:HA	2.04	0.58
4:A:25:PHE:CD2	4:A:88:ILE:HG21	2.38	0.58
4:A:326:LYS:NZ	4:A:328:ARG:HA	2.19	0.57
4:A:177:VAL:HG12	4:A:178:CYS:H	1.69	0.57
4:A:193:VAL:O	4:A:258:ARG:N	2.37	0.57
4:A:264:GLN:OE1	4:A:296:TYR:HB3	2.05	0.57
4:A:26:GLU:HA	4:A:30:SER:HB2	1.87	0.57
4:A:155:MET:HE1	4:A:188:SER:HB2	1.87	0.57
4:A:288:GLU:OE1	4:A:288:GLU:HA	2.04	0.56
4:A:19:LEU:HD12	4:A:43:ALA:HA	1.87	0.56
4:A:25:PHE:CE2	4:A:88:ILE:HG12	2.40	0.56
4:A:18:MET:HE1	4:A:82:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:228:LEU:HD22	4:A:237:GLY:HA2	1.87	0.56
4:A:200:PHE:CD2	4:A:259:LEU:HD21	2.41	0.56
4:A:228:LEU:HD23	4:A:237:GLY:HA2	1.87	0.56
4:A:299:ARG:HG2	4:A:310:PRO:HA	1.88	0.56
4:A:299:ARG:HG2	4:A:310:PRO:CA	2.36	0.55
2:P:1:DG:H8	2:P:1:DG:H5'	1.70	0.55
4:A:99:PHE:HD1	4:A:102:ARG:HD3	1.71	0.55
4:A:33:ILE:N	4:A:33:ILE:HD12	2.19	0.55
4:A:196:THR:HB	4:A:260:ILE:O	2.06	0.55
4:A:15:ILE:HG21	4:A:46:ILE:HD13	1.87	0.55
4:A:201:THR:HG22	4:A:204:SER:OG	2.07	0.54
4:A:259:LEU:HD12	4:A:260:ILE:N	2.23	0.54
4:A:206:LYS:O	4:A:208:PRO:HD3	2.07	0.54
4:A:169:VAL:HG23	4:A:213:GLN:NE2	2.21	0.54
4:A:323:ILE:O	4:A:324:GLN:HG2	2.06	0.54
4:A:259:LEU:HD12	4:A:260:ILE:H	1.72	0.54
4:A:23:ALA:O	4:A:36:TYR:HD1	1.90	0.54
3:D:1:DG:OP1	4:A:68:LYS:NZ	2.30	0.54
4:A:192:ASP:CB	4:A:258:ARG:HH22	2.20	0.54
4:A:134:HIS:ND1	4:A:138:ILE:HD11	2.22	0.54
4:A:12:ASN:HB3	4:A:46:ILE:HD12	1.90	0.54
4:A:326:LYS:HZ2	4:A:328:ARG:HA	1.71	0.54
4:A:12:ASN:HD21	4:A:53:ILE:H	1.55	0.54
4:A:123:GLU:O	4:A:127:LYS:HG3	2.08	0.54
4:A:169:VAL:CG1	4:A:214:VAL:HG12	2.30	0.53
1:T:7:DA:H2''	1:T:8:DC:O5'	2.07	0.53
4:A:18:MET:HG3	4:A:19:LEU:N	2.23	0.53
4:A:230:LYS:HB3	4:A:230:LYS:HZ1	1.71	0.53
4:A:240:GLN:HG2	4:A:241:LEU:N	2.24	0.53
4:A:21:GLU:HB3	4:A:85:LEU:HD21	1.90	0.53
4:A:164:ASN:O	4:A:167:LYS:HB3	2.08	0.53
4:A:241:LEU:HB2	4:A:250:TYR:CD2	2.42	0.53
4:A:38:ALA:O	4:A:41:LYS:N	2.41	0.53
4:A:305:GLY:O	4:A:306:VAL:HG13	2.08	0.53
4:A:298:ILE:HD13	4:A:322:TYR:HD2	1.72	0.53
4:A:115:VAL:HA	4:A:119:ILE:O	2.08	0.53
4:A:160:ASP:OD1	4:A:164:ASN:ND2	2.42	0.53
4:A:61:LYS:HG2	4:A:61:LYS:O	2.05	0.53
4:A:286:ALA:HB2	4:A:323:ILE:HG21	1.90	0.53
