

# Full wwPDB X-ray Structure Validation Report (i)

#### Jan 30, 2024 - 04:23 PM EST

PDB ID	:	1HUO
Title	:	CRYSTAL STRUCTURE OF DNA POLYMERASE BETA COMPLEXED
		WITH DNA AND CR-TMPPCP
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		C.; Tsai, MD.; Chan, M.K.
Deposited on	:	2001-01-04
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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

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.



Matria	Whole archive	Similar resolution
wietric	$(\# {\rm Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length		Qua	lity of chain		
1	С	11	9%	64%		27	%
1	Т	11	9%	36%	27%	27%	6
2	D	7		57%		43%	
2	Р	7		71%		29%	6
3	А	335		61%		33%	••
3	В	335		60%		32%	5% •



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# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5991 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 5'-D(\*AP\*AP\*TP\*AP\*GP\*GP\*CP\*GP\*TP\*CP\*G)-3'.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	т	0	Total	С	Ν	Ο	Р	0	0	0
	1	0	167	78	33	48	8	0		
1	C	0	Total	С	Ν	Ο	Р	0	0	0
		0	167	78	33	48	8	0	0	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	D	7	Total	С	Ν	Ο	Р	0	0	0
	1	1	141	66	27	41	7	0		
0	Л	7	Total	С	Ν	Ο	Р	0	0	0
	D	1	141	66	27	41	$\overline{7}$	0		

• Molecule 3 is a protein called DNA POLYMERASE BETA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	Δ	205	Total	С	Ν	0	S	0	0	0
0	A	323	2598	1639	457	493	9	0		
2	Р	205	Total	С	Ν	0	S	0	0	0
0	D	323	2598	1639	457	493	9	0		0

• Molecule 4 is CHROMIUM ION (three-letter code: CR) (formula: Cr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Cr 1 1	0	0
4	В	1	Total Cr 1 1	0	0

• Molecule 5 is PHOSPHOMETHYL PHOSPHONIC ACID DEOXYTHYMIDYLATE ESTER (three-letter code: TTE) (formula:  $C_{11}H_{19}N_2O_{13}P_3$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
Б	Δ	1	1 Total		Ν	Ο	Р	0	0	
0	A	1	29	11	2	13	3	0	0	
Б	D	1	Total	С	Ν	Ο	Р	0	0	
0	D	L	29	11	2	13	3	0	0	

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Т	4	Total O 4 4	0	0
6	Р	6	Total O 6 6	0	0
6	С	9	Total O 9 9	0	0
6	D	6	Total O 6 6	0	0
6	А	45	$\begin{array}{cc} \text{Total} & \text{O} \\ 45 & 45 \end{array}$	0	0
6	В	49	Total         O           49         49	0	0



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# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: 5'-D(\*AP\*AP\*TP\*AP\*GP\*GP\*CP\*GP\*TP\*CP\*G)-3'

Chain T:	9%	36%	27%	27%	
DA DA DA CS C7 C7 C7 C8	T9 C10 G11				
• Molecule	e 1: 5'-D(	*AP*AP*TP*AP*(	GP*GP*CP*GP*7	[P*CP*G)-3'	
Chain C:	9%	64%		27%	I
DA DA DA G5 G5 C7 C7	T9 C10 G11				
• Molecule	e 2: 5'-D(	P*CP*GP*AP*CP	*GP*CP*C)-3'		
Chain P:		71%		29%	I
C1 G2 G2 G5 G5 C6 C7					
• Molecule	e 2: 5'-D(	P*CP*GP*AP*CP	*GP*CP*C)-3'		
Chain D:		57%		43%	•
C1 62 64 65 65 65 65 67					
• Molecule	e 3: DNA	. POLYMERASE B	ETA		_
Chain A:	_	61%		33% • •	-
MET SER LYS LYS ALA PRO CIN	GLU GLU I15 M18	L19 L22 L22 K27 K27 N28 Y29 Y49 Y49 Y49	101 153 153 153 153 160 160 162 162 064 065 064 065 066 066 066 066	E71 K72 F76 L77 L77 C79 C80 C80 C81 C81 K81 K84 K84	L85 R89
T93 894 N98 F99 V103	R112 K113 L114 V115	1119 8123 8123 8124 8125 8125 8125 8125 8125 8125 1138 1138 1138 1138 1138	145 1150 1150 1150 1155 1155 1155 1155 1	V162 V162 L165 N164 N164 N166 D170 D171 D171 A175	T176 V177 C178
F181 R182 R183 S187 S187 D192	L194 L195 L195 T196 S205 K206	Q207 R213 V214 S229 R229 R255 R255 R255	1250 1257 1258 1269 1269 1269 7265 7265 7265 7273 7273 7273	S275 D276 F278 F278 F278 A284 A284 A284 A286 A286 C288 F291	T292 1293
			WORLDWIDE PROTEIN DATA BANK		

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• Molecule 3: DNA POLYMERASE BETA





# 4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	105.91Å $56.16$ Å $86.06$ Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $107.25^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	20.00 - 2.60	Depositor	
% Data completeness	(Not available) $(20.00-2.60)$	Depositor	
(in resolution range)	(1101 available) (20.00 2.00)		
$R_{merge}$	0.06	Depositor	
R <sub>sym</sub>	(Not available)	Depositor	
Refinement program	X-PLOR	Depositor	
$R, R_{free}$	0.226 , $0.288$	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	5991	wwPDB-VP	
Average B, all atoms $(Å^2)$	41.0	wwPDB-VP	



# 5 Model quality (i)

# 5.1 Standard geometry (i)

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

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).

