



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:21 pm GMT

PDB ID : 2BPG  
Title : STRUCTURES OF TERNARY COMPLEXES OF RAT DNA POLYMERASE BETA, A DNA TEMPLATE-PRIMER, AND DDCTP  
Authors : Pelletier, H.; Sawaya, M.R.; Kumar, A.; Wilson, S.H.; Kraut, J.  
Deposited on : 1994-05-19  
Resolution : 3.60 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

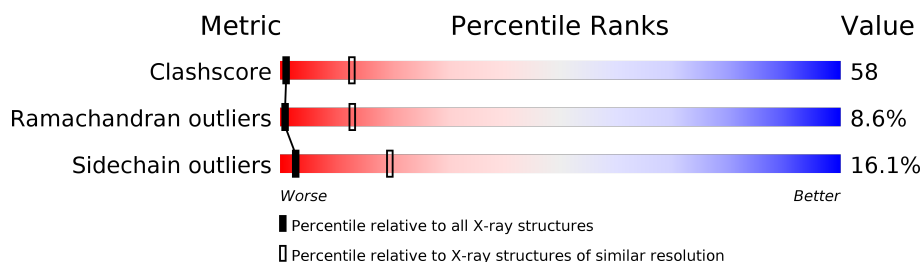
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	8	<div> <div>25%</div> <div>25%</div> <div>50%</div> </div>
1	T	8	<div> <div>13%</div> <div>25%</div> <div>13%</div> <div>50%</div> </div>
2	D	7	<div> <div>57%</div> <div>43%</div> </div>
2	P	7	<div> <div>43%</div> <div>43%</div> <div>14%</div> </div>
3	A	335	<div> <div>21%</div> <div>50%</div> <div>22%</div> <div>• •</div> </div>
3	B	335	<div> <div>26%</div> <div>45%</div> <div>22%</div> <div>• •</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5754 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(\*GP\*GP\*GP\*CP\*GP\*CP\*CP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	8	Total	C	N	O	P	0	0	0
			167	77	34	48	8			
1	C	8	Total	C	N	O	P	0	0	0
			167	77	34	48	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	P	0	0	0
			139	66	27	40	6			
2	D	7	Total	C	N	O	P	0	0	0
			139	66	27	40	6			

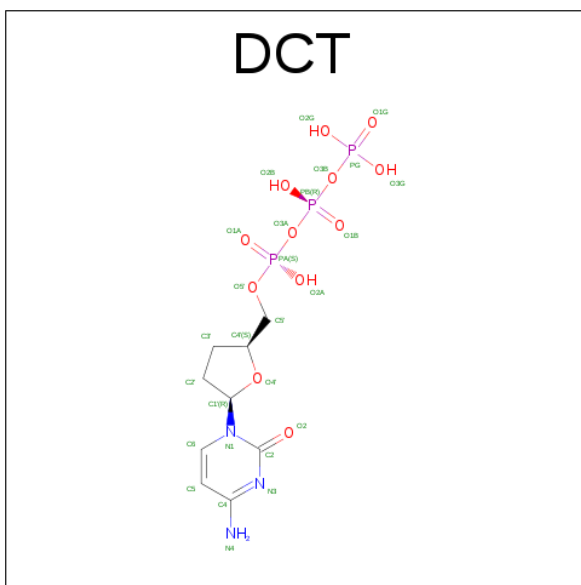
- Molecule 3 is a protein called DNA POLYMERASE BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	324	Total	C	N	O	S	0	0	0
			2542	1602	448	483	9			
3	B	324	Total	C	N	O	S	0	0	0
			2541	1601	448	483	9			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 2',3'-DIDEOXYCYTIDINE 5'-TRIPHOSPHATE (three-letter code: DCT) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 27	C 9	N 3	O 12	P 3	0	0
5	B	1	Total 27	C 9	N 3	O 12	P 3	0	0

- Molecule 6 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0
6	B	3	Total O 3 3	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 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.

Note EDS was not executed.

- Molecule 1: DNA (5'-D(\*GP\*GP\*GP\*CP\*GP\*CP\*CP\*G)-3')

Chain T: 



- Molecule 1: DNA (5'-D(\*GP\*GP\*GP\*CP\*GP\*CP\*CP\*G)-3')

Chain C: 



- Molecule 2: DNA (5'-D(\*CP\*GP\*GP\*CP\*GP\*CP\*C)-3')

Chain P: 



- Molecule 2: DNA (5'-D(\*CP\*GP\*GP\*CP\*GP\*CP\*C)-3')

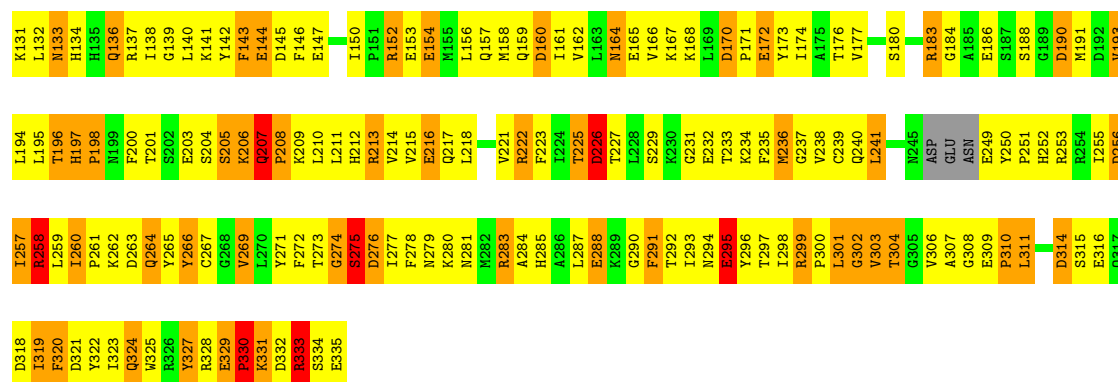
Chain D: 



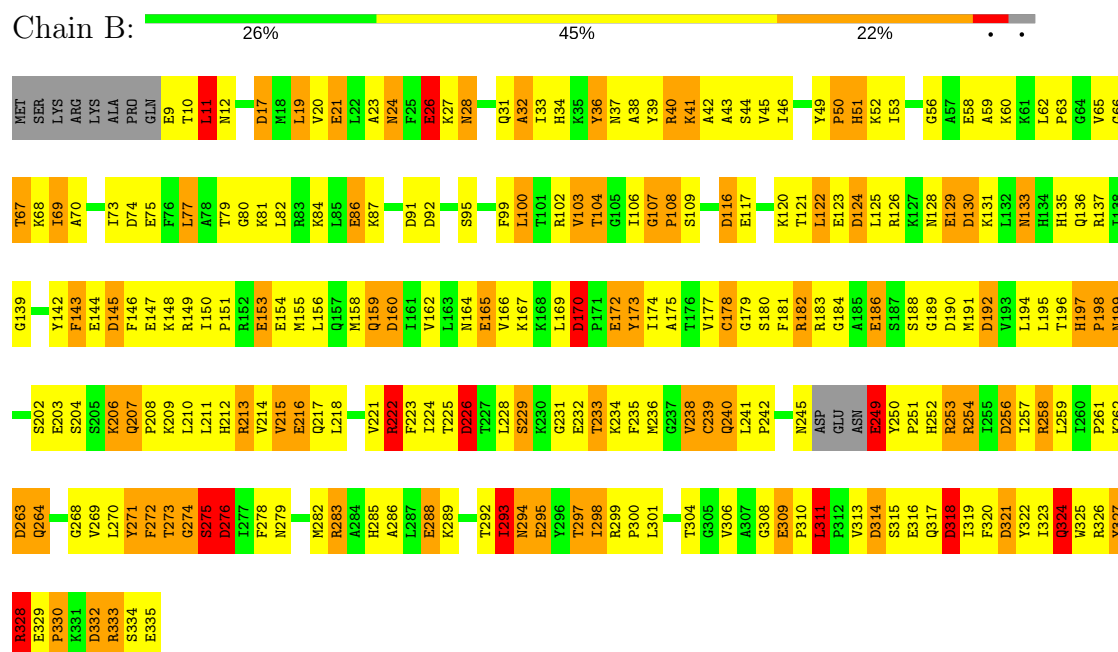
- Molecule 3: DNA POLYMERASE BETA

Chain A: 





## • Molecule 3: DNA POLYMERASE BETA



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.30Å 56.80Å 86.70Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	20.00 – 3.60	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5754	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	C	1.37	0/187	2.40	13/287 (4.5%)
1	T	1.82	3/187 (1.6%)	2.39	13/287 (4.5%)
2	D	1.70	2/155 (1.3%)	2.73	17/237 (7.2%)
2	P	1.22	0/155	2.15	8/237 (3.4%)
3	A	1.19	24/2588 (0.9%)	1.72	49/3491 (1.4%)
3	B	1.19	25/2587 (1.0%)	1.74	66/3490 (1.9%)
All	All	1.24	54/5859 (0.9%)	1.84	166/8029 (2.1%)

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
1	C	0	6
1	T	0	5
2	D	0	3
2	P	0	1
All	All	0	15