4:A:25:PHE:HE2	4:A:88:ILE:HG12	1.74	0.53
4:A:196:THR:HA	4:A:259:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:10:DT:H2"	2:P:11:DG:C8	2.44	0.53
4:A:302:GLY:HA2	4:A:307:ALA:HB3	1.91	0.53
4:A:298:ILE:HD13	4:A:322:TYR:CD2	2.44	0.53
4:A:193:VAL:O	4:A:257:ILE:HA	2.09	0.53
4:A:21:GLU:CB	4:A:85:LEU:HD21	2.38	0.53
4:A:196:THR:HG22	4:A:260:ILE:CB	2.38	0.52
4:A:140:LEU:O	4:A:140:LEU:HD12	2.08	0.52
4:A:102:ARG:HH21	4:A:147:GLU:CD	2.10	0.52
4:A:197:HIS:ND1	4:A:198:PRO:N	2.58	0.52
4:A:216:GLU:HA	4:A:219:GLN:HB2	1.90	0.52
4:A:287:LEU:HA	4:A:291:PHE:O	2.09	0.52
4:A:235:PHE:CZ	4:A:237:GLY:HA3	2.44	0.52
4:A:301:LEU:HD11	4:A:306:VAL:HA	1.90	0.52
4:A:121:THR:O	4:A:125:LEU:HG	2.10	0.52
4:A:138:ILE:H	4:A:138:ILE:CD1	2.18	0.52
4:A:209:LYS:O	4:A:213:GLN:N	2.29	0.52
4:A:33:ILE:H	4:A:33:ILE:CD1	2.13	0.52
4:A:110:ALA:HA	4:A:113:LYS:CE	2.39	0.52
4:A:278:PHE:CD2	4:A:333:ARG:HB3	2.45	0.52
4:A:122:LEU:HD22	4:A:126:ARG:NH1	2.25	0.52
4:A:116:ASP:C	4:A:118:GLY:H	2.14	0.52
4:A:221:VAL:HG22	4:A:221:VAL:O	2.09	0.51
1:T:8:DC:H5"	4:A:296:TYR:HH	1.75	0.51
4:A:150:ILE:HG21	4:A:155:MET:HG2	1.92	0.51
4:A:94:SER:O	4:A:98:ASN:N	2.40	0.51
4:A:22:LEU:HD11	4:A:85:LEU:HD13	1.91	0.51
4:A:126:ARG:O	4:A:129:GLU:OE1	2.28	0.51
4:A:173:TYR:CE1	4:A:210:LEU:HD22	2.45	0.51
4:A:25:PHE:CE2	4:A:88:ILE:HD13	2.46	0.51
4:A:267:CYS:O	4:A:270:LEU:HB3	2.11	0.51
4:A:194:LEU:HD13	4:A:195:LEU:N	2.23	0.51
4:A:296:TYR:CD1	4:A:296:TYR:N	2.79	0.51
4:A:173:TYR:OH	4:A:210:LEU:HD23	2.10	0.51
4:A:76:PHE:O	4:A:80:GLY:N	2.41	0.51
4:A:15:ILE:HG22	4:A:46:ILE:HD13	1.92	0.50
4:A:266:TYR:O	4:A:270:LEU:N	2.29	0.50
4:A:275:SER:N	4:A:278:PHE:HB3	2.26	0.50
4:A:162:VAL:HA	4:A:218:LEU:HD21	1.92	0.50
4:A:32:ALA:CB	4:A:35:LYS:HB2	2.40	0.50
4:A:110:ALA:O	4:A:113:LYS:N	2.44	0.50
4:A:134:HIS:O	4:A:137:ARG:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:33:ILE:O	4:A:37:ASN:OD1	2.30	0.50
1:T:15:DG:H2''	1:T:16:DC:C6	2.47	0.50
2:P:11:DG:O3'	4:A:272:PHE:O	2.29	0.50
4:A:151:PRO:O	4:A:154:GLU:N	2.44	0.50
4:A:314:ASP:O	4:A:315:SER:HB2	2.12	0.50
4:A:303:VAL:HG13	4:A:304:THR:HG23	1.92	0.50
4:A:196:THR:HG22	4:A:260:ILE:N	2.27	0.50