Mal	Mol Chain		ond lengths	Bond angles		
MOI Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5		
1	С	2.75	14/187~(7.5%)	3.07	36/287~(12.5%)	
1	Т	2.78	15/187~(8.0%)	3.05	28/287~(9.8%)	
2	D	3.34	17/157~(10.8%)	3.59	33/239~(13.8%)	
2	Р	3.29	19/157~(12.1%)	3.90	37/239~(15.5%)	
3	А	0.43	0/2645	0.64	0/3562	
3	В	0.41	0/2645	0.61	0/3562	
All	All	1.10	65/5978~(1.1%)	1.35	134/8176~(1.6%)	

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	С	0	7
1	Т	0	6
2	D	0	7
2	Р	0	7
All	All	0	27

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	DC	C5'-C4'	13.50	1.66	1.51
2	D	1	DC	P-O5'	11.98	1.71	1.59
2	Р	1	DC	C5'-C4'	11.41	1.63	1.51
1	С	10	DC	C4'-O4'	-10.83	1.34	1.45
2	D	1	DC	C4'-C3'	10.72	1.64	1.53
2	Р	1	DC	P-O5'	10.68	1.70	1.59
2	Р	1	DC	C4'-C3'	9.58	1.62	1.53
1	С	8	DG	N9-C4	8.82	1.45	1.38



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	Chain	<i>i previ</i>	Turne	Atoma	7	Obcomrod(Å)	
	D	res	DC	Co N7		Observed(A)	$1 \text{ luear}(\mathbf{A})$
2	P	5 0	DG	C8-N7	8.03	1.30	1.30
2	P	2	DG	C2-N3	8.61	1.39	1.32
2	D	4	DC	03'-P	-8.35	1.51	1.61
1	Т	11	DG	N9-C4	8.29	1.44	1.38
1	Т	9	DT	C2-N3	7.87	1.44	1.37
1	С	8	DG	C2-N3	7.85	1.39	1.32
2	Р	2	DG	N9-C8	-7.73	1.32	1.37
1	Т	10	DC	C4'-O4'	-7.34	1.37	1.45
2	Р	4	DC	N3-C4	7.29	1.39	1.33
2	D	1	DC	C4-C5	-7.24	1.37	1.43
2	Р	6	DC	C2-N3	7.06	1.41	1.35
2	D	4	DC	C4'-O4'	-6.99	1.38	1.45
1	С	11	DG	C6-N1	6.93	1.44	1.39
1	С	7	DC	C5'-C4'	6.91	1.58	1.51
2	Р	4	DC	C4'-C3'	-6.85	1.45	1.52
2	Р	1	DC	C4'-O4'	6.78	1.51	1.45
2	D	2	DG	N7-C5	-6.69	1.35	1.39
2	Р	5	DG	C6-N1	6.49	1.44	1.39
2	Р	4	DC	N1-C6	6.46	1.41	1.37
1	С	10	DC	C2'-C1'	-6.37	1.45	1.52
1	С	5	DG	N1-C2	6.35	1.42	1.37
2	Р	1	DC	O4'-C1'	6.26	1.49	1.42
1	Т	6	DG	N9-C4	6.07	1.42	1.38
1	Т	9	DT	C4-O4	5.94	1.28	1.23
2	Р	5	DG	P-O5'	-5.91	1.53	1.59
1	С	7	DC	C4'-O4'	5.90	1.50	1.45
1	Т	11	DG	N1-C2	5.89	1.42	1.37
1	С	6	DG	C6-N1	5.88	1.43	1.39
2	D	6	DC	C3'-C2'	-5.87	1.45	1.52
2	D	7	DC	C4-N4	5.84	1.39	1.33
2	Р	3	DA	C6-N6	5.72	1.38	1.33
1	Т	9	DT	N1-C2	5.65	1.42	1.38
2	D	1	DC	O4'-C1'	5.64	1.49	1.42
2	Р	4	DC	P-O5'	-5.63	1.54	1.59
1	Т	10	DC	O3'-P	-5.63	1.54	1.61
2	D	2	DG	N3-C4	5.62	1.39	1.35
1	С	9	DT	N1-C2	5.55	1.42	1.38
1	Т	5	DG	N7-C5	-5.54	1.35	1.39
2	D	4	DC	C4'-C3'	-5.43	1.47	1.52
2	Р	3	DA	N9-C4	5.41	1.41	1.37
2	D	7	DC	N3-C4	5.38	1.37	1.33
1	С	10	DC	N1-C6	5.35	1.40	1.37



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Т	10	DC	C4'-C3'	-5.35	1.47	1.52
1	С	6	DG	C2-N3	5.33	1.37	1.32
2	D	3	DA	N7-C5	-5.29	1.36	1.39
2	D	2	DG	C6-N1	5.25	1.43	1.39
1	Т	5	DG	N1-C2	5.24	1.42	1.37
1	С	5	DG	C5'-C4'	5.24	1.57	1.51
2	D	1	DC	C2-N3	5.24	1.40	1.35
1	Т	4	DA	N3-C4	-5.22	1.31	1.34
2	Р	4	DC	C4-N4	5.21	1.38	1.33
2	D	2	DG	N9-C8	-5.05	1.34	1.37
1	С	5	DG	C6-N1	5.04	1.43	1.39
2	Р	1	DC	N1-C6	-5.04	1.34	1.37
1	Т	10	DC	N1-C6	5.02	1.40	1.37
1	Т	11	DG	C2-N3	5.01	1.36	1.32
1	Т	5	DG	C6-N1	5.00	1.43	1.39