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	5	DG	C3'-O3'	-9.08	1.32	1.44
3	B	295	GLU	CD-OE2	7.36	1.33	1.25
3	A	335	GLU	CD-OE2	6.91	1.33	1.25
1	T	4	DG	C3'-O3'	-6.80	1.35	1.44
3	A	86	GLU	CD-OE2	6.75	1.33	1.25
3	B	21	GLU	CD-OE1	6.69	1.33	1.25
3	B	203	GLU	CD-OE2	6.68	1.33	1.25
3	A	249	GLU	CD-OE2	6.63	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	75	GLU	CD-OE1	6.62	1.32	1.25
2	D	4	DC	C3'-O3'	-6.57	1.35	1.44
3	A	203	GLU	CD-OE2	6.56	1.32	1.25
3	B	154	GLU	CD-OE2	6.56	1.32	1.25
3	A	9	GLU	CD-OE1	6.52	1.32	1.25
3	B	144	GLU	CD-OE2	6.52	1.32	1.25
3	A	144	GLU	CD-OE2	6.49	1.32	1.25
3	B	335	GLU	CD-OE2	6.43	1.32	1.25
3	A	129	GLU	CD-OE1	6.38	1.32	1.25
3	B	288	GLU	CD-OE1	6.38	1.32	1.25
3	A	147	GLU	CD-OE1	6.36	1.32	1.25
1	T	8	DG	C3'-O3'	6.21	1.52	1.44
3	A	154	GLU	CD-OE1	6.20	1.32	1.25
3	B	186	GLU	CD-OE2	6.17	1.32	1.25
3	A	153	GLU	CD-OE1	6.11	1.32	1.25
3	A	75	GLU	CD-OE1	6.04	1.32	1.25
3	B	232	GLU	CD-OE2	6.04	1.32	1.25
3	A	58	GLU	CD-OE1	6.02	1.32	1.25
3	B	153	GLU	CD-OE2	6.00	1.32	1.25
3	A	329	GLU	CD-OE1	5.98	1.32	1.25
3	B	147	GLU	CD-OE1	5.91	1.32	1.25
3	A	117	GLU	CD-OE1	5.89	1.32	1.25
3	B	9	GLU	CD-OE1	5.89	1.32	1.25
3	B	316	GLU	CD-OE1	5.88	1.32	1.25
3	A	216	GLU	CD-OE1	5.81	1.32	1.25
3	B	117	GLU	CD-OE2	5.71	1.31	1.25
3	A	232	GLU	CD-OE2	5.70	1.31	1.25
3	B	249	GLU	CD-OE1	5.66	1.31	1.25
3	A	21	GLU	CD-OE1	5.63	1.31	1.25
3	B	129	GLU	CD-OE2	5.61	1.31	1.25
3	B	309	GLU	CD-OE1	5.58	1.31	1.25
3	A	26	GLU	CD-OE2	5.55	1.31	1.25
3	A	295	GLU	CD-OE2	5.51	1.31	1.25
3	A	288	GLU	CD-OE1	5.48	1.31	1.25
3	A	165	GLU	CD-OE1	5.45	1.31	1.25
3	B	58	GLU	CD-OE1	5.44	1.31	1.25
3	A	309	GLU	CD-OE1	5.43	1.31	1.25
3	B	86	GLU	CD-OE1	5.40	1.31	1.25
3	B	165	GLU	CD-OE1	5.40	1.31	1.25
3	B	329	GLU	CD-OE1	5.31	1.31	1.25
2	D	6	DC	N1-C6	-5.22	1.34	1.37
3	A	172	GLU	CD-OE1	5.18	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	172	GLU	CD-OE2	5.18	1.31	1.25
3	A	186	GLU	CD-OE1	5.16	1.31	1.25
3	B	216	GLU	CD-OE1	5.13	1.31	1.25
3	B	26	GLU	CD-OE1	5.12	1.31	1.25

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	7	DC	C2-N1-C1'	-14.89	102.42	118.80
2	D	4	DC	C2-N1-C1'	-12.96	104.55	118.80
1	T	7	DC	C2-N1-C1'	12.62	132.69	118.80
2	D	1	DC	C6-N1-C1'	-12.09	106.29	120.80
1	C	7	DC	C6-N1-C1'	-11.61	106.87	120.80
2	D	1	DC	C2-N1-C1'	11.10	131.01	118.80
3	A	107	GLY	C-N-CD	-11.08	96.22	120.60
2	D	4	DC	C6-N1-C1'	10.73	133.68	120.80
1	T	7	DC	C6-N1-C1'	-10.27	108.47	120.80
1	C	7	DC	C2-N1-C1'	9.65	129.41	118.80
3	A	116	ASP	CB-CG-OD1	-9.40	109.84	118.30
3	B	190	ASP	CB-CG-OD2	-9.40	109.84	118.30
2	D	6	DC	O4'-C1'-N1	-9.36	101.45	108.00
1	C	8	DG	C8-N9-C4	-9.35	102.66	106.40
1	T	7	DC	P-O5'-C5'	-9.29	106.03	120.90
3	A	74	ASP	CB-CG-OD1	-9.10	110.11	118.30
2	D	5	DG	O4'-C1'-N9	8.91	114.24	108.00
3	A	256	ASP	CB-CG-OD2	-8.90	110.29	118.30
3	A	332	ASP	CB-CG-OD2	-8.48	110.66	118.30
3	B	91	ASP	CB-CG-OD2	-8.41	110.73	118.30
3	B	213	ARG	NE-CZ-NH1	8.39	124.50	120.30
3	B	254	ARG	NE-CZ-NH1	8.34	124.47	120.30
3	A	256	ASP	CB-CG-OD1	8.32	125.79	118.30
3	B	74	ASP	CB-CG-OD1	-8.27	110.86	118.30
3	B	124	ASP	CB-CG-OD1	-8.23	110.90	118.30
1	C	8	DG	O4'-C1'-N9	8.21	113.75	108.00
1	C	11	DG	O4'-C1'-N9	7.98	113.59	108.00
3	A	275	SER	N-CA-CB	7.94	122.41	110.50
1	T	11	DG	O4'-C1'-N9	7.93	113.55	108.00
1	C	5	DG	C4-N9-C1'	-7.86	116.28	126.50
2	D	6	DC	C2-N1-C1'	-7.83	110.19	118.80
3	A	197	HIS	C-N-CD	-7.81	103.43	120.60
1	T	5	DG	C1'-O4'-C4'	-7.73	102.37	110.10
3	A	332	ASP	CB-CG-OD1	7.66	125.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	91	ASP	CB-CG-OD2	-7.62	111.44	118.30
3	B	332	ASP	CB-CG-OD1	-7.52	111.53	118.30
3	B	328	ARG	NE-CZ-NH1	7.43	124.01	120.30
2	P	7	DC	C6-N1-C1'	7.37	129.65	120.80
3	B	116	ASP	CB-CG-OD1	-7.34	111.69	118.30
3	B	17	ASP	CB-CG-OD1	-7.33	111.70	118.30
3	A	283	ARG	NE-CZ-NH1	7.32	123.96	120.30
3	B	238	VAL	CB-CA-C	-7.21	97.71	111.40
3	B	104	THR	CA-CB-CG2	-7.20	102.31	112.40
3	B	74	ASP	CB-CG-OD2	7.19	124.77	118.30
3	A	160	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	T	5	DG	O4'-C4'-C3'	-7.14	101.64	104.50
3	B	40	ARG	NE-CZ-NH1	7.07	123.84	120.30
3	B	170	ASP	CB-CG-OD1	-7.05	111.95	118.30
3	B	263	ASP	CB-CG-OD1	-7.01	111.99	118.30
3	B	321	ASP	CB-CG-OD1	-6.94	112.05	118.30
3	A	276	ASP	CB-CG-OD2	-6.93	112.06	118.30
2	D	2	DG	C5'-C4'-C3'	-6.92	101.64	114.10
3	B	190	ASP	CB-CG-OD1	6.91	124.52	118.30
3	B	124	ASP	CB-CG-OD2	6.82	124.44	118.30
2	P	7	DC	C6-N1-C2	6.82	123.03	120.30
1	T	8	DG	C8-N9-C4	-6.80	103.68	106.40
3	A	318	ASP	CB-CG-OD1	-6.80	112.18	118.30
3	A	17	ASP	CB-CG-OD1	-6.69	112.28	118.30
3	B	318	ASP	CB-CG-OD2	6.66	124.29	118.30
3	A	74	ASP	CB-CG-OD2	6.65	124.28	118.30
2	D	6	DC	P-O3'-C3'	6.55	127.56	119.70
3	B	293	ILE	CB-CA-C	-6.52	98.56	111.60
3	B	332	ASP	CB-CG-OD2	6.51	124.16	118.30
3	A	190	ASP	CB-CG-OD1	-6.50	112.45	118.30
3	B	130	ASP	CB-CG-OD1	-6.39	112.55	118.30
2	P	7	DC	O4'-C4'-C3'	-6.39	101.95	104.50
3	B	276	ASP	CB-CG-OD2	-6.36	112.57	118.30
3	A	283	ARG	NE-CZ-NH2	-6.35	117.12	120.30
3	A	190	ASP	CB-CG-OD2	6.34	124.00	118.30
3	A	320	PHE	CB-CA-C	-6.31	97.77	110.40
1	T	8	DG	P-O3'-C3'	6.30	127.26	119.70
1	C	9	DC	C2-N1-C1'	6.28	125.71	118.80
1	T	11	DG	C8-N9-C1'	-6.27	118.85	127.00
3	B	253	ARG	NE-CZ-NH1	6.24	123.42	120.30
3	B	145	ASP	CB-CG-OD2	-6.21	112.71	118.30
3	A	121	THR	N-CA-CB	6.20	122.08	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	226	ASP	CB-CG-OD2	-6.20	112.72	118.30
3	B	197	HIS	C-N-CD	-6.18	106.99	120.60
3	B	137	ARG	NE-CZ-NH2	-6.15	117.22	120.30
3	B	283	ARG	NE-CZ-NH2	-6.13	117.24	120.30
2	D	5	DG	C8-N9-C4	-6.12	103.95	106.40
1	C	5	DG	P-O3'-C3'	6.10	127.02	119.70
3	A	333	ARG	NE-CZ-NH1	6.10	123.35	120.30
3	A	310	PRO	N-CA-CB	6.05	110.57	103.30
3	B	92	ASP	CB-CG-OD1	-6.01	112.89	118.30
3	B	192	ASP	CB-CG-OD1	5.97	123.68	118.30
3	B	251	PRO	N-CA-CB	5.96	110.45	103.30
3	A	170	ASP	CB-CG-OD1	-5.96	112.94	118.30
2	D	3	DG	C3'-C2'-C1'	-5.95	95.37	102.50
3	B	226	ASP	CB-CG-OD2	-5.93	112.96	118.30
3	A	152	ARG	NE-CZ-NH2	-5.92	117.34	120.30
3	A	213	ARG	NE-CZ-NH1	5.88	123.24	120.30
3	B	222	ARG	NE-CZ-NH1	5.80	123.20	120.30
3	B	276	ASP	CB-CG-OD1	5.79	123.52	118.30
3	B	116	ASP	CB-CG-OD2	5.76	123.48	118.30
3	B	17	ASP	CB-CG-OD2	5.75	123.47	118.30
3	B	36	TYR	CB-CG-CD2	-5.75	117.55	121.00
3	B	229	SER	N-CA-CB	5.75	119.12	110.50
3	A	236	MET	C-N-CA	-5.74	110.24	122.30
3	B	11	LEU	N-CA-C	5.74	126.49	111.00
3	A	116	ASP	CB-CG-OD2	5.72	123.45	118.30
3	A	241	LEU	C-N-CD	-5.71	108.03	120.60
1	T	10	DC	P-O5'-C5'	-5.67	111.82	120.90
3	A	291	PHE	CB-CA-C	-5.67	99.05	110.40
2	D	3	DG	C5'-C4'-C3'	5.65	124.27	114.10
3	B	311	LEU	C-N-CD	-5.63	108.21	120.60
3	B	256	ASP	CB-CG-OD1	-5.62	113.25	118.30
3	B	294	ASN	N-CA-CB	5.61	120.69	110.60
1	C	5	DG	O5'-P-OP1	-5.58	100.68	105.70
2	P	3	DG	O4'-C1'-N9	5.58	111.90	108.00
3	A	263	ASP	CB-CG-OD1	-5.57	113.28	118.30
3	A	152	ARG	NE-CZ-NH1	5.57	123.08	120.30
3	A	47	ALA	CB-CA-C	5.55	118.42	110.10
2	D	6	DC	C6-N1-C1'	5.54	127.45	120.80
3	A	91	ASP	CB-CG-OD1	5.51	123.26	118.30
3	B	297	THR	CB-CA-C	-5.50	96.74	111.60
2	D	7	DC	C6-N1-C1'	-5.49	114.21	120.80
3	A	92	ASP	CB-CG-OD2	5.49	123.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	8	DG	O4'-C1'-N9	5.49	111.84	108.00
3	B	69	ILE	CA-CB-CG1	-5.49	100.57	111.00
3	B	264	GLN	N-CA-CB	5.49	120.48	110.60
3	B	160	ASP	CB-CG-OD1	-5.48	113.37	118.30
3	B	321	ASP	CB-CG-OD2	5.48	123.23	118.30
1	C	5	DG	P-O5'-C5'	-5.46	112.17	120.90
3	A	183	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	T	10	DC	C6-N1-C1'	-5.42	114.30	120.80
3	A	266	TYR	CB-CA-C	5.42	121.24	110.40
3	B	318	ASP	CB-CG-OD1	-5.41	113.43	118.30
3	B	229	SER	CB-CA-C	5.39	120.34	110.10
3	B	40	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	11	DG	C4-N9-C1'	5.36	133.47	126.50
3	B	333	ARG	NE-CZ-NH2	-5.36	117.62	120.30
3	B	182	ARG	NE-CZ-NH1	5.34	122.97	120.30
3	A	333	ARG	N-CA-C	5.33	125.40	111.00
2	P	6	DC	C2-N1-C1'	5.33	124.66	118.80
2	P	6	DC	C6-N1-C1'	-5.31	114.43	120.80
2	D	2	DG	C4'-C3'-C2'	5.31	107.88	103.10
3	B	51	HIS	CA-CB-CG	5.30	122.61	113.60
3	A	130	ASP	CB-CG-OD2	-5.29	113.54	118.30
3	A	276	ASP	CB-CG-OD1	5.28	123.05	118.30
3	B	301	LEU	N-CA-C	-5.28	96.74	111.00
3	A	251	PRO	N-CA-CB	5.28	109.63	103.30
3	B	314	ASP	CB-CG-OD2	5.25	123.02	118.30
3	B	107	GLY	N-CA-C	-5.22	100.04	113.10
3	B	256	ASP	CB-CG-OD2	5.22	123.00	118.30
3	B	91	ASP	CB-CG-OD1	5.22	123.00	118.30
3	A	128	ASN	CA-CB-CG	-5.21	101.95	113.40
3	A	258	ARG	NE-CZ-NH2	-5.21	117.70	120.30
3	B	170	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	11	DG	P-O5'-C5'	-5.15	112.66	120.90
3	B	251	PRO	C-N-CA	-5.15	108.82	121.70
3	B	108	PRO	N-CA-C	5.15	125.49	112.10
3	B	239	CYS	N-CA-CB	-5.14	101.35	110.60
1	C	9	DC	C6-N1-C1'	-5.13	114.64	120.80
2	D	6	DC	C6-N1-C2	5.12	122.35	120.30
3	A	330	PRO	N-CA-CB	5.11	109.43	103.30
3	B	36	TYR	CB-CA-C	-5.06	100.29	110.40
1	T	10	DC	C6-N1-C2	5.04	122.31	120.30
3	A	145	ASP	CB-CG-OD1	-5.04	113.77	118.30
3	B	298	ILE	N-CA-C	-5.04	97.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	5	DG	O4'-C1'-N9	5.03	111.52	108.00
2	D	1	DC	O4'-C4'-C3'	-5.02	102.49	104.50
3	A	260	ILE	CB-CA-C	-5.02	101.55	111.60
3	A	314	ASP	CB-CG-OD1	-5.02	113.78	118.30
3	B	261	PRO	N-CA-CB	5.02	109.32	103.30
3	A	226	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	11	DG	Sidechain
1	C	4	DG	Sidechain
1	C	5	DG	Sidechain
1	C	7	DC	Sidechain
1	C	8	DG	Sidechain
1	C	9	DC	Sidechain
2	D	1	DC	Sidechain
2	D	2	DG	Sidechain
2	D	7	DC	Sidechain
2	P	7	DC	Sidechain
1	T	10	DC	Sidechain
1	T	11	DG	Sidechain
1	T	4	DG	Sidechain
1	T	5	DG	Sidechain
1	T	8	DG	Sidechain