4:A:329:GLU:O	4:A:333:ARG:HG3	2.11	0.49
4:A:87:LYS:O	4:A:90:GLN:HG3	2.12	0.49
4:A:289:LYS:N	4:A:289:LYS:HD3	2.19	0.49
2:P:1:DG:H2'	2:P:2:DC:C6	2.47	0.49
4:A:150:ILE:HG22	4:A:155:MET:CG	2.42	0.49
4:A:285:HIS:HB2	4:A:325:TRP:CZ2	2.48	0.49
4:A:96:SER:HB3	4:A:120:LYS:HB2	1.94	0.49
4:A:209:LYS:HD2	4:A:209:LYS:H	1.77	0.49
4:A:285:HIS:CE1	4:A:289:LYS:NZ	2.80	0.49
4:A:58:GLU:O	4:A:61:LYS:HB3	2.13	0.49
4:A:112:ARG:O	4:A:116:ASP:OD1	2.30	0.49
4:A:207:GLN:HB2	4:A:209:LYS:HZ2	1.74	0.49
4:A:183:ARG:O	4:A:185:ALA:N	2.45	0.49
4:A:132:LEU:HA	4:A:136:GLN:HE21	1.78	0.49
4:A:297:THR:HB	4:A:310:PRO:HB3	1.94	0.49
4:A:165:GLU:CB	4:A:218:LEU:HG	2.43	0.49
4:A:155:MET:O	4:A:158:MET:HB2	2.12	0.48
4:A:241:LEU:HD23	4:A:242:PRO:HD2	1.94	0.48
4:A:28:ASN:OD1	4:A:98:ASN:ND2	2.46	0.48
4:A:285:HIS:CD2	4:A:325:TRP:CE2	3.01	0.48
4:A:194:LEU:CD1	4:A:195:LEU:N	2.77	0.48
4:A:202:SER:N	4:A:261:PRO:HB3	2.27	0.48
4:A:202:SER:OG	4:A:264:GLN:NE2	2.46	0.48
4:A:275:SER:OG	4:A:276:ASP:N	2.38	0.48
4:A:294:ASN:ND2	4:A:297:THR:O	2.46	0.48
2:P:11:DG:OP1	4:A:190:ASP:OD2	2.31	0.48
4:A:201:THR:HA	4:A:261:PRO:CB	2.44	0.48
4:A:240:GLN:CG	4:A:241:LEU:N	2.76	0.48
4:A:243:SER:OG	4:A:247:GLU:O	2.31	0.48
4:A:132:LEU:HD13	4:A:136:GLN:HB3	1.96	0.48
4:A:209:LYS:H	4:A:209:LYS:CD	2.27	0.48
4:A:49:TYR:CD2	4:A:53:ILE:HD11	2.48	0.48
4:A:302:GLY:HA2	4:A:307:ALA:CB	2.44	0.48
4:A:62:LEU:HB3	4:A:63:PRO:HD2	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:202:SER:HG	4:A:264:GLN:NE2	2.12	0.48
4:A:195:LEU:O	4:A:259:LEU:HA	2.13	0.48
4:A:225:THR:OG1	4:A:226:ASP:OD1	2.28	0.48
4:A:200:PHE:CZ	4:A:261:PRO:HD3	2.49	0.48
4:A:328:ARG:NH1	4:A:332:ASP:O	2.46	0.48
4:A:132:LEU:HA	4:A:136:GLN:NE2	2.29	0.48
4:A:99:PHE:O	4:A:102:ARG:HG3	2.14	0.48
4:A:9:GLU:C	4:A:11:LEU:H	2.18	0.47
4:A:133:ASN:HD22	4:A:135:HIS:N	2.13	0.47
4:A:196:THR:HG22	4:A:260:ILE:CA	2.43	0.47
4:A:165:GLU:O	4:A:217:GLN:HG2	2.15	0.47
4:A:19:LEU:HD12	4:A:43:ALA:HB2	1.97	0.47
4:A:285:HIS:CG	4:A:325:TRP:CE2	3.03	0.47
2:P:1:DG:C8	2:P:1:DG:H5'	2.48	0.47
2:P:1:DG:H2'	2:P:2:DC:C5	2.50	0.47
4:A:150:ILE:HD12	4:A:155:MET:HE2	1.96	0.47