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Р	1	DC	O4'-C1'-N1	17.98	120.58	108.00
2	Р	2	DG	N3-C2-N2	15.38	130.66	119.90
2	D	2	DG	N3-C2-N2	13.02	129.01	119.90
2	D	1	DC	O4'-C1'-N1	12.64	116.85	108.00
2	Р	1	DC	O4'-C4'-C3'	-12.29	98.62	106.00
1	С	8	DG	N3-C2-N2	11.91	128.24	119.90
2	Р	1	DC	C6-N1-C2	-11.47	115.71	120.30
2	Р	4	DC	N3-C4-N4	11.04	125.73	118.00
1	С	10	DC	O4'-C4'-C3'	-10.72	99.57	106.00
2	D	1	DC	N3-C4-N4	10.67	125.47	118.00
2	D	5	DG	O4'-C1'-C2'	-10.65	97.38	105.90
2	D	3	DA	N1-C6-N6	10.47	124.88	118.60
2	Р	1	DC	N3-C4-C5	-10.17	117.83	121.90
1	С	4	DA	N1-C6-N6	9.74	124.44	118.60
2	Р	7	DC	O4'-C4'-C3'	-9.43	100.34	106.00
1	Т	11	DG	N3-C2-N2	9.21	126.35	119.90
2	Р	1	DC	N3-C4-N4	9.15	124.41	118.00
2	Р	1	DC	N3-C2-O2	-9.13	115.51	121.90
2	D	5	DG	N3-C2-N2	9.06	126.25	119.90
2	Р	3	DA	N1-C6-N6	8.75	123.85	118.60
2	Р	2	DG	N1-C2-N2	-8.74	108.34	116.20
2	D	1	DC	P-O5'-C5'	8.70	134.81	120.90
1	Т	8	DG	N3-C2-N2	8.66	125.96	119.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Р	5	DG	N3-C2-N2	8.59	125.91	119.90
2	D	4	DC	O4'-C4'-C3'	-8.52	100.89	106.00
2	D	1	DC	O4'-C4'-C3'	-8.48	100.91	106.00
1	С	6	DG	C5-C6-O6	-8.43	123.55	128.60
1	С	10	DC	N3-C4-N4	8.41	123.89	118.00
2	D	7	DC	N3-C4-C5	-8.40	118.54	121.90
2	D	6	DC	N3-C4-N4	8.32	123.83	118.00
2	D	2	DG	N1-C2-N2	-8.21	108.81	116.20
2	D	1	DC	C5-C4-N4	-8.15	114.49	120.20
1	С	6	DG	N1-C6-O6	8.10	124.76	119.90
2	D	3	DA	C8-N9-C4	-8.08	102.57	105.80
1	С	11	DG	N3-C2-N2	8.04	125.53	119.90
1	С	6	DG	N3-C2-N2	8.04	125.53	119.90
1	Т	5	DG	N3-C2-N2	7.93	125.45	119.90
1	Т	6	DG	P-O5'-C5'	-7.90	108.27	120.90
2	D	7	DC	N3-C4-N4	7.87	123.51	118.00
1	Т	4	DA	C5-C6-N1	-7.85	113.77	117.70
1	Т	9	DT	O4'-C1'-N1	7.84	113.49	108.00
1	Т	10	DC	N3-C4-C5	-7.69	118.82	121.90
1	С	9	DT	O4'-C1'-C2'	-7.66	99.77	105.90
2	Р	4	DC	N3-C4-C5	-7.43	118.93	121.90
1	С	6	DG	N1-C2-N3	-7.41	119.45	123.90
2	D	4	DC	O5'-P-OP1	7.21	119.35	110.70
1	Т	9	DT	N3-C4-O4	7.09	124.15	119.90
2	Р	4	DC	C5-C4-N4	-7.02	115.29	120.20
2	Р	1	DC	P-O3'-C3'	7.00	128.10	119.70
2	Р	1	DC	O5'-P-OP2	6.92	119.01	110.70
2	Р	2	DG	O3'-P-O5'	-6.87	90.94	104.00
1	С	11	DG	N1-C6-O6	6.84	124.00	119.90
2	Р	3	DA	C5-C6-N1	-6.80	114.30	117.70
1	Т	10	DC	N3-C4-N4	6.80	122.76	118.00
1	С	8	DG	O4'-C1'-N9	-6.80	103.24	108.00
2	Р	6	DC	N3-C4-C5	-6.79	119.19	121.90
2	Р	3	DA	P-O5'-C5'	-6.75	110.11	120.90
1	С	5	DG	N1-C2-N3	-6.64	119.91	123.90
1	Т	5	DG	N1-C6-O6	6.58	123.84	119.90
2	D	5	DG	C8-N9-C4	-6.48	103.81	106.40
2	Р	6	DC	N3-C4-N4	6.46	122.52	118.00
1	Т	6	DG	N1-C6-O6	6.40	123.74	119.90
1	С	8	DG	N3-C4-C5	-6.37	125.42	128.60
2	D	5	DG	OP1-P-O3 <sup>7</sup>	6.32	119.10	105.20
2	Р	3	DA	O4'-C1'-C2'	-6.32	100.85	105.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	D	6	DC	N3-C4-C5	-6.31	119.38	121.90
1	С	5	DG	C2-N3-C4	6.26	115.03	111.90
1	Т	9	DT	N3-C4-C5	-6.25	111.45	115.20
2	Р	4	DC	C4'-C3'-C2'	-6.19	97.53	103.10
1	С	11	DG	C5-C6-O6	-6.13	124.92	128.60
1	Т	6	DG	N3-C2-N2	6.13	124.19	119.90
1	С	11	DG	C2-N3-C4	6.08	114.94	111.90
1	С	10	DC	C2-N3-C4	6.08	122.94	119.90
1	Т	11	DG	N1-C2-N3	-6.08	120.25	123.90
1	С	7	DC	C6-N1-C2	-6.04	117.89	120.30
1	Т	8	DG	N1-C2-N3	-6.02	120.29	123.90
1	Т	8	DG	N1-C6-O6	6.01	123.51	119.90
1	С	11	DG	N1-C2-N3	-6.00	120.30	123.90
2	Р	2	DG	N1-C2-N3	-5.99	120.31	123.90
1	С	8	DG	N1-C2-N3	-5.95	120.33	123.90
1	С	10	DC	N3-C4-C5	-5.95	119.52	121.90
2	D	2	DG	P-O3'-C3'	5.92	126.80	119.70
1	С	8	DG	N3-C4-N9	5.91	129.55	126.00
1	Т	9	DT	C4-C5-C6	5.91	121.55	118.00
2	D	1	DC	C4'-C3'-C2'	5.88	108.39	103.10
2	Р	4	DC	P-O3'-C3'	5.87	126.75	119.70
1	Т	5	DG	O4'-C1'-N9	5.80	112.06	108.00
1	Т	7	DC	P-O5'-C5'	-5.74	111.71	120.90
1	С	5	DG	N1-C6-O6	5.74	123.34	119.90
1	С	7	DC	C5-C6-N1	5.71	123.86	121.00
2	D	4	DC	O4'-C1'-N1	5.70	111.99	108.00
1	С	5	DG	N3-C2-N2	5.68	123.88	119.90
2	D	1	DC	O5'-P-OP2	5.68	117.52	110.70
2	Р	2	DG	P-O3'-C3'	5.64	126.47	119.70
1	С	4	DA	C5-C6-N1	-5.62	114.89	117.70
1	C	6	DG	C3'-C2'-C1'	-5.62	95.76	102.50
1	Т	4	DA	P-O5'-C5'	-5.61	111.92	120.90
2	D	1	DC	C6-N1-C2	-5.61	118.06	120.30
2	D	3	DA	C5-C6-N6	-5.56	119.25	123.70
1	С	7	DC	N3-C4-N4	5.55	121.88	118.00
2	D	2	DG	C8-N9-C4	-5.54	104.18	106.40
2	Р	1	DC	C4'-C3'-C2'	5.54	108.08	103.10
2	Р	5	DG	N1-C2-N2	-5.50	111.25	116.20
2	D	7	DC	04'-C1'-N1	5.50	111.85	108.00
2	Р	1	DC	O5'-C5'-C4'	5.49	$1\overline{24.72}$	111.00
1	C	9	DT	N3-C2-O2	$-5.\overline{47}$	119.02	122.30
1	Т	4	DA	C4-C5-C6	5.38	119.69	117.00



Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
2	D	5	DG	C1'-O4'-C4'	-5.37	104.73	110.10
1	Т	6	DG	P-O3'-C3'	-5.37	113.26	119.70
2	Р	2	DG	N3-C4-N9	5.34	129.21	126.00
2	D	2	DG	O4'-C1'-N9	-5.34	104.26	108.00
2	Р	1	DC	P-O5'-C5'	5.33	129.42	120.90
2	Р	4	DC	OP1-P-O3'	5.33	116.91	105.20
1	С	8	DG	N1-C2-N2	-5.30	111.43	116.20
1	Т	10	DC	C6-N1-C2	-5.30	118.18	120.30
2	D	2	DG	N1-C6-O6	5.29	123.08	119.90
1	С	10	DC	N1-C2-O2	5.28	122.07	118.90
1	С	4	DA	P-O5'-C5'	-5.28	112.46	120.90
1	Т	5	DG	O3'-P-O5'	-5.28	93.98	104.00
1	Т	9	DT	C4'-C3'-C2'	5.27	107.85	103.10
2	Р	1	DC	N1-C2-N3	5.25	122.88	119.20
2	Р	1	DC	O4'-C1'-C2'	-5.24	101.71	105.90
1	Т	8	DG	C5-C6-O6	-5.23	125.46	128.60
2	Р	1	DC	C5-C6-N1	5.17	123.58	121.00
1	С	5	DG	P-O3'-C3'	5.16	125.90	119.70
1	С	10	DC	C5-C4-N4	-5.16	116.59	120.20
2	D	2	DG	N7-C8-N9	5.15	115.67	113.10
2	D	3	DA	P-O5'-C5'	-5.07	112.78	120.90
1	С	6	DG	P-O5'-C5'	-5.07	112.79	120.90
2	Р	4	DC	P-O5'-C5'	-5.07	112.79	120.90
2	Р	4	DC	C5-C6-N1	5.05	123.53	121.00
2	D	6	DC	C5-C4-N4	-5.04	116.67	120.20
1	Т	10	DC	O4'-C1'-C2'	-5.01	101.89	105.90
1	Т	8	DG	N9-C1'-C2'	5.00	122.10	112.60

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There are no chirality outliers.

All (	(27)	planarity	outliers	are	listed	below:
1 TII (	<u> </u>	pranarity	outifiers	arc	moucu	00101.

Mol	Chain	Res	Type	Group
1	С	10	DC	Sidechain
1	С	11	DG	Sidechain
1	С	5	DG	Sidechain
1	С	6	DG	Sidechain
1	С	7	DC	Sidechain
1	С	8	DG	Sidechain
1	С	9	DT	Sidechain
2	D	1	DC	Sidechain
2	D	2	DG	Sidechain
2	D	3	DA	Sidechain



Mol	Chain	Res	Type	Group
2	D	4	DC	Sidechain
2	D	5	DG	Sidechain
2	D	6	DC	Sidechain
2	D	7	DC	Sidechain
2	Р	1	DC	Sidechain
2	Р	2	DG	Sidechain
2	Р	3	DA	Sidechain
2	Р	4	DC	Sidechain
2	Р	5	DG	Sidechain
2	Р	6	DC	Sidechain
2	Р	7	DC	Sidechain
1	Т	10	DC	Sidechain
1	Т	11	DG	Sidechain
1	Т	5	DG	Sidechain
1	Т	6	DG	Sidechain
1	Т	7	DC	Sidechain
1	Т	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	С	167	0	90	0	0
1	Т	167	0	90	3	0
2	D	141	0	78	4	0
2	Р	141	0	78	4	0
3	А	2598	0	2604	89	0
3	В	2598	0	2604	92	0
4	А	1	0	0	0	0
4	В	1	0	0	0	0
5	А	29	0	15	7	0
5	В	29	0	15	6	0
6	А	45	0	0	4	0
6	В	49	0	0	4	0
6	С	9	0	0	0	0
6	D	6	0	0	0	0
6	Р	6	0	0	0	0
6	Т	4	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5991	0	5574	194	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 17.