## 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	C	167	0	89	13	0
1	T	167	0	89	9	0
2	D	139	0	79	13	0
2	P	139	0	79	18	2
3	A	2542	0	2488	321	2
3	B	2541	0	2486	285	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
5	A	27	0	12	8	0
5	B	27	0	12	1	0
6	A	1	0	0	2	0
6	B	3	0	0	0	0
All	All	5754	0	5334	642	2

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 58.

All (642) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:330:PRO:HD3	3:A:333:ARG:HH21	1.16	1.05
3:A:62:LEU:HD12	3:A:63:PRO:HD2	1.42	1.00
2:D:5:DG:H5''	3:B:107:GLY:H	1.29	0.97
2:D:1:DC:H2''	2:D:2:DG:N7	1.81	0.95
3:A:320:PHE:CD2	3:A:327:TYR:HA	2.03	0.94
1:C:8:DG:H5'	3:B:234:LYS:HB3	1.49	0.93
3:A:218:LEU:HD22	3:A:223:PHE:CD2	2.04	0.92
3:B:183:ARG:HH21	3:B:275:SER:HA	1.31	0.92
3:A:191:MET:HG2	3:A:193:VAL:HG12	1.52	0.91
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.53	0.90
3:A:299:ARG:HG3	3:A:307:ALA:HB1	1.54	0.90
3:A:330:PRO:HD3	3:A:333:ARG:NH2	1.86	0.89
3:B:271:TYR:HA	3:B:279:ASN:HD21	1.35	0.89
3:B:278:PHE:CZ	3:B:333:ARG:HD3	2.08	0.89
2:D:5:DG:H5''	3:B:107:GLY:N	1.86	0.89
3:B:271:TYR:HA	3:B:279:ASN:ND2	1.86	0.89
3:B:235:PHE:HD2	3:B:257:ILE:HG12	1.33	0.88
3:A:214:VAL:HG22	3:A:218:LEU:HD12	1.55	0.88
1:T:8:DG:H5''	3:A:231:GLY:HA3	1.56	0.87
3:B:67:THR:HG23	3:B:68:LYS:H	1.39	0.87
3:B:169:LEU:HD13	3:B:213:ARG:HH21	1.40	0.84
3:B:300:PRO:HG2	3:B:308:GLY:HA3	1.59	0.84
3:B:169:LEU:HB3	3:B:213:ARG:NH2	1.93	0.84
3:A:167:LYS:HG2	3:A:171:PRO:HA	1.59	0.83
3:A:194:LEU:HD13	3:A:195:LEU:N	1.93	0.83
2:D:1:DC:H2''	2:D:2:DG:C8	2.13	0.83
3:A:62:LEU:HD12	3:A:63:PRO:CD	2.07	0.83
3:A:201:THR:HA	3:A:261:PRO:HB3	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:121:THR:H	3:B:124:ASP:HB2	1.44	0.81
3:A:240:GLN:HG2	3:A:241:LEU:N	1.95	0.81
3:A:329:GLU:HB3	3:A:331:LYS:NZ	1.95	0.81
3:A:193:VAL:HG22	3:A:257:ILE:HG23	1.61	0.81
3:B:182:ARG:HH22	3:B:269:VAL:HG11	1.45	0.80
3:B:41:LYS:HD2	3:B:42:ALA:N	1.96	0.80
3:B:62:LEU:HD12	3:B:63:PRO:CD	2.11	0.80
3:B:241:LEU:HD23	3:B:250:TYR:CE2	2.17	0.80
3:B:62:LEU:HD12	3:B:63:PRO:HD2	1.64	0.79
3:A:329:GLU:HB3	3:A:331:LYS:HZ2	1.45	0.79
3:A:158:MET:O	3:A:162:VAL:HG23	1.83	0.79
3:B:199:ASN:HB2	3:B:207:GLN:OE1	1.83	0.79
3:A:24:ASN:HA	3:A:27:LYS:HB3	1.65	0.78
3:B:256:ASP:O	3:B:257:ILE:HD13	1.84	0.78
3:B:197:HIS:CD2	3:B:198:PRO:HD2	2.18	0.78
3:A:291:PHE:HA	3:A:301:LEU:HD13	1.66	0.78
3:A:240:GLN:HB2	3:A:252:HIS:HA	1.63	0.77
3:B:217:GLN:O	3:B:221:VAL:HG22	1.85	0.77
3:A:11:LEU:HD23	3:A:12:ASN:CG	2.05	0.77
3:B:158:MET:O	3:B:162:VAL:HG23	1.85	0.77
2:D:3:DG:H2''	2:D:4:DC:H6	1.50	0.76
3:A:11:LEU:CD2	3:A:12:ASN:H	1.98	0.76
3:A:300:PRO:HD2	3:A:308:GLY:HA3	1.69	0.75
3:B:100:LEU:O	3:B:103:VAL:HG23	1.87	0.75
3:A:298:ILE:HG23	3:A:311:LEU:HB2	1.69	0.74
3:A:295:GLU:HG2	3:A:296:TYR:CE1	2.23	0.74
3:B:320:PHE:HD1	3:B:323:ILE:HD11	1.52	0.74
3:B:211:LEU:O	3:B:214:VAL:HG12	1.88	0.74
3:A:66:GLY:H	3:A:69:ILE:HG13	1.53	0.74
3:A:11:LEU:HD23	3:A:12:ASN:H	1.52	0.73
3:B:299:ARG:HB2	3:B:300:PRO:HD2	1.70	0.73
2:D:3:DG:H2''	2:D:4:DC:C6	2.22	0.73
3:A:156:LEU:O	3:A:159:GLN:HB3	1.87	0.73
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.24	0.73
3:B:175:ALA:HB2	3:B:195:LEU:HD13	1.70	0.73
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.69	0.72
3:B:324:GLN:HE21	3:B:324:GLN:HA	1.53	0.72
3:A:74:ASP:HA	3:A:77:LEU:HB2	1.71	0.72
3:A:69:ILE:O	3:A:73:ILE:HG13	1.89	0.72
3:A:323:ILE:HG13	3:A:325:TRP:HB2	1.70	0.72
3:A:59:ALA:O	3:A:62:LEU:HB3	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:110:ALA:O	3:A:114:LEU:HG	1.90	0.72
3:B:313:VAL:HG11	3:B:319:ILE:HG12	1.70	0.72
3:B:174:ILE:O	3:B:195:LEU:HD12	1.90	0.72
3:A:209:LYS:HG2	3:A:212:HIS:HB2	1.73	0.71
3:A:320:PHE:HB3	3:A:325:TRP:O	1.91	0.71
3:B:206:LYS:C	3:B:208:PRO:HD3	2.10	0.71
3:A:15:ILE:HG12	3:A:46:ILE:CD1	2.21	0.71
1:T:8:DG:H4'	3:A:229:SER:OG	1.91	0.71
2:P:2:DG:H2'	2:P:3:DG:H8	1.55	0.71
3:A:218:LEU:HD22	3:A:223:PHE:HD2	1.53	0.71
3:B:172:GLU:HB3	3:B:197:HIS:CD2	2.26	0.70
3:A:156:LEU:HD13	3:A:159:GLN:NE2	2.05	0.70
2:P:2:DG:H2'	2:P:3:DG:C8	2.27	0.70
3:B:197:HIS:CG	3:B:198:PRO:HD2	2.26	0.69
3:B:153:GLU:O	3:B:156:LEU:HB3	1.92	0.69
3:A:26:GLU:OE2	3:A:35:LYS:HD2	1.92	0.69
3:A:258:ARG:HH21	3:A:295:GLU:HG3	1.55	0.69
3:A:300:PRO:HD2	3:A:308:GLY:CA	2.23	0.68
3:B:103:VAL:HB	3:B:106:ILE:HD12	1.74	0.68
3:B:150:ILE:HG21	3:B:155:MET:HG2	1.74	0.68
2:P:1:DC:H2'	2:P:2:DG:C8	2.29	0.68
3:A:264:GLN:HB3	3:A:296:TYR:O	1.92	0.68
3:A:320:PHE:HA	3:A:323:ILE:HG12	1.74	0.68
3:A:172:GLU:HB3	3:A:198:PRO:CG	2.24	0.68
3:A:240:GLN:HG2	3:A:241:LEU:H	1.58	0.67
5:A:338:DCT:H6	5:A:338:DCT:C5'	2.24	0.67
3:B:24:ASN:O	3:B:27:LYS:HB3	1.94	0.67
3:A:70:ALA:O	3:A:73:ILE:HB	1.94	0.67
2:P:7:DC:C6	5:A:338:DCT:H5	2.29	0.67
3:A:233:THR:O	3:A:258:ARG:HG3	1.94	0.67
3:A:206:LYS:C	3:A:208:PRO:HD3	2.15	0.67
3:A:18:MET:O	3:A:22:LEU:HD13	1.95	0.66
3:A:302:GLY:O	3:A:304:THR:N	2.29	0.66
3:A:260:ILE:HG22	3:A:261:PRO:N	2.10	0.66
3:B:258:ARG:NH2	3:B:295:GLU:HG3	2.10	0.66
3:A:214:VAL:CG2	3:A:218:LEU:HD12	2.24	0.66
3:B:212:HIS:O	3:B:215:VAL:HG22	1.96	0.66
3:A:285:HIS:CE1	3:A:325:TRP:HE1	2.15	0.65
3:A:237:GLY:O	3:A:255:ILE:N	2.30	0.65
3:B:150:ILE:CG2	3:B:155:MET:HG2	2.26	0.65
3:B:67:THR:O	3:B:70:ALA:HB3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:182:ARG:NH2	3:B:269:VAL:HG11	2.10	0.65
3:A:25:PHE:O	3:A:29:VAL:N	2.29	0.65
3:B:180:SER:HB2	3:B:188:SER:OG	1.95	0.65
3:A:183:ARG:HH11	3:A:273:THR:HG22	1.61	0.65
3:A:330:PRO:CD	3:A:333:ARG:HE	2.10	0.65
3:A:138:ILE:O	3:A:141:LYS:HB3	1.97	0.65
3:B:199:ASN:N	3:B:199:ASN:OD1	2.29	0.65
3:A:195:LEU:HD23	3:A:259:LEU:HB2	1.79	0.64
3:A:209:LYS:HA	3:A:212:HIS:HB2	1.78	0.64
3:A:239:CYS:O	3:A:253:ARG:N	2.31	0.64
3:B:165:GLU:HB3	3:B:217:GLN:HG2	1.78	0.64
3:A:294:ASN:ND2	3:A:297:THR:O	2.30	0.64
3:A:15:ILE:O	3:A:19:LEU:HD13	1.97	0.64
3:A:65:VAL:HG23	3:A:69:ILE:HB	1.80	0.64
2:D:4:DC:H5''	3:B:109:SER:CB	2.28	0.64
3:B:67:THR:HG23	3:B:68:LYS:N	2.11	0.64
3:A:174:ILE:HD12	3:A:174:ILE:N	2.13	0.64
3:A:70:ALA:HA	3:A:73:ILE:HD12	1.78	0.64
3:B:174:ILE:N	3:B:196:THR:O	2.28	0.64
3:B:62:LEU:HD12	3:B:63:PRO:HD3	1.80	0.63
3:A:266:TYR:CE1	3:A:315:SER:HA	2.34	0.63
3:B:210:LEU:O	3:B:213:ARG:HB2	1.98	0.63
3:A:294:ASN:OD1	3:A:296:TYR:HB2	1.99	0.63
3:B:206:LYS:HE2	3:B:207:GLN:HG3	1.81	0.63
2:P:6:DC:H2''	2:P:7:DC:C5'	2.28	0.63
3:A:207:GLN:O	3:A:210:LEU:HG	1.98	0.63
3:A:174:ILE:O	3:A:195:LEU:HD12	1.99	0.63
3:A:217:GLN:O	3:A:221:VAL:HG23	1.99	0.63
3:A:83:ARG:O	3:A:86:GLU:N	2.32	0.63
3:B:182:ARG:NH1	3:B:273:THR:OG1	2.31	0.63
3:B:174:ILE:O	3:B:195:LEU:HA	1.99	0.63
3:B:135:HIS:CE1	3:B:228:LEU:HD22	2.33	0.63
3:A:99:PHE:O	3:A:102:ARG:N	2.32	0.63
3:B:17:ASP:N	3:B:17:ASP:OD1	2.30	0.63
2:P:5:DG:H5''	3:A:107:GLY:H	1.64	0.63
3:A:191:MET:CG	3:A:193:VAL:HG12	2.28	0.63
3:A:201:THR:CA	3:A:261:PRO:HB3	2.27	0.62
3:A:258:ARG:NH2	3:A:295:GLU:HG3	2.14	0.62
3:B:37:ASN:HA	3:B:40:ARG:HG2	1.81	0.62
3:A:115:VAL:HG22	3:A:120:LYS:HD3	1.81	0.62
3:B:182:ARG:HB3	3:B:273:THR:HG23	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:194:LEU:HD13	3:B:195:LEU:N	2.15	0.62