4:A:326:LYS:O	4:A:328:ARG:N	2.48	0.47
4:A:65:VAL:CG1	4:A:66:GLY:N	2.78	0.47
4:A:133:ASN:HD22	4:A:133:ASN:C	2.18	0.47
4:A:236:MET:HE3	4:A:254:ARG:NH2	2.30	0.47
4:A:200:PHE:CD2	4:A:259:LEU:HG	2.50	0.47
4:A:151:PRO:O	4:A:153:GLU:N	2.47	0.47
4:A:240:GLN:CG	4:A:241:LEU:H	2.27	0.47
4:A:197:HIS:ND1	4:A:198:PRO:HD2	2.29	0.47
4:A:75:GLU:OE1	4:A:82:LEU:HD12	2.15	0.47
4:A:169:VAL:HG11	4:A:214:VAL:CG1	2.33	0.47
4:A:186:GLU:O	4:A:187:SER:HB3	2.15	0.47
4:A:91:ASP:OD2	4:A:94:SER:N	2.37	0.47
4:A:232:GLU:HG3	4:A:233:THR:HG23	1.97	0.47
4:A:19:LEU:HD12	4:A:43:ALA:CB	2.45	0.46
4:A:201:THR:CA	4:A:261:PRO:HB3	2.46	0.46
4:A:294:ASN:HD22	4:A:294:ASN:C	2.17	0.46
3:D:2:DT:H4'	4:A:41:LYS:NZ	2.31	0.46
4:A:255:ILE:CG1	4:A:256:ASP:N	2.78	0.46
4:A:196:THR:CG2	4:A:265:TYR:CD1	2.99	0.46
4:A:170:ASP:CB	4:A:173:TYR:CD2	2.99	0.46
4:A:72:LYS:HD3	4:A:82:LEU:HD21	1.97	0.46
2:P:1:DG:C2'	2:P:2:DC:C6	2.99	0.46
4:A:138:ILE:HG23	4:A:142:TYR:CE2	2.50	0.46
4:A:18:MET:CG	4:A:19:LEU:N	2.79	0.46
4:A:165:GLU:OE1	4:A:168:LYS:NZ	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:59:ALA:O	4:A:62:LEU:HB2	2.16	0.46
4:A:59:ALA:O	4:A:62:LEU:HD23	2.16	0.46
4:A:152:ARG:NH2	4:A:181:PHE:O	2.49	0.46
4:A:279:ASN:HD22	4:A:279:ASN:HA	1.54	0.46
4:A:161:ILE:HG22	4:A:218:LEU:CD2	2.46	0.46
4:A:165:GLU:OE1	4:A:221:VAL:HG11	2.16	0.46
4:A:317:LYS:HD3	4:A:327:TYR:CB	2.44	0.46
4:A:122:LEU:O	4:A:126:ARG:HG2	2.15	0.46
4:A:317:LYS:O	4:A:321:ASP:OD1	2.34	0.46
4:A:197:HIS:ND1	4:A:198:PRO:CD	2.79	0.46
4:A:238:VAL:CG1	4:A:239:CYS:N	2.79	0.46
4:A:212:HIS:NE2	4:A:216:GLU:OE2	2.49	0.45
4:A:285:HIS:CB	4:A:325:TRP:CZ2	3.00	0.45
4:A:293:ILE:CG2	4:A:294:ASN:H	2.27	0.45
4:A:18:MET:HE3	4:A:82:LEU:HD13	1.93	0.45
4:A:285:HIS:CE1	4:A:289:LYS:HE3	2.52	0.45
4:A:6:ALA:HB2	4:A:48:LYS:HE2	1.98	0.45
4:A:228:LEU:HD23	4:A:237:GLY:CA	2.47	0.45
4:A:192:ASP:OD1	4:A:192:ASP:N	2.44	0.45
4:A:196:THR:HG21	4:A:265:TYR:CD1	2.52	0.45
3:D:4:DG:H2''	3:D:5:DG:H8	1.75	0.45
4:A:241:LEU:CB	4:A:250:TYR:CD2	2.99	0.45
1:T:15:DG:C2'	1:T:16:DC:C6	2.99	0.45
2:P:10:DT:C2'	2:P:11:DG:C8	3.00	0.45
4:A:289:LYS:HD3	4:A:289:LYS:HA	1.54	0.45
4:A:254:ARG:NH1	4:A:255:ILE:O	2.40	0.45