All (194) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:A:338:TTE:O4'	5:A:338:TTE:C4'	1.64	1.38
5:B:338:TTE:O4'	5:B:338:TTE:C4'	1.64	1.27
3:B:300:PRO:HD3	3:B:311:LEU:HD23	1.58	0.83
3:A:125:LEU:HD23	3:A:140:LEU:HD13	1.62	0.80
3:A:323:ILE:HG13	3:A:325:TRP:HB2	1.63	0.80
3:A:192:ASP:HB3	3:A:272:PHE:CE1	2.16	0.79
3:A:169:LEU:HD21	3:A:213:ARG:HB3	1.65	0.77
3:A:150:ILE:HG12	3:A:253:ARG:HD2	1.68	0.76
3:A:183:ARG:HD3	3:A:274:GLY:O	1.86	0.75
3:A:293:ILE:HG12	3:A:298:ILE:HD13	1.68	0.74
3:B:229:SER:HB2	3:B:236:MET:HB2	1.67	0.73
3:A:256:ASP:HB2	6:A:1004:HOH:O	1.87	0.72
5:A:338:TTE:H6	5:A:338:TTE:H3'	1.72	0.72
3:B:20:VAL:HG13	3:B:40:ARG:HH12	1.56	0.69
3:B:293:ILE:HG12	3:B:298:ILE:HD13	1.76	0.68
3:B:129:GLU:HB3	3:B:137:ARG:HD2	1.76	0.68
3:A:297:THR:HB	3:A:310:PRO:HB3	1.75	0.67
3:B:150:ILE:HG21	3:B:155:MET:SD	2.33	0.67
2:D:7:DC:C2'	5:B:338:TTE:H5'2	2.24	0.67
3:B:152:ARG:HH22	3:B:184:GLY:HA2	1.60	0.67
2:P:7:DC:H2'	5:A:338:TTE:H5'2	1.77	0.66
3:A:153:GLU:HA	3:A:156:LEU:HD12	1.77	0.66
3:A:194:LEU:HD11	3:A:260:ILE:CG1	2.26	0.66
3:A:229:SER:HB2	3:A:236:MET:HB2	1.78	0.65
3:A:291:PHE:HA	3:A:300:PRO:HA	1.77	0.65
3:B:271:TYR:HA	3:B:279:ASN:HD21	1.63	0.64
3:B:60:LYS:HA	3:B:65:VAL:HG22	1.80	0.64
3:B:151:PRO:HG2	3:B:154:GLU:HB2	1.80	0.64
3:A:174:ILE:HB	3:A:196:THR:HG22	1.79	0.63
3:B:28:ASN:HD22	3:B:98:ASN:ND2	1.96	0.63
3:B:106:ILE:HG23	3:B:110:ALA:HB3	1.81	0.63
3:B:99:PHE:O	3:B:102:ARG:HB2	2.00	0.61
3:B:81:LYS:NZ	3:B:81:LYS:HB3	2.15	0.60



	to as pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:P:7:DC:C2'	5:A:338:TTE:H5'2	2.31	0.60
3:A:152:ARG:HH11	3:A:152:ARG:HG3	1.66	0.60
3:A:275:SER:HB3	3:A:278:PHE:HB3	1.83	0.59
3:A:60:LYS:HA	3:A:65:VAL:HG22	1.85	0.59
3:B:82:LEU:O	3:B:86:GLU:HG2	2.02	0.59
3:B:122:LEU:HD23	3:B:126:ARG:NH1	2.18	0.59
3:B:129:GLU:HB3	3:B:137:ARG:CD	2.33	0.59
3:A:164:ASN:O	3:A:167:LYS:HG2	2.03	0.58
3:A:278:PHE:HE1	3:A:328:ARG:HD3	1.67	0.58
3:B:201:THR:HG22	3:B:202:SER:H	1.68	0.58
3:B:208:PRO:HB3	3:B:232:GLU:HG2	1.84	0.58
3:A:320:PHE:CD2	3:A:327:TYR:HA	2.37	0.58
3:B:193:VAL:HG13	3:B:257:ILE:HG12	1.84	0.58
3:B:194:LEU:HD11	3:B:260:ILE:HG13	1.84	0.58
3:A:22:LEU:HD13	3:A:39:TYR:HE2	1.68	0.57
3:B:154:GLU:HA	3:B:157:GLN:HE21	1.69	0.57
2:D:7:DC:H2"	5:B:338:TTE:H5'2	1.85	0.57
3:A:194:LEU:HD11	3:A:260:ILE:HG12	1.87	0.57
3:A:18:MET:CE	3:A:82:LEU:HB2	2.35	0.57
3:B:271:TYR:HA	3:B:279:ASN:ND2	2.20	0.56
3:A:15:ILE:O	3:A:19:LEU:HG	2.06	0.55
3:B:18:MET:HE2	3:B:82:LEU:HB2	1.88	0.55
3:B:174:ILE:HB	3:B:196:THR:CG2	2.36	0.55
3:A:299:ARG:HG2	3:A:299:ARG:HH11	1.71	0.55
3:A:164:ASN:HA	3:A:167:LYS:HE2	1.89	0.55
3:A:261:PRO:HG2	3:A:264:GLN:NE2	2.22	0.55
3:A:330:PRO:HD3	3:A:333:ARG:NH2	2.23	0.54
3:B:182:ARG:HD3	3:B:273:THR:OG1	2.07	0.54
3:B:112:ARG:HH11	3:B:112:ARG:HG3	1.72	0.54
3:A:53:ILE:HG21	3:A:59:ALA:HB2	1.88	0.54
3:B:18:MET:CE	3:B:82:LEU:HB2	2.37	0.53
3:A:177:VAL:HG13	3:A:177:VAL:O	2.09	0.53
5:A:338:TTE:H6	5:A:338:TTE:C3'	2.37	0.53
3:B:158:MET:HE1	3:B:253:ARG:HG3	1.91	0.53
3:A:67:THR:O	3:A:71:GLU:HG3	2.09	0.53
3:A:194:LEU:HD11	3:A:260:ILE:HG13	1.89	0.53
3:A:275:SER:HB3	3:A:278:PHE:CB	2.39	0.53
3:B:49:TYR:CE1	3:B:62:LEU:HD11	2.44	0.53
2:P:6:DC:H2"	2:P:7:DC:H5'	1.91	0.52
3:A:28:ASN:HD22	3:A:98:ASN:ND2	2.07	0.52
3:B:211:LEU:HD23	3:B:231:GLY:O	2.10	0.52