1:C:8:DG:OP1	3:B:233:THR:N	2.28	0.62
3:A:293:ILE:HG22	3:A:294:ASN:N	2.14	0.62
3:A:115:VAL:O	3:A:118:GLY:N	2.31	0.62
3:B:103:VAL:HG12	3:B:139:GLY:HA3	1.82	0.62
3:A:42:ALA:O	3:A:46:ILE:HG23	2.00	0.61
3:A:174:ILE:HB	3:A:196:THR:HG22	1.81	0.61
3:B:11:LEU:HD13	3:B:11:LEU:N	2.15	0.61
1:T:8:DG:C5'	3:A:231:GLY:HA3	2.29	0.61
3:A:16:THR:HG23	3:A:46:ILE:CG1	2.31	0.61
3:A:299:ARG:CG	3:A:307:ALA:HB1	2.28	0.61
3:B:274:GLY:HA2	3:B:278:PHE:CD2	2.36	0.61
3:B:50:PRO:O	3:B:51:HIS:ND1	2.28	0.61
3:A:112:ARG:O	3:A:115:VAL:N	2.33	0.61
3:A:195:LEU:HG	3:A:196:THR:N	2.16	0.61
1:T:10:DC:H2''	1:T:11:DG:C8	2.36	0.61
3:A:183:ARG:HH11	3:A:273:THR:CG2	2.14	0.61
3:B:311:LEU:HB3	3:B:322:TYR:CE1	2.36	0.61
3:A:31:GLN:HG3	3:A:32:ALA:H	1.66	0.61
3:A:287:LEU:HD23	3:A:301:LEU:HD21	1.83	0.61
1:T:4:DG:H1	5:A:338:DCT:HN41	1.47	0.61
3:B:297:THR:O	3:B:299:ARG:NH1	2.34	0.61
3:A:164:ASN:N	3:A:164:ASN:OD1	2.32	0.60
3:B:297:THR:HG21	3:B:310:PRO:HB3	1.83	0.60
3:A:164:ASN:O	3:A:168:LYS:HG3	2.00	0.60
3:A:67:THR:O	3:A:70:ALA:HB3	2.02	0.60
3:B:172:GLU:O	3:B:198:PRO:HD3	2.01	0.60
3:A:26:GLU:HG2	3:A:35:LYS:HB2	1.84	0.60
3:A:79:THR:O	3:A:81:LYS:N	2.31	0.60
3:A:197:HIS:ND1	3:A:198:PRO:HD2	2.17	0.60
3:A:281:ASN:O	3:A:284:ALA:HB3	2.01	0.60
3:B:174:ILE:O	3:B:196:THR:N	2.29	0.60
3:B:326:ARG:HH12	3:B:328:ARG:HA	1.66	0.60
3:A:275:SER:O	3:A:278:PHE:N	2.34	0.60
3:A:330:PRO:HA	3:A:333:ARG:CG	2.29	0.60
3:B:315:SER:O	3:B:318:ASP:HB2	2.02	0.60
3:A:293:ILE:HG22	3:A:294:ASN:H	1.67	0.60
3:B:17:ASP:HA	3:B:20:VAL:HG12	1.84	0.60
3:B:38:ALA:HA	3:B:41:LYS:HE3	1.83	0.59
3:A:17:ASP:O	3:A:20:VAL:HG12	2.02	0.59
3:A:330:PRO:HD3	3:A:333:ARG:HE	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:309:GLU:OE1	3:B:310:PRO:HD2	2.01	0.59
3:B:258:ARG:NH2	3:B:295:GLU:OE2	2.32	0.59
3:B:294:ASN:ND2	3:B:299:ARG:HH22	2.00	0.59
2:P:6:DC:H2''	2:P:7:DC:O5'	2.01	0.59
3:A:191:MET:HG2	3:A:193:VAL:CG1	2.30	0.59
3:A:154:GLU:O	3:A:157:GLN:N	2.36	0.58
3:A:31:GLN:HG3	3:A:32:ALA:N	2.18	0.58
3:B:148:LYS:HB3	3:B:253:ARG:HH12	1.67	0.58
3:B:235:PHE:CD2	3:B:257:ILE:HG12	2.26	0.58
3:A:320:PHE:CE2	3:A:327:TYR:HA	2.37	0.58
3:B:99:PHE:O	3:B:102:ARG:HB2	2.04	0.58
3:B:257:ILE:HG22	3:B:258:ARG:N	2.18	0.58
3:B:330:PRO:O	3:B:333:ARG:N	2.31	0.58
3:B:172:GLU:HG3	3:B:198:PRO:HG3	1.84	0.58
3:B:240:GLN:O	3:B:242:PRO:HD3	2.03	0.58
3:B:228:LEU:HB2	3:B:236:MET:HB2	1.85	0.58
3:B:70:ALA:O	3:B:73:ILE:HB	2.03	0.58
3:A:320:PHE:CA	3:A:323:ILE:HG12	2.33	0.58
3:A:20:VAL:O	3:A:23:ALA:N	2.36	0.58
3:B:326:ARG:NH2	3:B:327:TYR:O	2.37	0.57
3:A:19:LEU:O	3:A:22:LEU:HB2	2.04	0.57
3:A:16:THR:HG23	3:A:46:ILE:HG13	1.86	0.57
3:B:103:VAL:HB	3:B:106:ILE:CD1	2.33	0.57
3:A:207:GLN:N	3:A:208:PRO:HD3	2.19	0.57
3:A:25:PHE:O	3:A:29:VAL:HB	2.05	0.57
3:B:268:GLY:O	3:B:271:TYR:HB3	2.04	0.57
3:B:313:VAL:HG12	3:B:318:ASP:HB3	1.86	0.57
3:B:174:ILE:C	3:B:195:LEU:HD12	2.24	0.57
3:B:169:LEU:CD1	3:B:213:ARG:HH21	2.16	0.57
3:B:235:PHE:HD2	3:B:257:ILE:CG1	2.11	0.57
3:B:42:ALA:HA	3:B:45:VAL:HG12	1.86	0.57
3:B:172:GLU:HG3	3:B:198:PRO:CG	2.34	0.57
3:A:139:GLY:O	3:A:143:PHE:N	2.36	0.57
3:A:234:LYS:HE2	3:A:236:MET:CG	2.34	0.57
3:A:280:LYS:O	3:A:284:ALA:N	2.35	0.57
3:B:213:ARG:O	3:B:216:GLU:HB2	2.05	0.57
3:B:223:PHE:CZ	3:B:239:CYS:HB2	2.40	0.57
3:A:297:THR:O	3:A:299:ARG:NH1	2.36	0.57
3:B:274:GLY:HA3	3:B:279:ASN:OD1	2.05	0.57
3:A:209:LYS:O	3:A:213:ARG:N	2.37	0.56
3:B:160:ASP:O	3:B:164:ASN:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:180:SER:HA	3:B:183:ARG:NH1	2.20	0.56
3:B:271:TYR:CE2	3:B:272:PHE:HD1	2.23	0.56
3:B:323:ILE:HG13	3:B:324:GLN:N	2.19	0.56
3:B:49:TYR:HE1	3:B:51:HIS:HB2	1.70	0.56
3:A:156:LEU:HD13	3:A:159:GLN:HE22	1.69	0.56
1:T:4:DG:N2	5:A:338:DCT:N3	2.48	0.56
3:A:84:LYS:NZ	6:A:401:HOH:O	2.38	0.56
1:C:10:DC:H2''	1:C:11:DG:O5'	2.05	0.56
3:A:174:ILE:N	3:A:196:THR:O	2.35	0.56
3:A:241:LEU:HD22	3:A:250:TYR:CD2	2.40	0.56
3:A:55:SER:O	3:A:58:GLU:HB3	2.05	0.56
3:B:121:THR:OG1	3:B:124:ASP:N	2.37	0.56
3:B:139:GLY:O	3:B:143:PHE:N	2.33	0.56
3:B:206:LYS:HG3	3:B:207:GLN:N	2.21	0.56
3:B:324:GLN:O	3:B:325:TRP:HD1	1.89	0.56
3:A:133:ASN:OD1	3:A:134:HIS:N	2.39	0.56
3:B:169:LEU:HB3	3:B:213:ARG:HH21	1.67	0.56
3:A:157:GLN:O	3:A:160:ASP:HB2	2.05	0.56
3:A:217:GLN:HG2	3:A:221:VAL:HG23	1.87	0.56
3:A:218:LEU:O	3:A:223:PHE:HB3	2.06	0.56
3:A:22:LEU:N	3:A:22:LEU:HD12	2.21	0.56
3:B:299:ARG:HB2	3:B:300:PRO:CD	2.34	0.56
3:A:200:PHE:HE2	3:A:259:LEU:HG	1.70	0.56
3:A:291:PHE:CA	3:A:301:LEU:HD13	2.36	0.56
3:A:158:MET:O	3:A:161:ILE:HB	2.06	0.55
3:B:121:THR:O	3:B:124:ASP:N	2.39	0.55
3:A:330:PRO:N	3:A:333:ARG:HE	2.04	0.55
1:C:8:DG:OP1	3:B:234:LYS:N	2.33	0.55
3:A:45:VAL:HG13	3:A:62:LEU:HD21	1.89	0.55
3:A:24:ASN:O	3:A:27:LYS:HB3	2.07	0.55
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.87	0.55
3:A:283:ARG:NE	3:A:293:ILE:HB	2.21	0.55
3:B:182:ARG:CB	3:B:273:THR:HG23	2.36	0.55
2:P:6:DC:H2''	2:P:7:DC:H5'	1.89	0.55
3:A:162:VAL:O	3:A:166:VAL:HG23	2.07	0.55
3:B:325:TRP:CZ3	3:B:328:ARG:HD2	2.41	0.55
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.41	0.55
3:A:238:VAL:HG12	3:A:239:CYS:N	2.21	0.55
3:B:121:THR:N	3:B:124:ASP:HB2	2.19	0.55
3:B:195:LEU:O	3:B:259:LEU:HA	2.07	0.55
3:A:267:CYS:HB3	3:A:294:ASN:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:283:ARG:HE	3:A:293:ILE:HB	1.72	0.54
3:A:330:PRO:HD3	3:A:333:ARG:NE	2.23	0.54
3:B:142:TYR:CE1	3:B:252:HIS:CG	2.95	0.54
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.37	0.54
3:B:225:THR:OG1	3:B:226:ASP:N	2.40	0.54
3:B:99:PHE:HE2	3:B:122:LEU:HD23	1.72	0.54
3:A:316:GLU:OE1	3:A:333:ARG:NH1	2.38	0.54
3:A:266:TYR:O	3:A:269:VAL:HG23	2.07	0.54
3:A:215:VAL:HG23	3:A:216:GLU:N	2.22	0.54
3:A:330:PRO:HD3	3:A:333:ARG:CZ	2.37	0.54
3:B:62:LEU:CD1	3:B:63:PRO:HD2	2.36	0.54
3:B:245:ASN:O	3:B:249:GLU:N	2.41	0.54
3:A:302:GLY:O	3:A:304:THR:HG22	2.08	0.54
3:B:26:GLU:O	3:B:32:ALA:HB3	2.08	0.54
3:B:294:ASN:ND2	3:B:299:ARG:HH12	2.06	0.54
3:A:294:ASN:HD22	3:A:299:ARG:NH2	2.06	0.53
3:A:132:LEU:HD22	3:A:136:GLN:HB3	1.89	0.53
3:B:271:TYR:CD2	3:B:272:PHE:N	2.77	0.53
3:A:234:LYS:HG2	3:A:235:PHE:N	2.22	0.53
1:C:10:DC:H2'	1:C:11:DG:C8	2.44	0.53
3:A:115:VAL:HG23	3:A:120:LYS:HB3	1.91	0.53
3:B:56:GLY:O	3:B:60:LYS:N	2.33	0.53
3:A:27:LYS:HG3	3:A:28:ASN:N	2.24	0.53
3:B:28:ASN:HB3	3:B:108:PRO:HG3	1.90	0.53
3:A:258:ARG:NH1	3:A:296:TYR:OH	2.35	0.53
3:A:330:PRO:O	3:A:333:ARG:HG3	2.09	0.53
3:B:211:LEU:O	3:B:215:VAL:HG13	2.09	0.53
3:B:263:ASP:N	3:B:263:ASP:OD1	2.41	0.53
3:A:193:VAL:HG22	3:A:257:ILE:CG2	2.37	0.53
3:B:235:PHE:C	3:B:236:MET:HG3	2.29	0.53
3:A:133:ASN:O	3:A:137:ARG:HG3	2.10	0.52
3:A:226:ASP:N	3:A:226:ASP:OD1	2.42	0.52
3:B:194:LEU:HA	3:B:258:ARG:O	2.09	0.52
3:B:328:ARG:CG	3:B:328:ARG:HH11	2.22	0.52
1:C:10:DC:N3	1:C:11:DG:C6	2.77	0.52
3:B:183:ARG:HE	3:B:275:SER:HB2	1.73	0.52
1:C:6:DG:H4'	3:B:295:GLU:CD	2.29	0.52
3:A:130:ASP:OD1	3:A:131:LYS:HG3	2.08	0.52
3:B:195:LEU:N	3:B:258:ARG:O	2.39	0.52
3:B:133:ASN:CG	3:B:136:GLN:HE21	2.10	0.52