4:A:278:PHE:CA	4:A:335:GLU:HA	2.46	0.45
4:A:163:LEU:CD2	4:A:163:LEU:N	2.80	0.45
4:A:302:GLY:CA	4:A:307:ALA:HB3	2.47	0.45
4:A:274:GLY:HA3	4:A:275:SER:HA	1.64	0.45
4:A:202:SER:HG	4:A:263:ASP:CG	2.20	0.45
4:A:106:ILE:HG23	4:A:110:ALA:HB3	1.99	0.45
4:A:99:PHE:CD1	4:A:102:ARG:HD3	2.50	0.45
4:A:207:GLN:HG3	4:A:210:LEU:HG	1.98	0.45
4:A:236:MET:CE	4:A:254:ARG:NH2	2.80	0.45
4:A:254:ARG:NH2	4:A:256:ASP:OD2	2.48	0.45
4:A:138:ILE:N	4:A:138:ILE:CD1	2.77	0.45
4:A:12:ASN:HB3	4:A:46:ILE:CD1	2.47	0.45
4:A:106:ILE:HG22	4:A:107:GLY:O	2.17	0.45
4:A:182:ARG:NE	4:A:273:THR:HG21	2.10	0.44
4:A:202:SER:N	4:A:261:PRO:CB	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:300:PRO:HD2	4:A:309:GLU:O	2.17	0.44
4:A:96:SER:CB	4:A:120:LYS:HB2	2.47	0.44
4:A:194:LEU:HD13	4:A:258:ARG:O	2.16	0.44
4:A:241:LEU:HA	4:A:241:LEU:HD23	1.66	0.44
4:A:90:GLN:NE2	4:A:91:ASP:CA	2.79	0.44
4:A:103:VAL:HG22	4:A:143:PHE:CD1	2.52	0.44
4:A:299:ARG:HG2	4:A:310:PRO:N	2.32	0.44
4:A:96:SER:O	4:A:100:LEU:HB2	2.18	0.44
4:A:152:ARG:NH2	4:A:184:GLY:CA	2.77	0.44
4:A:161:ILE:HG22	4:A:165:GLU:CG	2.40	0.44
4:A:25:PHE:CE2	4:A:88:ILE:CG2	3.00	0.44
4:A:228:LEU:HD22	4:A:228:LEU:H	1.80	0.44
4:A:22:LEU:HA	4:A:22:LEU:HD12	1.78	0.44
4:A:25:PHE:CE2	4:A:88:ILE:CG1	3.00	0.44
4:A:177:VAL:HG13	4:A:192:ASP:O	2.17	0.44
4:A:150:ILE:HG12	4:A:253:ARG:CZ	2.47	0.44
4:A:19:LEU:O	4:A:22:LEU:HB2	2.17	0.44
3:D:1:DG:P	4:A:68:LYS:HD3	2.58	0.44
2:P:4:DG:N7	6:P:506:HOH:O	2.35	0.44
4:A:317:LYS:HE3	4:A:321:ASP:OD1	2.17	0.44
4:A:197:HIS:CG	4:A:198:PRO:CD	2.99	0.44
4:A:271:TYR:CD2	4:A:295:GLU:CB	3.00	0.44
4:A:241:LEU:HB3	4:A:250:TYR:CE2	2.54	0.43
4:A:27:LYS:HB3	4:A:28:ASN:H	1.53	0.43
4:A:301:LEU:HA	4:A:301:LEU:HD13	1.89	0.43
4:A:218:LEU:CD2	4:A:223:PHE:CD2	2.99	0.43
4:A:76:PHE:HA	4:A:81:LYS:O	2.18	0.43
4:A:195:LEU:HA	4:A:265:TYR:OH	2.18	0.43
4:A:150:ILE:HA	4:A:151:PRO:HD2	1.90	0.43
4:A:279:ASN:O	4:A:283:ARG:HG3	2.18	0.43
4:A:161:ILE:O	4:A:165:GLU:HG2	2.18	0.43
1:T:1:DC:H6	1:T:1:DC:O5'	1.97	0.43
4:A:179:GLY:O	4:A:183:ARG:HG3	2.18	0.43
4:A:87:LYS:CA	4:A:90:GLN:HG3	2.47	0.43
4:A:295:GLU:HG2	4:A:296:TYR:CD1	2.51	0.43