	to do pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.91	0.52
3:B:132:LEU:HB2	3:B:137:ARG:HG2	1.92	0.52
3:B:193:VAL:CG1	3:B:257:ILE:HG12	2.40	0.51
3:A:143:PHE:O	3:A:147:GLU:HG2	2.10	0.51
3:A:315:SER:HB2	3:A:317:GLN:OE1	2.11	0.51
3:B:86:GLU:O	3:B:90:GLN:HG3	2.11	0.51
3:A:22:LEU:O	3:A:26:GLU:HG2	2.09	0.51
3:B:169:LEU:HD21	3:B:213:ARG:HB3	1.93	0.51
3:A:158:MET:O	3:A:162:VAL:HG23	2.11	0.51
3:A:266:TYR:CE2	3:A:315:SER:HA	2.45	0.51
3:A:291:PHE:HB3	3:A:298:ILE:HD11	1.92	0.51
3:A:49:TYR:CD1	3:A:62:LEU:HD11	2.46	0.51
3:B:85:LEU:O	3:B:89:ARG:HG3	2.11	0.51
3:B:152:ARG:HB2	3:B:186:GLU:O	2.11	0.51
3:B:18:MET:CE	3:B:76:PHE:HB2	2.41	0.50
3:A:299:ARG:HB3	3:A:310:PRO:HA	1.93	0.50
3:A:285:HIS:O	3:A:288:GLU:HB3	2.12	0.50
2:D:7:DC:H2'	5:B:338:TTE:H5'2	1.91	0.50
5:B:338:TTE:H3'	5:B:338:TTE:H6	1.92	0.50
3:B:129:GLU:O	3:B:137:ARG:HD3	2.12	0.50
3:A:163:LEU:HD12	3:A:175:ALA:HB3	1.93	0.50
3:B:164:ASN:O	3:B:168:LYS:HG3	2.12	0.50
3:B:277:ILE:HG22	3:B:281:ASN:HD21	1.76	0.50
2:D:5:DG:H2"	2:D:6:DC:O5'	2.11	0.49
3:A:300:PRO:HD3	3:A:311:LEU:HD23	1.94	0.49
3:B:201:THR:HG22	3:B:202:SER:N	2.26	0.49
3:A:81:LYS:HB3	3:A:81:LYS:NZ	2.26	0.49
3:B:158:MET:CE	3:B:253:ARG:HG3	2.42	0.49
3:A:134:HIS:CE1	3:A:138:ILE:HD11	2.47	0.49
3:A:150:ILE:O	3:A:187:SER:HA	2.11	0.49
3:B:135:HIS:CD2	3:B:228:LEU:HD22	2.48	0.48
3:B:166:VAL:HG13	3:B:173:TYR:HB3	1.94	0.48
3:A:68:LYS:O	3:A:72:LYS:HG3	2.13	0.48
3:B:125:LEU:HG	3:B:132:LEU:HD11	1.94	0.48
3:B:276:ASP:HB3	5:B:338:TTE:C5	2.43	0.48
3:B:177:VAL:HG21	3:B:191:MET:HE2	1.95	0.48
3:B:150:ILE:HG12	3:B:253:ARG:HD2	1.96	0.48
3:B:122:LEU:HD23	3:B:126:ARG:HH12	1.79	0.47
3:A:112:ARG:HG3	3:A:112:ARG:HH11	1.80	0.47
3:B:69:ILE:O	3:B:73:ILE:HG13	2.14	0.47
3:B:103:VAL:HG22	3:B:143:PHE:HD1	1.80	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:B:177:VAL:O	3:B:177:VAL:HG13	2.14	0.47
3:A:283:ARG:O	3:A:287:LEU:HD12	2.15	0.47
3:B:22:LEU:HG	3:B:85:LEU:HD13	1.96	0.47
3:B:311:LEU:HD13	3:B:312:PRO:HD2	1.96	0.47
3:B:206:LYS:O	3:B:208:PRO:HD3	2.15	0.47
3:A:22:LEU:HD13	3:A:39:TYR:CE2	2.50	0.46
3:B:279:ASN:O	3:B:283:ARG:HG3	2.15	0.46
3:B:297:THR:HB	3:B:310:PRO:HB3	1.97	0.46
3:B:174:ILE:HB	3:B:196:THR:HG22	1.97	0.46
3:B:323:ILE:HG13	3:B:325:TRP:HB2	1.98	0.46
3:B:152:ARG:HH11	3:B:152:ARG:HG3	1.79	0.46
3:B:300:PRO:HD3	3:B:311:LEU:CD2	2.39	0.46
3:A:154:GLU:O	3:A:158:MET:HG3	2.16	0.46
3:A:195:LEU:HD21	3:A:214:VAL:HG21	1.96	0.46
3:A:76:PHE:O	3:A:79:THR:O	2.34	0.46
3:A:178:CYS:HA	3:A:182:ARG:HB2	1.98	0.46
3:B:192:ASP:HB3	3:B:272:PHE:CZ	2.51	0.45
3:A:114:LEU:O	3:A:119:ILE:HB	2.16	0.45
3:B:107:GLY:O	3:B:108:PRO:C	2.55	0.45
3:B:209:LYS:HB2	6:B:1025:HOH:O	2.16	0.45
3:A:60:LYS:O	3:A:60:LYS:HG2	2.17	0.45
3:A:278:PHE:CE1	3:A:328:ARG:HD3	2.51	0.45
3:B:53:ILE:HG22	3:B:54:LYS:N	2.32	0.44
3:A:18:MET:HE1	3:A:82:LEU:HB2	1.98	0.44
3:A:49:TYR:CE1	3:A:62:LEU:HD11	2.52	0.44
3:A:112:ARG:HG3	3:A:112:ARG:NH1	2.33	0.44
3:B:18:MET:HE1	3:B:76:PHE:HB2	2.00	0.44
3:B:154:GLU:HG2	3:B:157:GLN:NE2	2.33	0.44
3:B:158:MET:O	3:B:162:VAL:HG23	2.17	0.44
3:A:299:ARG:HG2	3:A:299:ARG:NH1	2.32	0.44
3:B:204:SER:OG	3:B:207:GLN:OE1	2.36	0.44
3:B:103:VAL:HG22	3:B:143:PHE:CD1	2.53	0.44
3:B:239:CYS:SG	3:B:255:ILE:HB	2.58	0.43
3:B:240:GLN:HG2	3:B:241:LEU:N	2.34	0.43
3:A:18:MET:HE2	3:A:82:LEU:HB2	1.99	0.43
3:B:182:ARG:HH11	3:B:273:THR:HG21	1.82	0.43
3:B:298:ILE:O	3:B:311:LEU:HB2	2.18	0.43
3:B:294:ASN:HB2	3:B:299:ARG:HH12	1.83	0.43
3:A:276:ASP:N	3:A:276:ASP:OD1	2.51	0.43
3:B:49:TYR:HA	3:B:50:PRO:HD3	1.75	0.43
3:A:103:VAL:HG22	3:A:143:PHE:CD1	2.54	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:B:254:ARG:HB3	3:B:254:ARG:NH1	2.34	0.42
1:T:9:DT:H2"	1:T:10:DC:C6	2.54	0.42
3:A:170:ASP:HA	3:A:171:PRO:HD3	1.86	0.42
3:A:99:PHE:CD2	3:A:99:PHE:C	2.93	0.42
3:A:205:SER:O	3:A:206:LYS:HB2	2.19	0.42
3:B:221:VAL:HG12	3:B:221:VAL:O	2.19	0.42
3:A:123:GLU:OE2	3:A:127:LYS:HE3	2.20	0.42
3:A:221:VAL:HG12	3:A:221:VAL:O	2.19	0.42
3:A:83:ARG:HB2	6:A:1000:HOH:O	2.19	0.42
1:T:8:DG:H4'	3:A:229:SER:HB3	2.01	0.42
3:B:112:ARG:HG3	3:B:112:ARG:NH1	2.34	0.42
3:B:178:CYS:HA	3:B:182:ARG:HB2	2.00	0.42
3:A:152:ARG:HH11	3:A:152:ARG:CG	2.29	0.42
3:B:34:HIS:HD2	6:B:1023:HOH:O	2.02	0.42
3:A:158:MET:CE	3:A:253:ARG:HG3	2.49	0.42
3:B:210:LEU:HD23	3:B:210:LEU:HA	1.93	0.42
3:A:146:PHE:CE2	3:A:254:ARG:HG2	2.55	0.41
3:B:24:ASN:HB3	6:B:1022:HOH:O	2.20	0.41
3:B:123:GLU:O	3:B:127:LYS:HG3	2.20	0.41
3:B:166:VAL:CG1	3:B:173:TYR:HB3	2.49	0.41
1:T:5:DG:OP1	3:A:292:THR:HG23	2.20	0.41
3:B:81:LYS:HB3	3:B:81:LYS:HZ3	1.82	0.41
3:B:205:SER:O	3:B:206:LYS:HB2	2.19	0.41
3:A:27:LYS:HB3	3:A:27:LYS:HE2	1.75	0.41
2:P:7:DC:H5"	3:A:254:ARG:NH2	2.36	0.41
3:A:85:LEU:HA	3:A:85:LEU:HD12	1.81	0.41
3:B:73:ILE:O	3:B:77:LEU:HD22	2.20	0.41
3:A:89:ARG:HA	6:A:1017:HOH:O	2.19	0.41
3:A:177:VAL:HA	3:A:192:ASP:O	2.21	0.41
3:A:302:GLY:HA3	6:A:1020:HOH:O	2.21	0.41
3:A:45:VAL:HG11	3:A:63:PRO:O	2.20	0.41
3:A:115:VAL:HA	3:A:119:ILE:O	2.21	0.40
3:A:266:TYR:CD2	3:A:315:SER:HA	2.57	0.40
3:A:276:ASP:HB3	5:A:338:TTE:C5	2.51	0.40
3:B:92:ASP:HB3	6:B:1005:HOH:O	2.21	0.40
3:B:211:LEU:HB2	3:B:259:LEU:HD22	2.04	0.40
3:A:180:SER:HB3	5:A:338:TTE:HCC2	2.03	0.40
3:B:197:HIS:HA	3:B:198:PRO:HD3	1.98	0.40