3:B:169:LEU:O	3:B:170:ASP:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:223:PHE:CE2	3:B:239:CYS:HB2	2.44	0.52
3:A:115:VAL:CG2	3:A:120:LYS:HB3	2.39	0.52
3:A:194:LEU:HD13	3:A:195:LEU:H	1.74	0.52
3:B:258:ARG:HG3	3:B:259:LEU:N	2.24	0.52
1:C:4:DG:C2	1:C:5:DG:C6	2.97	0.52
3:B:196:THR:OG1	3:B:262:LYS:HB2	2.10	0.52
3:B:297:THR:CG2	3:B:310:PRO:HB3	2.39	0.52
3:A:134:HIS:O	3:A:137:ARG:HB2	2.10	0.52
3:B:158:MET:HB2	3:B:191:MET:HE1	1.92	0.52
3:B:330:PRO:HA	3:B:333:ARG:HG3	1.92	0.52
3:B:178:CYS:SG	3:B:272:PHE:HB3	2.50	0.52
3:A:146:PHE:N	3:A:146:PHE:HD1	2.08	0.52
3:B:317:GLN:H	3:B:317:GLN:CD	2.13	0.52
3:B:278:PHE:CE1	3:B:333:ARG:HD3	2.44	0.52
3:B:69:ILE:O	3:B:73:ILE:HG13	2.09	0.52
3:B:239:CYS:SG	3:B:253:ARG:HB2	2.49	0.51
3:B:285:HIS:CE1	3:B:325:TRP:HE1	2.28	0.51
3:A:125:LEU:HD23	3:A:140:LEU:HD13	1.91	0.51
3:A:75:GLU:HG2	3:A:81:LYS:O	2.10	0.51
3:B:79:THR:O	3:B:81:LYS:N	2.43	0.51
3:B:12:ASN:OD1	3:B:53:ILE:HG13	2.10	0.51
3:A:132:LEU:HD22	3:A:136:GLN:CB	2.40	0.51
3:A:146:PHE:N	3:A:146:PHE:CD1	2.77	0.51
3:A:227:THR:HG23	3:A:235:PHE:HE1	1.76	0.51
1:C:6:DG:H4'	3:B:295:GLU:OE1	2.10	0.51
3:B:82:LEU:O	3:B:86:GLU:HG2	2.11	0.51
3:A:290:GLY:O	3:A:301:LEU:N	2.32	0.51
3:B:121:THR:O	3:B:124:ASP:HB2	2.11	0.51
5:A:338:DCT:H6	5:A:338:DCT:H5''	1.93	0.51
3:B:179:GLY:O	3:B:182:ARG:HB2	2.11	0.51
3:B:212:HIS:N	3:B:212:HIS:CD2	2.78	0.51
3:A:233:THR:HG22	3:A:233:THR:O	2.10	0.51
3:A:266:TYR:CD1	3:A:315:SER:HA	2.46	0.51
3:B:159:GLN:HG3	3:B:177:VAL:HG11	1.92	0.51
1:C:8:DG:H5''	3:B:231:GLY:HA3	1.93	0.51
3:B:20:VAL:O	3:B:23:ALA:N	2.44	0.51
3:B:66:GLY:O	3:B:69:ILE:N	2.43	0.51
3:A:316:GLU:O	3:A:319:ILE:HB	2.11	0.50
3:A:87:LYS:O	3:A:91:ASP:N	2.44	0.50
3:B:318:ASP:O	3:B:321:ASP:HB2	2.10	0.50
2:P:5:DG:OP1	3:A:107:GLY:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:35:LYS:NZ	6:A:401:HOH:O	2.44	0.50
3:B:207:GLN:OE1	3:B:210:LEU:HD11	2.10	0.50
3:B:40:ARG:O	3:B:43:ALA:HB3	2.10	0.50
3:A:209:LYS:HG2	3:A:212:HIS:CB	2.41	0.50
3:B:20:VAL:O	3:B:23:ALA:HB3	2.12	0.50
3:B:332:ASP:C	3:B:334:SER:H	2.14	0.50
3:B:26:GLU:HG3	3:B:32:ALA:CB	2.41	0.50
3:B:279:ASN:O	3:B:283:ARG:HG3	2.11	0.50
3:B:324:GLN:HE21	3:B:324:GLN:CA	2.17	0.50
3:B:46:ILE:HG22	3:B:62:LEU:HD23	1.92	0.50
3:A:319:ILE:O	3:A:322:TYR:HB2	2.12	0.50
3:A:98:ASN:O	3:A:101:THR:OG1	2.29	0.50
2:D:5:DG:H5''	3:B:107:GLY:CA	2.41	0.50
3:A:40:ARG:HG3	3:A:41:LYS:N	2.26	0.50
3:B:121:THR:OG1	3:B:124:ASP:OD1	2.30	0.50
3:A:266:TYR:CZ	3:A:315:SER:HA	2.46	0.50
3:A:294:ASN:ND2	3:A:299:ARG:NH2	2.60	0.50
3:A:62:LEU:HG	3:A:65:VAL:HG12	1.93	0.50
3:B:173:TYR:CD1	3:B:197:HIS:HB2	2.47	0.50
3:B:271:TYR:CE2	3:B:272:PHE:CD1	3.00	0.50
3:A:295:GLU:HG2	3:A:296:TYR:CD1	2.47	0.50
3:B:178:CYS:O	3:B:181:PHE:HB3	2.11	0.50
3:B:79:THR:C	3:B:81:LYS:H	2.14	0.50
3:A:127:LYS:HD2	3:A:128:ASN:HD22	1.76	0.49
3:A:183:ARG:NH1	3:A:273:THR:O	2.45	0.49
3:B:177:VAL:HA	3:B:192:ASP:O	2.12	0.49
3:B:40:ARG:HG3	3:B:41:LYS:N	2.27	0.49
3:B:53:ILE:HG21	3:B:59:ALA:HB2	1.94	0.49
2:P:5:DG:O5'	3:A:107:GLY:HA3	2.12	0.49
3:B:129:GLU:C	3:B:131:LYS:H	2.16	0.49
3:B:17:ASP:O	3:B:20:VAL:HG12	2.12	0.49
3:B:300:PRO:O	3:B:308:GLY:N	2.45	0.49
3:A:11:LEU:HD23	3:A:12:ASN:OD1	2.12	0.49
3:B:159:GLN:N	3:B:191:MET:HE1	2.27	0.49
3:B:292:THR:O	3:B:298:ILE:HA	2.12	0.49
3:B:37:ASN:HD22	3:B:40:ARG:HD3	1.77	0.49
3:A:239:CYS:O	3:A:252:HIS:HA	2.12	0.49
3:B:320:PHE:CD2	3:B:327:TYR:HA	2.48	0.49
3:A:316:GLU:OE1	3:A:333:ARG:NH2	2.46	0.49
3:A:294:ASN:HD22	3:A:299:ARG:NH1	2.11	0.49
3:A:323:ILE:O	3:A:324:GLN:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:129:GLU:O	3:A:131:LYS:N	2.46	0.49
3:A:320:PHE:CE1	3:A:327:TYR:CD2	3.00	0.49
2:D:6:DC:C2	2:D:7:DC:C5	3.00	0.49
3:B:84:LYS:O	3:B:87:LYS:HB3	2.13	0.49
3:B:146:PHE:HE1	3:B:252:HIS:O	1.95	0.48
2:P:2:DG:H2''	2:P:3:DG:O4'	2.13	0.48
3:A:292:THR:O	3:A:292:THR:HG23	2.13	0.48
3:A:328:ARG:HH11	3:A:328:ARG:HG2	1.78	0.48
3:A:183:ARG:NH1	3:A:273:THR:HG22	2.28	0.48
3:A:261:PRO:HB2	3:A:264:GLN:NE2	2.29	0.48
3:A:164:ASN:C	3:A:168:LYS:HG3	2.33	0.48
3:A:106:ILE:HG12	3:A:136:GLN:HG2	1.96	0.48
3:A:142:TYR:HB3	3:A:146:PHE:CE1	2.49	0.48
3:B:292:THR:HG22	3:B:292:THR:O	2.13	0.48
3:B:298:ILE:O	3:B:298:ILE:HG23	2.14	0.48
3:B:285:HIS:CD2	3:B:325:TRP:NE1	2.81	0.48
1:T:10:DC:H2''	1:T:11:DG:N7	2.28	0.48
3:B:122:LEU:HD22	3:B:122:LEU:HA	1.58	0.48
2:P:5:DG:H5''	3:A:107:GLY:N	2.29	0.48
1:C:6:DG:H4'	3:B:295:GLU:OE2	2.14	0.48
3:A:127:LYS:HD2	3:A:128:ASN:ND2	2.28	0.48
3:B:156:LEU:O	3:B:159:GLN:HB3	2.14	0.48
3:B:27:LYS:HG3	3:B:28:ASN:N	2.29	0.48
3:A:103:VAL:CB	3:A:106:ILE:HD12	2.41	0.47
3:B:299:ARG:HA	3:B:311:LEU:HD22	1.96	0.47
3:A:67:THR:HG23	3:A:68:LYS:N	2.29	0.47
3:A:215:VAL:CG2	3:A:216:GLU:N	2.77	0.47
3:B:39:TYR:O	3:B:43:ALA:HB2	2.15	0.47
3:A:90:GLN:HE21	3:A:90:GLN:HA	1.80	0.47
3:A:93:THR:O	3:A:96:SER:HB2	2.15	0.47
3:B:49:TYR:HE1	3:B:51:HIS:O	1.97	0.47
2:D:3:DG:C2'	2:D:4:DC:C6	2.96	0.47
3:A:160:ASP:O	3:A:164:ASN:OD1	2.32	0.47
3:B:12:ASN:HD21	3:B:53:ILE:H	1.61	0.47
3:B:221:VAL:O	3:B:222:ARG:HB2	2.14	0.47
3:A:159:GLN:O	3:A:162:VAL:HB	2.15	0.47
3:A:215:VAL:HA	3:A:218:LEU:HB2	1.96	0.47
3:B:19:LEU:HA	3:B:19:LEU:HD12	1.30	0.47
3:B:41:LYS:O	3:B:44:SER:HB3	2.15	0.47
1:T:9:DC:H2''	1:T:10:DC:C5'	2.44	0.47
3:A:150:ILE:CD1	3:A:190:ASP:HA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:62:LEU:CD1	3:A:63:PRO:HD2	2.29	0.47
3:B:11:LEU:HD13	3:B:11:LEU:H	1.79	0.47
3:B:128:ASN:HB3	3:B:131:LYS:HD2	1.95	0.47
3:B:223:PHE:O	3:B:239:CYS:HA	2.14	0.47
3:B:262:LYS:HG2	3:B:262:LYS:O	2.15	0.47
3:B:328:ARG:HG2	3:B:328:ARG:HH11	1.80	0.47
2:D:5:DG:H2'	2:D:6:DC:H6	1.80	0.47
3:A:260:ILE:CG2	3:A:261:PRO:N	2.77	0.47
3:B:320:PHE:HA	3:B:323:ILE:HG12	1.95	0.46
3:B:311:LEU:HB3	3:B:322:TYR:CZ	2.50	0.46
3:A:33:ILE:CG2	3:A:34:HIS:N	2.77	0.46
3:A:240:GLN:NE2	3:A:241:LEU:O	2.44	0.46
3:A:255:ILE:CG1	3:A:256:ASP:N	2.79	0.46
3:B:196:THR:HG21	3:B:262:LYS:HG3	1.97	0.46
3:B:37:ASN:O	3:B:40:ARG:HG2	2.16	0.46
3:A:294:ASN:ND2	3:A:299:ARG:CZ	2.79	0.46
3:A:66:GLY:H	3:A:69:ILE:CG1	2.27	0.46
3:B:225:THR:OG1	3:B:238:VAL:HB	2.14	0.46
3:B:315:SER:N	3:B:318:ASP:OD1	2.49	0.46
3:A:20:VAL:HG13	3:A:21:GLU:N	2.31	0.46
3:A:258:ARG:NH2	3:A:295:GLU:CG	2.79	0.46
3:A:320:PHE:HA	3:A:323:ILE:CG1	2.42	0.46
3:A:323:ILE:CG1	3:A:325:TRP:HB2	2.43	0.46
3:A:300:PRO:CD	3:A:308:GLY:HA3	2.43	0.46
3:B:278:PHE:CE2	3:B:333:ARG:HD3	2.51	0.46
2:P:5:DG:H5''	3:A:105:GLY:O	2.15	0.46
3:A:132:LEU:CD2	3:A:136:GLN:HE21	2.29	0.46
3:B:11:LEU:CD1	3:B:11:LEU:H	2.29	0.46
3:A:115:VAL:C	3:A:117:GLU:H	2.19	0.46
3:A:271:TYR:O	5:A:338:DCT:H2''	2.15	0.46
3:A:77:LEU:HD12	3:A:77:LEU:HA	1.40	0.45
3:B:142:TYR:O	3:B:145:ASP:N	2.38	0.45
3:B:234:LYS:CG	3:B:235:PHE:N	2.78	0.45
3:A:256:ASP:OD1	3:A:257:ILE:N	2.49	0.45
3:B:123:GLU:O	3:B:126:ARG:HB2	2.15	0.45
3:B:174:ILE:HB	3:B:196:THR:HG22	1.97	0.45
3:B:240:GLN:HG2	3:B:241:LEU:N	2.30	0.45
3:A:16:THR:HA	3:A:46:ILE:HD11	1.97	0.45
3:A:167:LYS:HA	3:A:170:ASP:O	2.16	0.45
3:B:197:HIS:HA	3:B:198:PRO:HD3	1.47	0.45
3:A:170:ASP:OD1	3:A:171:PRO:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:18:MET:HE2	3:A:72:LYS:O	2.16	0.45