4:A:141:LYS:HB3	4:A:142:TYR:H	1.52	0.43
4:A:85:LEU:HA	4:A:85:LEU:HD12	1.58	0.43
4:A:270:LEU:HD23	4:A:319:ILE:HD13	1.98	0.43
4:A:196:THR:HA	4:A:259:LEU:HD11	2.01	0.43
4:A:11:LEU:HA	4:A:11:LEU:HD23	1.78	0.43
4:A:213:GLN:O	4:A:216:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:123:GLU:CD	4:A:123:GLU:H	2.22	0.43
4:A:122:LEU:HD23	4:A:140:LEU:HD11	1.99	0.43
4:A:10:THR:HG22	4:A:10:THR:H	1.56	0.43
4:A:259:LEU:HA	4:A:259:LEU:HD12	1.72	0.43
4:A:224:ILE:HA	4:A:239:CYS:HA	2.00	0.43
1:T:9:DG:H2"	1:T:10:DC:H6	1.84	0.43
4:A:33:ILE:CD1	4:A:33:ILE:N	2.82	0.43
4:A:165:GLU:HB3	4:A:218:LEU:HG	2.01	0.43
4:A:25:PHE:CE2	4:A:88:ILE:CD1	3.01	0.43
4:A:301:LEU:CD1	4:A:306:VAL:HA	2.48	0.42
4:A:165:GLU:CG	4:A:218:LEU:CD2	2.97	0.42
4:A:294:ASN:HD22	4:A:294:ASN:N	2.16	0.42
4:A:37:ASN:HA	4:A:40:ARG:CG	2.45	0.42
4:A:301:LEU:HD12	4:A:301:LEU:C	2.32	0.42
4:A:228:LEU:O	4:A:229:SER:HB3	2.18	0.42
4:A:122:LEU:CD2	4:A:126:ARG:CZ	2.97	0.42
4:A:23:ALA:C	4:A:36:TYR:HD1	2.22	0.42
3:D:2:DT:H5"	4:A:64:GLY:O	2.20	0.42
4:A:29:VAL:HG12	4:A:29:VAL:O	2.19	0.42
4:A:269:VAL:O	4:A:273:THR:OG1	2.30	0.42
4:A:320:PHE:CD2	4:A:327:TYR:HA	2.54	0.42
1:T:15:DG:H2"	1:T:16:DC:O5'	2.20	0.42
4:A:191:MET:HG3	4:A:192:ASP:N	2.34	0.42
4:A:142:TYR:CE1	4:A:252:HIS:ND1	2.87	0.42
4:A:289:LYS:CD	4:A:289:LYS:N	2.79	0.42
4:A:97:ILE:HD13	4:A:97:ILE:HG21	1.47	0.42
4:A:150:ILE:CG1	4:A:253:ARG:HD3	2.47	0.42
4:A:196:THR:CG2	4:A:265:TYR:CE1	2.99	0.42
4:A:156:LEU:HA	4:A:156:LEU:HD23	1.74	0.42
4:A:278:PHE:CD2	4:A:333:ARG:CB	3.02	0.42
1:T:14:DA:H2"	1:T:15:DG:C5'	2.50	0.42
3:D:1:DG:OP2	4:A:68:LYS:HD3	2.19	0.42
1:T:9:DG:C4	1:T:10:DC:C5	3.08	0.42
4:A:195:LEU:N	4:A:258:ARG:O	2.47	0.42
4:A:60:LYS:HA	4:A:65:VAL:HB	2.01	0.41
4:A:132:LEU:CA	4:A:136:GLN:HE21	2.33	0.41
4:A:200:PHE:HD2	4:A:259:LEU:HD11	1.85	0.41
4:A:294:ASN:ND2	4:A:294:ASN:N	2.67	0.41
4:A:197:HIS:CD2	4:A:198:PRO:HD2	2.55	0.41
4:A:150:ILE:N	4:A:188:SER:O	2.32	0.41
4:A:128:ASN:O	4:A:130:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:158:MET:HE1	4:A:253:ARG:HD2	2.00	0.41
4:A:149:ARG:NH2	4:A:187:SER:O	2.32	0.41
4:A:37:ASN:CA	4:A:40:ARG:HG3	2.43	0.41