There are no symmetry-related clashes.



# 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	А	323/335~(96%)	293 (91%)	24 (7%)	6(2%)	8 15
3	В	323/335~(96%)	288 (89%)	30~(9%)	5(2%)	10 21
All	All	646/670~(96%)	581 (90%)	54 (8%)	11 (2%)	9 18

All (11) Ramachandran outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
3	А	331	LYS
3	В	143	PHE
3	В	274	GLY
3	В	331	LYS
3	А	274	GLY
3	В	78	ALA
3	А	178	CYS
3	А	304	THR
3	А	330	PRO
3	В	330	PRO
3	А	303	VAL

#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
3	А	283/296~(96%)	265~(94%)	18 (6%)	17	35
3	В	283/296~(96%)	264 (93%)	19 (7%)	16	33



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Mol	Chain	Analysed	lysed Rotameric Outliers		Perce	entiles
All	All	566/592~(96%)	529~(94%)	37~(6%)	17	34

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	А	51	HIS
3	А	62	LEU
3	А	65	VAL
3	А	67	THR
3	А	77	LEU
3	А	81	LYS
3	А	92	ASP
3	А	93	THR
3	А	95	SER
3	А	123	GLU
3	А	152	ARG
3	А	176	THR
3	А	207	GLN
3	А	258	ARG
3	А	272	PHE
3	А	298	ILE
3	А	324	GLN
3	А	325	TRP
3	В	62	LEU
3	В	65	VAL
3	В	67	THR
3	В	77	LEU
3	В	81	LYS
3	В	92	ASP
3	В	93	THR
3	В	108	PRO
3	В	122	LEU
3	В	125	LEU
3	В	152	ARG
3	В	173	TYR
3	В	193	VAL
3	В	269	VAL
3	В	272	PHE
3	В	298	ILE
3	В	311	LEU
3	В	324	GLN
3	В	325	TRP



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
3	А	98	ASN
3	А	134	HIS
3	А	159	GLN
3	А	264	GLN
3	В	31	GLN
3	В	34	HIS
3	В	51	HIS
3	В	98	ASN
3	В	135	HIS
3	В	157	GLN
3	В	264	GLN
3	В	281	ASN
3	В	324	GLN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are 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).



