

Full wwPDB NMR Structure Validation Report (i)

Feb 19, 2022 – 03:09 PM EST

PDB ID	:	1RCS
Title	:	NMR STUDY OF TRP REPRESSOR-OPERATOR DNA COMPLEX
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Deposited on	:	1995-05-12

This is a Full wwPDB NMR 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/NMRValidationReportHelp with specific help available everywhere you see the (i) symbol.

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)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $SOLUTION\ NMR$

The overall completeness of chemical shifts assignment was not calculated.

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	NMR archive (#Entries)		
Clashscore	158937	12864		
Ramachandran outliers	154571	11451		
Sidechain outliers	154315	11428		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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%

Mol	Chain	Length	Quality of chain				
1	Е	20	70%		30%)	
1	F	20	75%		20%)	5%
2	А	105	50%	29%	5%	15%	
2	В	105	49%	31%	•	15%	•



2 Ensemble composition and analysis (i)

This entry contains 15 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues								
Well-defined core	Vell-defined core Residue range (total)			Medoid model				
1	A:18-A:105, (176)	B:518-B:605	0.40	1				

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 1 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 6, 7, 8, 9, 10, 11, 12, 13, 14
Single-model clusters	5; 15



3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4704 atoms, of which 2188 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms				Trace		
1	F	20	Total	С	Η	Ν	0	Р	0
	20	635	196	228	74	118	19	0	
1	1 E	F 90	Total	С	Η	Ν	0	Р	0
Г	20	635	196	228	74	118	19		

• Molecule 2 is a protein called TRP REPRESSOR.

Mol	Chain	Residues	Atoms				Trace		
0	Δ	104	Total	С	Η	Ν	0	S	0
	Z A	104	1690	524	854	152	157	3	0
0	В	104	Total	С	Η	Ν	0	S	0
2 B	104	1690	524	854	152	157	3		

• Molecule 3 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				
2	Δ	1	Total	С	Η	Ν	0
3	3 A	1	27	11	12	2	2
9	D	D 1	Total	С	Η	Ν	0
0 D	1	27	11	12	2	2	



4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

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

Chain E:	70%		30%	
C1 C2 C2 C2 C2 C2 C3 C3 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	619 619 620			
• Molecule 1: DNA (5 *TP*AP*CP*G)-3')	'-D(*CP*GP*TP*A	AP*CP*TP*AP*G	P*TP*TP*AP*AP	*CP*TP*AP*GP
Chain F:	75%		20% 5%	
C1 C2 C2 C2 C5 C5 C5 C3 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	619 619 620			
• Molecule 2: TRP RE	EPRESSOR			
Chain A:	50%	29%	5% 15% •	
04 55 55 77 75 75 75 86 410 412 413 614 614 614 700	R21 F22 V23 V23 V23 V23 V23 V23 V23 R26 R33 R33 R33 R33 R33 R33 R33 R33 R33 R3	1.38 1.39 1.40 1.44 1.44 1.44 1.44 1.44 1.44 1.44	15 (V58 863 863 863 869 870 872 872 878 179 81	2 2 1
K90 L96 R97 R97 Q98 N99 L100 L100 K106 S107 ASP				
• Molecule 2: TRP RE	EPRESSOR			
Chain B:	49%	31%	• 15% •	
9504 8505 7507 7507 7506 7506 7506 7506 7509 8513 8513 8513 8513 8513 8513 8513 8513	1521 1522 1522 1528 1528 1534 1534 1534 1534	L525 L541 L542 L543 L544 L544 R544 R554 R555 R555 R555 R555	1557 V558 R563 R563 R563 R563 R563 L571 L571 K572 A580 A580 A580	2
K590 K597 K597 K599 K599 K599 E601 E603 E604 E604 E604 E604 E604 E604 E604 K506 S607 ASP				