4:A:158:MET:HE3	4:A:253:ARG:CD	2.47	0.41
4:A:289:LYS:HG3	4:A:323:ILE:O	2.21	0.41
4:A:240:GLN:HG2	4:A:241:LEU:H	1.86	0.41
1:T:3:DG:N2	6:T:509:HOH:O	2.46	0.41
4:A:133:ASN:HD21	4:A:135:HIS:HB3	1.86	0.41
4:A:269:VAL:HG11	4:A:316:GLU:OE2	2.20	0.41
4:A:207:GLN:CB	4:A:209:LYS:NZ	2.79	0.41
4:A:62:LEU:HA	4:A:63:PRO:HD3	1.72	0.41
2:P:8:DC:H2''	2:P:9:DG:O5'	2.20	0.41
4:A:332:ASP:C	4:A:334:SER:H	2.24	0.41
4:A:298:ILE:O	4:A:298:ILE:HG23	2.20	0.41
4:A:222:HIS:N	4:A:222:HIS:ND1	2.68	0.41
4:A:201:THR:HA	4:A:261:PRO:HB3	2.03	0.41
4:A:67:THR:H	4:A:67:THR:HG22	1.31	0.41
4:A:128:ASN:O	4:A:131:LYS:HG2	2.21	0.40
4:A:235:PHE:CE1	4:A:237:GLY:HA3	2.56	0.40
4:A:169:VAL:HG21	4:A:213:GLN:HG3	2.03	0.40
4:A:122:LEU:O	4:A:125:LEU:HB2	2.21	0.40
4:A:6:ALA:HA	4:A:7:PRO:HD3	1.60	0.40
4:A:100:LEU:HD22	4:A:115:VAL:CG2	2.51	0.40
4:A:130:ASP:OD1	4:A:131:LYS:HG2	2.22	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
4	A	329/335 (98%)	248 (75%)	58 (18%)	23 (7%)	<b>1</b> <b>1</b>

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	7	PRO
4	A	8	GLN
4	A	141	LYS
4	A	152	ARG
4	A	302	GLY
4	A	129	GLU
4	A	142	TYR
4	A	184	GLY
4	A	202	SER
4	A	265	TYR
4	A	327	TYR
4	A	27	LYS
4	A	42	ALA
4	A	117	GLU
4	A	222	HIS
4	A	187	SER
4	A	143	PHE
4	A	221	VAL
4	A	250	TYR
4	A	266	TYR
4	A	309	GLU
4	A	50	PRO
4	A	242	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
4	A	291/295 (99%)	238 (82%)	53 (18%)	<b>2</b> <b>3</b>

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	10	THR
4	A	16	THR

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Mol	Chain	Res	Type
4	A	22	LEU
4	A	40	ARG
4	A	41	LYS
4	A	46	ILE
4	A	61	LYS
4	A	67	THR
4	A	77	LEU
4	A	90	GLN
4	A	94	SER
4	A	96	SER
4	A	98	ASN
4	A	109	SER
4	A	122	LEU
4	A	127	LYS
4	A	131	LYS
4	A	132	LEU
4	A	133	ASN
4	A	140	LEU
4	A	151	PRO
4	A	153	GLU
4	A	164	ASN
4	A	169	VAL
4	A	176	THR
4	A	186	GLU
4	A	187	SER
4	A	192	ASP
4	A	194	LEU
4	A	201	THR
4	A	203	GLU
4	A	206	LYS
4	A	213	GLN
4	A	226	ASP
4	A	230	LYS
4	A	232	GLU
4	A	236	MET
4	A	245	ASN
4	A	246	ASP
4	A	253	ARG
4	A	265	TYR
4	A	273	THR
4	A	277	ILE
4	A	287	LEU

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Mol	Chain	Res	Type