3:A:173:TYR:HA	3:A:196:THR:O	2.16	0.45
3:A:200:PHE:O	3:A:201:THR:HG23	2.17	0.45
3:A:214:VAL:CG2	3:A:218:LEU:CD1	2.95	0.45
3:B:34:HIS:O	3:B:37:ASN:HB2	2.16	0.45
3:B:49:TYR:CE1	3:B:51:HIS:HB2	2.50	0.45
3:A:197:HIS:HA	3:A:198:PRO:HD3	1.64	0.45
3:A:18:MET:SD	3:A:19:LEU:HD12	2.56	0.45
3:A:294:ASN:HD22	3:A:299:ARG:CZ	2.29	0.45
3:A:292:THR:O	3:A:299:ARG:NH1	2.49	0.45
3:A:291:PHE:HA	3:A:299:ARG:O	2.16	0.45
3:A:133:ASN:H	3:A:136:GLN:NE2	2.15	0.45
3:B:148:LYS:CB	3:B:253:ARG:HH12	2.29	0.45
3:B:325:TRP:CE3	3:B:328:ARG:HD2	2.52	0.45
2:P:1:DC:C2'	2:P:2:DG:C8	2.98	0.45
3:B:269:VAL:O	3:B:273:THR:N	2.48	0.45
3:B:328:ARG:HH11	3:B:328:ARG:CB	2.30	0.45
3:A:67:THR:CG2	3:A:68:LYS:N	2.79	0.45
3:B:170:ASP:O	3:B:173:TYR:HB2	2.17	0.45
3:B:182:ARG:C	3:B:184:GLY:H	2.19	0.45
3:B:175:ALA:CB	3:B:195:LEU:HD13	2.45	0.45
3:B:33:ILE:HG23	3:B:34:HIS:N	2.32	0.44
3:A:225:THR:HB	3:A:226:ASP:OD1	2.16	0.44
3:A:234:LYS:HE2	3:A:236:MET:HG3	1.99	0.44
3:B:269:VAL:O	3:B:273:THR:OG1	2.34	0.44
3:B:325:TRP:CZ3	3:B:328:ARG:CD	3.00	0.44
3:B:79:THR:HG23	3:B:81:LYS:O	2.17	0.44
1:C:10:DC:C4	1:C:11:DG:C6	3.04	0.44
3:A:132:LEU:HD22	3:A:136:GLN:HE21	1.81	0.44
3:A:183:ARG:NH1	3:A:273:THR:CG2	2.79	0.44
3:A:330:PRO:CA	3:A:333:ARG:HG3	2.36	0.44
3:A:62:LEU:HD12	3:A:63:PRO:N	2.31	0.44
3:B:11:LEU:N	3:B:11:LEU:CD1	2.80	0.44
3:B:286:ALA:O	3:B:289:LYS:N	2.51	0.44
3:B:20:VAL:HG13	3:B:21:GLU:N	2.33	0.44
3:A:150:ILE:HD11	3:A:190:ASP:HA	1.99	0.44
3:B:146:PHE:HA	3:B:146:PHE:HD1	1.47	0.44
3:B:17:ASP:O	3:B:21:GLU:HG3	2.17	0.44
3:A:213:ARG:O	3:A:216:GLU:N	2.51	0.44
3:A:277:ILE:HG12	3:A:277:ILE:H	1.45	0.44
3:A:283:ARG:HD3	3:A:293:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:321:ASP:O	3:A:324:GLN:N	2.37	0.44
3:A:330:PRO:CD	3:A:333:ARG:HH21	2.06	0.44
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.76	0.44
3:A:11:LEU:HD22	3:A:12:ASN:H	1.80	0.44
3:A:174:ILE:N	3:A:174:ILE:CD1	2.81	0.44
3:A:241:LEU:CD2	3:A:250:TYR:CD2	3.00	0.44
3:B:304:THR:HG23	3:B:306:VAL:HB	1.99	0.44
3:A:320:PHE:CE1	3:A:327:TYR:HD2	2.36	0.43
3:A:62:LEU:O	3:A:65:VAL:HG13	2.18	0.43
3:A:194:LEU:HA	3:A:194:LEU:HD22	1.78	0.43
3:A:201:THR:HA	3:A:261:PRO:CB	2.39	0.43
3:A:177:VAL:HG13	3:A:177:VAL:O	2.18	0.43
3:B:53:ILE:H	3:B:53:ILE:HG13	1.62	0.43
2:P:7:DC:C4	5:A:338:DCT:N4	2.86	0.43
3:A:126:ARG:HA	3:A:140:LEU:HD21	2.01	0.43
3:A:213:ARG:O	3:A:217:GLN:N	2.43	0.43
3:B:194:LEU:HD22	3:B:194:LEU:HA	1.81	0.43
3:A:217:GLN:HG2	3:A:221:VAL:CG2	2.48	0.43
3:B:103:VAL:CB	3:B:106:ILE:HD12	2.47	0.43
3:B:33:ILE:O	3:B:36:TYR:HB3	2.18	0.43
3:A:133:ASN:C	3:A:137:ARG:HG3	2.39	0.43
3:A:212:HIS:O	3:A:216:GLU:HG3	2.19	0.43
2:P:2:DG:C2'	2:P:3:DG:C8	3.01	0.43
3:B:207:GLN:HB3	3:B:210:LEU:HD12	2.01	0.43
3:B:23:ALA:HB1	3:B:36:TYR:HD1	1.83	0.43
3:A:166:VAL:HG12	3:A:167:LYS:N	2.34	0.43
3:A:174:ILE:O	3:A:195:LEU:HA	2.18	0.43
3:A:283:ARG:CD	3:A:293:ILE:HB	2.49	0.43
3:B:270:LEU:HD12	3:B:333:ARG:HH12	1.84	0.43
3:B:77:LEU:HA	3:B:77:LEU:HD13	1.68	0.43
3:A:200:PHE:HA	3:A:204:SER:HG	1.83	0.43
3:B:313:VAL:C	3:B:315:SER:H	2.21	0.43
3:A:138:ILE:HG23	3:A:138:ILE:HD12	1.63	0.43
3:A:279:ASN:N	3:A:279:ASN:OD1	2.41	0.43
3:B:228:LEU:HD23	3:B:228:LEU:HA	1.72	0.43
3:B:294:ASN:HD22	3:B:299:ARG:HH22	1.67	0.43
3:A:172:GLU:HB3	3:A:198:PRO:CD	2.49	0.42
3:A:294:ASN:ND2	3:A:297:THR:H	2.17	0.42
3:B:257:ILE:HG22	3:B:258:ARG:H	1.83	0.42
3:A:274:GLY:HA3	3:A:279:ASN:HD21	1.84	0.42
3:A:294:ASN:HD22	3:A:299:ARG:HH22	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:299:ARG:HB2	3:A:300:PRO:HD2	2.01	0.42
3:B:328:ARG:HB3	3:B:328:ARG:HH11	1.84	0.42
3:A:238:VAL:CG1	3:A:239:CYS:N	2.81	0.42
3:A:264:GLN:HE21	3:A:264:GLN:HB2	1.65	0.42
2:P:7:DC:C5	5:A:338:DCT:H5	2.54	0.42
3:B:133:ASN:OD1	3:B:133:ASN:O	2.37	0.42
5:B:338:DCT:O1A	5:B:338:DCT:O1G	2.37	0.42
3:A:206:LYS:HG3	3:A:207:GLN:H	1.83	0.42
3:B:128:ASN:O	3:B:131:LYS:N	2.52	0.42
3:B:20:VAL:C	3:B:23:ALA:H	2.23	0.42
3:B:324:GLN:NE2	3:B:324:GLN:HA	2.28	0.42
3:A:172:GLU:HB3	3:A:198:PRO:HG3	2.01	0.42
3:A:301:LEU:O	3:A:303:VAL:N	2.52	0.42
3:A:316:GLU:O	3:A:320:PHE:HD1	2.02	0.42
3:A:316:GLU:CD	3:A:333:ARG:HH22	2.21	0.42
3:A:99:PHE:HD2	3:A:100:LEU:CD1	2.32	0.42
3:B:166:VAL:HG12	3:B:167:LYS:N	2.34	0.42
3:B:270:LEU:HD21	3:B:282:MET:HE3	2.01	0.42
3:A:330:PRO:HA	3:A:333:ARG:CD	2.50	0.42
3:A:66:GLY:O	3:A:69:ILE:HG12	2.19	0.42
2:D:5:DG:O5'	3:B:107:GLY:HA3	2.20	0.42
3:A:200:PHE:CE2	3:A:259:LEU:HG	2.51	0.42
3:A:316:GLU:HB3	3:A:320:PHE:HE1	1.85	0.42
3:B:317:GLN:HG3	3:B:327:TYR:CD1	2.55	0.42
3:B:320:PHE:CZ	3:B:328:ARG:HB2	2.53	0.42
3:B:330:PRO:HA	3:B:333:ARG:NE	2.35	0.42
3:B:62:LEU:HA	3:B:63:PRO:HD3	1.74	0.42
3:B:69:ILE:O	3:B:69:ILE:HG22	2.19	0.42
3:A:146:PHE:H	3:A:146:PHE:HD1	1.67	0.42
3:A:237:GLY:N	3:A:255:ILE:O	2.33	0.42
3:A:33:ILE:O	3:A:37:ASN:N	2.47	0.42
3:B:207:GLN:N	3:B:208:PRO:HD3	2.35	0.42
3:B:283:ARG:CZ	3:B:294:ASN:HA	2.49	0.42
2:D:5:DG:H2'	2:D:6:DC:C6	2.55	0.42
1:T:9:DC:H2''	1:T:10:DC:H5'	2.02	0.42
3:A:20:VAL:O	3:A:23:ALA:HB3	2.20	0.41
3:A:24:ASN:CA	3:A:27:LYS:HB3	2.40	0.41
3:A:294:ASN:ND2	3:A:299:ARG:NH1	2.68	0.41
3:B:294:ASN:ND2	3:B:299:ARG:NH2	2.68	0.41
3:A:267:CYS:HB2	3:A:295:GLU:C	2.40	0.41
2:P:4:DC:H2'	2:P:5:DG:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:180:SER:OG	3:A:188:SER:HB3	2.20	0.41
3:A:291:PHE:N	3:A:301:LEU:HD22	2.35	0.41
3:A:285:HIS:O	3:A:288:GLU:HB3	2.20	0.41
3:B:133:ASN:CB	3:B:136:GLN:HE21	2.33	0.41
3:B:133:ASN:OD1	3:B:136:GLN:NE2	2.44	0.41
3:B:23:ALA:HA	3:B:39:TYR:HD2	1.86	0.41
3:A:15:ILE:HG23	3:A:16:THR:N	2.35	0.41
3:A:319:ILE:HG21	3:A:319:ILE:HD13	1.73	0.41
3:B:173:TYR:CE1	3:B:197:HIS:HB2	2.55	0.41
3:B:235:PHE:CD2	3:B:257:ILE:CG1	2.97	0.41
3:B:202:SER:OG	3:B:263:ASP:OD2	2.30	0.41
3:A:22:LEU:CD1	3:A:22:LEU:N	2.82	0.41
3:B:150:ILE:HG13	3:B:189:GLY:O	2.21	0.41
3:B:172:GLU:HB3	3:B:197:HIS:NE2	2.36	0.41
3:B:172:GLU:HA	3:B:172:GLU:OE1	2.21	0.41
3:A:11:LEU:HD23	3:A:12:ASN:N	2.27	0.41
3:A:238:VAL:CG1	3:A:252:HIS:HB3	2.51	0.41
3:A:320:PHE:O	3:A:325:TRP:N	2.50	0.41
3:B:149:ARG:O	3:B:151:PRO:HD3	2.20	0.41
3:B:234:LYS:HG3	3:B:235:PHE:N	2.35	0.41
3:B:270:LEU:HD12	3:B:333:ARG:NH1	2.36	0.41
3:B:37:ASN:CA	3:B:40:ARG:HG2	2.49	0.41
3:A:9:GLU:HB3	3:A:10:THR:H	1.73	0.41
3:A:125:LEU:CD2	3:A:140:LEU:HD13	2.51	0.41
3:B:136:GLN:O	3:B:139:GLY:N	2.54	0.41
3:B:182:ARG:NH2	3:B:269:VAL:CG1	2.80	0.41
3:B:218:LEU:HB3	3:B:224:ILE:HG13	2.03	0.40
3:B:239:CYS:SG	3:B:253:ARG:O	2.78	0.40
3:A:134:HIS:HA	3:A:137:ARG:HD2	2.03	0.40
3:A:331:LYS:HG3	3:A:331:LYS:H	1.21	0.40
3:A:23:ALA:O	3:A:36:TYR:HB2	2.20	0.40
3:A:292:THR:HG22	3:A:301:LEU:HD11	2.04	0.40
3:A:152:ARG:NH2	3:A:184:GLY:HA2	2.36	0.40
3:B:149:ARG:HH21	3:B:188:SER:HA	1.85	0.40
3:B:197:HIS:CD2	3:B:198:PRO:CD	2.99	0.40
3:B:285:HIS:O	3:B:288:GLU:HB3	2.22	0.40
3:B:293:ILE:HG22	3:B:294:ASN:N	2.37	0.40
1:C:7:DC:H2'	1:C:7:DC:O5'	2.22	0.40
3:A:134:HIS:O	3:A:137:ARG:N	2.54	0.40
3:A:211:LEU:O	3:A:214:VAL:HG12	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:2:DG:C5'	3:A:66:GLY:CA[2_655]	2.09	0.11
2:P:2:DG:O5'	3:A:66:GLY:CA[2_655]	2.15	0.05