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

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

Chain E: 65% 35% • Molecule 1: DNA (5'-D(*CP*GP*TP*AP*CP*TP*AP*GP*TP*TP*AP*AP*CP*TP*AP*GP *TP*AP*CP*G)-3') Chain F: 80% 15% 5% • Molecule 2: TRP REPRESSOR Chain A: 51% 26% 7% 15% • Molecule 2: TRP REPRESSOR Chain B: 50% 24% 10% 15%

4.2.2 Score per residue for model 2

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

Chain E:	70%	25%	5%



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

Chain F:	80%		15	% 5%	
C1 C2 C2 C5 A7 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5	C13 114 114 115 117 117 117 019 020				
• Molecule 2: T	RP REPRESSOR				
Chain A:	50%	23%	10% •	15% •	I
04 85 85 85 88 88 810 811 8112 8113 8115 8115	H16 117 119 119 119 119 119 126 126 126 126 126 126 126 126 126 126	L34 H35 L38 L38 L38 L38 L38 L41 L41 L41 L43 L43 L43 L43	R48 R54 R56 R56 R56 R56 T57 V58 V58	R63 R69 E70 L71 K72	179 A80 181 182
K90 K97 R97 R97 R97 Q98 U99 L100 L100 L104 L105 K106	ASP ASP				
• Molecule 2: T	RP REPRESSOR				
Chain B:	47%	28%	9% •	15%	
q504 S505 P506 P506 A509 A510 A511 A512 A512 E513 E513 B515 R515 R515	H5 16 05 17 05 17 15 20 15 20 15 20 15 22 15 25 15 25 15 25 15 25 15 23 15 33	H535 L538 L538 L541 M542 L543 L543 L543 E547 R548	L551 (552 (552 1553 R554 R556 1557 V558	R563 G564 E565 R569 R569 E570	L571 K572 I579 A580
T581 1582 1583 R584 R584 R587 Q588 Q598 Q598 C509 L600	E602 K606 ASP				

4.2.3 Score per residue for model 3

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

Chain E:	65%	35%
C1 C2 C5 A4 A7 C5 A12 A12 A12 A12 A12 A12 A12 A13 A15 A15 A15 A15 C19 C19 C19 C20 C20		
• Molecule 1: DNA (5'-D(*C *TP*AP*CP*G)-3')	CP*GP*TP*AP*CP*TP*AP*GI	P*TP*TP*AP*AP*CP*TP*AP*GP
Chain F:	75%	20% 5%
C1 C2 C5 C5 C5 C5 C5 C5 C5 C5 C5 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2		
• Molecule 2: TRP REPRES	SSOR	



Chain A:	51%	22%	10%	15% •	
94 85 85 77 75 88 81 81 81 81 81 81 81 81 81 81 81 81	F22 V23 V23 K27 K27 N26 N26 N28 N28 N28 N28 N28 N28 N28 N28 N28 N28	R56 I57 V58 R63	R69 E70 L71 K72	L75 C78 C78 A80 A80 182 182 182 K90	196
R97 098 1099 1004 1104 1105 8107 8107 8107					
• Molecule 2: TRP REF	PRESSOR				
Chain B:	50%	25%	7% •	15% •	
Q504 7505 7505 7507 7507 7507 7507 8508 8513 8513 8514 8513 8514 8513 8514 8513 8514 8513 8514 8515 8518 8518 8518 8518 8518 8518	F522 L525 L526 L526 A529 Y530 D533 L534 H536 L543 L541 M542 L543	1644 R548 L551 R554 R554	1557 V558 L561 L562 R563	R569 E570 L571 K572 L575 L575 C578	1579 A580
1581 1682 8597 0598 0598 0599 0599 0599 0599 0599 0599					

4.2.4 Score per residue for model 4

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

Cha	in	E):												65%	35%
1 8 8 1 8 8	A4	T6 T6	A7	29 19	T10	A11 A12	613	T14	A15	G16	T17	A18	C19	G20		