4	A	289	LYS
4	A	294	ASN
4	A	296	TYR
4	A	301	LEU
4	A	311	LEU
4	A	321	ASP
4	A	324	GLN
4	A	327	TYR
4	A	332	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	12	ASN
4	A	28	ASN
4	A	37	ASN
4	A	90	GLN
4	A	98	ASN
4	A	133	ASN
4	A	136	GLN
4	A	164	ASN
4	A	213	GLN
4	A	245	ASN
4	A	264	GLN
4	A	279	ASN
4	A	281	ASN
4	A	285	HIS
4	A	294	ASN
4	A	324	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	T	16/16 (100%)	0.43	1 (6%) 23 17	27, 45, 91, 92	0
2	P	11/11 (100%)	0.19	0 100 100	30, 38, 66, 92	0
3	D	5/5 (100%)	-0.49	0 100 100	18, 26, 37, 38	0
4	A	331/335 (98%)	1.01	66 (19%) 1 1	16, 57, 99, 100	75 (22%)
All	All	363/367 (98%)	0.94	67 (18%) 2 1	16, 55, 99, 100	75 (20%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	313	VAL	10.9
4	A	299	ARG	6.7
4	A	301	LEU	6.7
4	A	291	PHE	6.3
4	A	204	SER	5.8
4	A	287	LEU	5.5
4	A	314	ASP	5.5
4	A	315	SER	5.4
4	A	282	MET	5.3
4	A	316	GLU	5.2
4	A	277	ILE	5.1
4	A	300	PRO	5.1
4	A	201	THR	5.1
4	A	330	PRO	4.7
4	A	183	ARG	4.6
4	A	184	GLY	4.4
4	A	208	PRO	4.4
4	A	202	SER	4.2
4	A	160	ASP	4.2
4	A	292	THR	4.2
4	A	324	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
4	A	244	LYS	3.8
4	A	281	ASN	3.7
4	A	307	ALA	3.7
4	A	246	ASP	3.6
4	A	329	GLU	3.6
4	A	286	ALA	3.6
1	T	7	DA	3.6
4	A	273	THR	3.5
4	A	180	SER	3.5
4	A	303	VAL	3.5
4	A	265	TYR	3.5
4	A	173	TYR	3.5
4	A	205	THR	3.4
4	A	280	LYS	3.4
4	A	289	LYS	3.3
4	A	325	TRP	3.2
4	A	8	GLN	3.2
4	A	331	LYS	3.1
4	A	247	GLU	3.0
4	A	302	GLY	3.0
4	A	288	GLU	2.9
4	A	9	GLU	2.8
4	A	334	SER	2.8
4	A	276	ASP	2.8
4	A	323	ILE	2.7
4	A	5	LYS	2.7
4	A	262	LYS	2.7
4	A	116	ASP	2.7
4	A	269	VAL	2.7
4	A	304	THR	2.7
4	A	312	PRO	2.6
4	A	152	ARG	2.5
4	A	10	THR	2.5
4	A	248	LYS	2.5
4	A	272	PHE	2.5
4	A	200	PHE	2.5
4	A	283	ARG	2.4
4	A	274	GLY	2.4
4	A	335	GLU	2.2
4	A	295	GLU	2.2
4	A	322	TYR	2.2
4	A	290	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
4	A	327	TYR	2.1
4	A	207	GLN	2.1
4	A	236	MET	2.0
4	A	245	ASN	2.0

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NA	A	341	1/1	0.96	0.16	-0.18	22,22,22,22	0
5	NA	A	342	1/1	0.96	0.11	-2.29	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.