## 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	320/335 (96%)	234 (73%)	55 (17%)	31 (10%)	1	11
3	B	320/335 (96%)	248 (78%)	48 (15%)	24 (8%)	1	16
All	All	640/670 (96%)	482 (75%)	103 (16%)	55 (9%)	1	13

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	11	LEU
3	A	127	LYS
3	A	130	ASP
3	A	143	PHE
3	A	198	PRO
3	A	206	LYS
3	A	207	GLN
3	A	222	ARG
3	A	275	SER
3	A	276	ASP
3	A	303	VAL
3	A	333	ARG
3	A	334	SER
3	B	11	LEU
3	B	32	ALA
3	B	50	PRO
3	B	143	PHE

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Mol	Chain	Res	Type
3	B	186	GLU
3	B	207	GLN
3	A	80	GLY
3	A	164	ASN
3	A	205	SER
3	A	265	TYR
3	A	306	VAL
3	A	330	PRO
3	B	10	THR
3	B	67	THR
3	B	80	GLY
3	B	204	SER
3	B	276	ASP
3	B	327	TYR
3	A	10	THR
3	A	116	ASP
3	A	262	LYS
3	A	274	GLY
3	A	302	GLY
3	A	310	PRO
3	B	206	LYS
3	B	240	GLN
3	B	273	THR
3	B	274	GLY
3	B	275	SER
3	A	32	ALA
3	A	93	THR
3	B	52	LYS
3	A	12	ASN
3	B	120	LYS
3	B	130	ASP
3	B	198	PRO
3	B	324	GLN
3	A	108	PRO
3	A	319	ILE
3	B	330	PRO
3	A	208	PRO
3	B	170	ASP