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

Chain F:	80%		159	% 5%	
01 02 02 05 05 05 05 05 01 01 013 015 013 015 015 015 015 015 015 015 015 015	A18 C19 G20				
• Molecule 2: TRP RE	PRESSOR				
Chain A:	49%	27%	8% •	15% •	
94 55 77 77 76 85 810 811 8112 813 813 813 814 815 813 815 813 815 813 815 813 817 817 817 817 817 817 817 817 817 817	R21 F22 V23 V23 L26 L26 L26 L26 L26 L26 L33 L36 L36 L36 L36 L36 L36 L36	L39 N40 L41 L43 L43 T44 P45 R46 R46 R46 R46 R46	R54 157 V58	nos M66 R69 K72	G78 179 A80
181 182 182 182 182 196 196 199 199 199 199 199 199 199 199					
• Molecule 2: TRP RE	PRESSOR				
Chain B:	49%	30%	6%	15% •	



1581 4504 1582 7505 7583 7505 7583 7506 7583 7506 7593 7506 7503 7506 7504 7506 7503 7506 7504 7506 7505 7514 7506 7514 7507 8507 7508 7514 7509 7514 7509 7514 7509 7514 7509 7514 7509 753 7509 753 7509 753 7509 753 7509 753 7509 753 7538 753 7539 753 7538 753 7539 753 7538 753 7539 753 7539 753 7539 753 7539 <td

4.2.5 Score per residue for model 5

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

Chain E:	70%	_	20%	10%			
C1 G2 G2 G2 G2 G2 G1 G1 G1 G1 G1 G1 G1 G1 G1 G1 G1 G1 G1	111/ 118 619 620						
• Molecule 1: DNA (5 *TP*AP*CP*G)-3')	o'-D(*CP*GP*TP*AP*C	CP*TP*AP*(GP*TP*′	ГР*АР	*AP*C	P*TP*AI	°*G
Chain F:	75%		25%)			
C1 C1 C2 C2 C2 C5 C5 C5 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	111 718 718 720						
• Molecule 2: TRP RI	EPRESSOR						
Chain A:	53%	23%	8%	15% •			
94 55 77 75 75 75 75 838 711 712 7112 7113 7115 7115 7115 7115 7115 7115 7115	V22 V22 D24 D24 L25 L25 V20 V23 V23 V23 V23 V23 V23 V23 V23 V23 V24 V24 V24 V24 V24 V24 V24 V24 V24 V24	M42 R48 L51 R54 V55 R56 R56	V58 R63 M66	R69 K72 I79	A80 181 182 K90		
R97 098 099 0103 1104 1105 8107 ASP							
• Molecule 2: TRP RI	EPRESSOR						
Chain B:	48%	27%	9% •	15%			
9504 8505 7505 7506 7506 7506 7506 7506 7506 7	L520 R521 F522 V523 V523 L526 L526 L526 L526 L534 H533 L538 L538 L538 L538	M542 L543 T544 E547 E547 R554 R554 R555 R555 R555	V558 R563 G564 R569	E570 L571 K572 G578	1579 4580 1581 1582		
K590 R597 R597 R597 R597 V503 L604 L604 L604 L605 K605 S607 ASP							