Mal	Turne	Chain	Dec	Tinle	B	ond leng	gths	E	Bond ang	gles
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
5	TTE	В	338	4	27,30,30	2.94	12 (44%)	40,47,47	2.83	14 (35%)
5	TTE	А	338	4	27,30,30	2.90	11 (40%)	40,47,47	2.76	13 (32%)

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	TTE	В	338	4	-	6/19/34/34	0/2/2/2
5	TTE	А	338	4	-	6/19/34/34	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
5	А	338	TTE	O4'-C4'	8.92	1.64	1.45
5	В	338	TTE	O4'-C4'	8.83	1.64	1.45
5	А	338	TTE	PG-01G	6.18	1.63	1.50
5	В	338	TTE	PG-O1G	5.84	1.62	1.50
5	А	338	TTE	PB-O1B	4.64	1.62	1.51
5	В	338	TTE	PB-O1B	4.41	1.62	1.51
5	В	338	TTE	PB-O3A	4.34	1.63	1.58
5	А	338	TTE	C4-C5	3.96	1.51	1.44
5	В	338	TTE	C4-C5	3.55	1.50	1.44
5	А	338	TTE	C1'-N1	-3.54	1.39	1.48
5	А	338	TTE	PG-O3G	3.31	1.62	1.54
5	В	338	TTE	C1'-N1	-3.23	1.39	1.48
5	А	338	TTE	C2-N3	-3.13	1.32	1.38
5	В	338	TTE	PG-O3G	3.11	1.62	1.54
5	В	338	TTE	O4'-C1'	-2.77	1.36	1.42
5	В	338	TTE	C2-N3	-2.73	1.33	1.38
5	А	338	TTE	O4'-C1'	-2.70	1.36	1.42
5	В	338	TTE	PA-O1A	2.64	1.60	1.50
5	В	338	TTE	PG-O2G	2.61	1.60	1.54
5	А	338	TTE	PA-O1A	2.50	1.59	1.50
5	А	338	TTE	PG-O2G	2.39	1.60	1.54
5	В	338	TTE	C2-N1	-2.29	1.34	1.38
5	А	338	TTE	C2-N1	-2.18	1.35	1.38

All (27) bond angle outliers are listed below:



1H	UO	
111	00	

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	В	338	TTE	O3G-PG-O2G	10.17	137.77	108.08
5	А	338	TTE	O3G-PG-O2G	9.89	136.96	108.08
5	А	338	TTE	O2B-PB-CC	7.40	136.85	106.58
5	В	338	TTE	O2B-PB-CC	7.31	136.47	106.58
5	В	338	TTE	N3-C2-N1	5.31	121.94	114.89
5	А	338	TTE	N3-C2-N1	5.18	121.76	114.89
5	А	338	TTE	O1G-PG-CC	-4.46	101.63	111.24
5	В	338	TTE	O3G-PG-O1G	-4.36	100.87	112.39
5	В	338	TTE	O1G-PG-CC	-4.28	102.02	111.24
5	А	338	TTE	O3G-PG-O1G	-3.88	102.14	112.39
5	В	338	TTE	C2'-C3'-C4'	3.52	110.09	102.76
5	А	338	TTE	O4'-C4'-C3'	-3.51	97.49	105.67
5	А	338	TTE	O4'-C1'-N1	3.39	113.92	107.86
5	В	338	TTE	O4'-C4'-C3'	-3.39	97.77	105.67
5	В	338	TTE	O4'-C1'-N1	3.23	113.63	107.86
5	В	338	TTE	C6-N1-C2	-2.98	118.28	121.30
5	А	338	TTE	C2'-C3'-C4'	2.95	108.91	102.76
5	В	338	TTE	O2G-PG-O1G	-2.95	104.59	112.39
5	А	338	TTE	O2G-PG-O1G	-2.86	104.82	112.39
5	А	338	TTE	C6-N1-C2	-2.63	118.63	121.30
5	В	338	TTE	O1B-PB-CC	-2.52	102.41	109.07
5	В	338	TTE	C4-N3-C2	-2.46	124.17	127.35
5	В	338	TTE	O2-C2-N1	-2.42	119.57	122.79
5	А	338	TTE	C4-N3-C2	-2.41	124.24	127.35
5	А	338	TTE	O2-C2-N1	-2.14	119.94	122.79
5	А	338	TTE	O1B-PB-CC	-2.11	103.50	109.07
5	В	338	TTE	O3G-PG-CC	-2.08	101.36	106.40

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	А	338	TTE	C5'-O5'-PA-O1A
5	А	338	TTE	C5'-O5'-PA-O2A
5	А	338	TTE	PB-CC-PG-O3G
5	В	338	TTE	C5'-O5'-PA-O1A
5	В	338	TTE	PB-CC-PG-O3G
5	А	338	TTE	C3'-C4'-C5'-O5'
5	А	338	TTE	O4'-C4'-C5'-O5'
5	В	338	TTE	C3'-C4'-C5'-O5'
5	В	338	TTE	O4'-C4'-C5'-O5'
5	В	338	TTE	C5'-O5'-PA-O2A
5	А	338	TTE	C5'-O5'-PA-O3A



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Mol	Chain	Res	Type	Atoms
5	В	338	TTE	C5'-O5'-PA-O3A

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	В	338	TTE	6	0
5	А	338	TTE	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







# 5.7 Other polymers (i)

There are no such residues in this entry.

# 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

# 6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

#### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