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	267/296 (90%)	222 (83%)	45 (17%)	2	17
3	B	267/296 (90%)	226 (85%)	41 (15%)	3	22
All	All	534/592 (90%)	448 (84%)	86 (16%)	3	19

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	11	LEU
3	A	16	THR
3	A	26	GLU
3	A	31	GLN
3	A	36	TYR
3	A	41	LYS
3	A	45	VAL
3	A	67	THR
3	A	74	ASP
3	A	77	LEU
3	A	85	LEU
3	A	90	GLN
3	A	91	ASP
3	A	93	THR
3	A	100	LEU
3	A	104	THR
3	A	115	VAL
3	A	122	LEU
3	A	128	ASN
3	A	130	ASP
3	A	133	ASN
3	A	136	GLN
3	A	144	GLU
3	A	176	THR
3	A	193	VAL
3	A	196	THR
3	A	205	SER

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Mol	Chain	Res	Type
3	A	207	GLN
3	A	222	ARG
3	A	225	THR
3	A	226	ASP
3	A	257	ILE
3	A	258	ARG
3	A	264	GLN
3	A	269	VAL
3	A	272	PHE
3	A	295	GLU
3	A	299	ARG
3	A	301	LEU
3	A	304	THR
3	A	311	LEU
3	A	314	ASP
3	A	324	GLN
3	A	327	TYR
3	A	331	LYS
3	B	11	LEU
3	B	19	LEU
3	B	24	ASN
3	B	26	GLU
3	B	28	ASN
3	B	31	GLN
3	B	41	LYS
3	B	65	VAL
3	B	77	LEU
3	B	95	SER
3	B	100	LEU
3	B	103	VAL
3	B	104	THR
3	B	116	ASP
3	B	122	LEU
3	B	125	LEU
3	B	133	ASN
3	B	159	GLN
3	B	173	TYR
3	B	178	CYS
3	B	199	ASN
3	B	209	LYS
3	B	215	VAL
3	B	222	ARG

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Mol	Chain	Res	Type
3	B	226	ASP
3	B	229	SER
3	B	233	THR
3	B	249	GLU
3	B	254	ARG
3	B	258	ARG
3	B	264	GLN
3	B	271	TYR
3	B	272	PHE
3	B	275	SER
3	B	276	ASP
3	B	293	ILE
3	B	311	LEU
3	B	314	ASP
3	B	318	ASP
3	B	324	GLN
3	B	328	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	37	ASN
3	A	90	GLN
3	A	98	ASN
3	A	128	ASN
3	A	157	GLN
3	A	159	GLN
3	A	207	GLN
3	A	264	GLN
3	A	294	ASN
3	A	324	GLN
3	B	28	ASN
3	B	31	GLN
3	B	37	ASN
3	B	136	GLN
3	B	159	GLN
3	B	197	HIS
3	B	212	HIS
3	B	264	GLN
3	B	281	ASN
3	B	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	DCT	A	338	-	22,28,28	1.33	3 (13%)	20,43,43	1.35	3 (15%)
5	DCT	B	338	-	22,28,28	0.98	1 (4%)	20,43,43	1.03	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DCT	A	338	-	-	0/18/31/31	0/2/2/2
5	DCT	B	338	-	-	0/18/31/31	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	338	DCT	PG-O3B	-3.40	1.54	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	338	DCT	PG-O2G	-2.41	1.44	1.54
5	A	338	DCT	O5'-C5'	-2.41	1.35	1.44
5	A	338	DCT	C6-N1	2.39	1.39	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	338	DCT	C5-C6-N1	-2.25	115.50	120.67
5	A	338	DCT	C6-N1-C2	2.44	125.23	121.28
5	A	338	DCT	O2G-PG-O1G	2.53	120.39	110.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	338	DCT	8	0
5	B	338	DCT	1	0

## 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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.