4.2.6 Score per residue for model 6

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



Chain E:	70%		25%	5%	
C1 C1 C2 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5	C13 715 716 716 717 713 713 720				
• Molecule 1: Dl *TP*AP*CP*G)	NA (5'-D(*CP*GP*TP* -3')	AP*CP*TP*AP'	*GP*TP*T	P*AP*AP*C	P*TP*AP*(
Chain F:	70%		30%		
C1 C1 C2 C2 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5	T13 114 115 116 117 117 117 117 019 020				
• Molecule 2: Th	RP REPRESSOR				
Chain A:	50%	26%	8% • 1	•	
94 55 77 77 88 89 810 811 811 8113 914 914 8115	0116 0116 0118 0118 0118 0118 0118 0118	L38 L39 L39 L41 M42 L43 L43 F44 F48 R48 R48 R48 R48 R48	R63 R69 E70 K72 K72	L75 G78 179 A80 T81 182 T83 R84	
R97 98 499 100 100 104 104 104 104 106 8107 8107 8107					
• Molecule 2: TI	RP REPRESSOR				
Chain B:	52%	24%	7% • 1	5% •	
9504 8505 8505 7506 7508 8508 8508 8508 8510 8511 8512 8513 8515 8515	8616 8616 8618 8519 8520 8520 8521 8522 8522 8526 8526 8529 8529 8529 8533 8533 8533 8533 8533 8533 8533 853	L538 L538 M642 L543 L543 L543 L544 L551 L551 R554 V555	1557 V558 N558 E570 L571 K572	1579 4580 1581 1582 1596 1596 R597 0598 W599	

L604 L605 K606 S607 ASP

4.2.7Score per residue for model 7

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

Chain E:	65%	35%
C1 62 74 74 75 75 75 75 71 71 71 71 71 71 71 71 71 71 71 71 71		

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

DB

Chain F:	75%	20%	5%
01 13 13 13 13 13 13 14 14 14 14 14 14 14 14 14 14 14 14 14			

• Molecule 2: TRP REPRESSOR



4.2.8 Score per residue for model 8

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

Chain E:	70%	30%
C1 C1 C2 C5 C5 C5 C5 C5 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1		

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

Chain F:	80%		15	% 5%
C1 C2 C2 C5 C5 C5 C5 C5 C1 C12 C13 C13 C13 C13 C13 C13 C13 C13 C13 C13	A18 C19 G20			
• Molecule 2: TRP RE	PRESSOR			
Chain A:	49%	30%	5%•	15% •
94 55 77 77 85 85 85 81 81 81 813 813 813 813 813 813 813 81	R21 F22 V23 L26 A29 Y30 D33 L34	H35 L38 L38 L39 L43 M42 L41 M40 L41 M42 L43 M42 R44 T44 T44 T55 T55 T55	R63 R69 K72	L75 G78 G78 179 179 181 181 182 182 K90
196 897 999 1100 1100 1100 1100 1100 1100 110				
• Molecule 2: TRP RE	PRESSOR			
Chain B:	48%	27%	9% •	15% •
		WORLDWIDE PROTEIN DATA BANK		

1596 4504 1596 4505 1596 7504 1500 7504 1600 7504 1600 7504 1600 7504 1600 7504 1600 7504 1600 7504 1600 7504 1600 7504 1600 750 1601 851 1602 851 1603 851 1614 852 1624 852 1625 852 1633 1634 1634 1634 1634 1634 1635 1634 1634 1634 1635 1634 1635 1634 1635 1644 1636 1656 1644 1656 1657 1658 1656 1657 1657 1658 1658

4.2.9 Score per residue for model 9

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

Chain E:	70%	25%	5%
C1 C2 C2 C2 C5 C5 A1 C5 C5 C5 C5 C5 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	019 020		
• Molecule 1: DNA (5'-1 *TP*AP*CP*G)-3')	D(*CP*GP*TP*AP*CP	*TP*AP*GP*TP*TP	*AP*AP*CP*TP*AP*GP
Chain F:	80%	15%	5%
C1 C1 C2 C5 C5 A7 A12 C5 A12 C13 A11 C13 A15 A15 A15 A15 A15 A15 A15 A15 A15 A15	C19 G20		
• Molecule 2: TRP REF	PRESSOR		
Chain A:	50%	26% 8% 15%	6 ·
94 55 55 77 75 75 74 40 411 813 813 814 815 914 815 813 815 813 815 817 812 813	F22 V23 V23 V23 V30 V30 V30 L26 L38 L38 L38 L38 L38 L38 L38 L38 L38 L38	L43 144 144 157 157 157 157 157 157 157 157 157 157	L75 179 A80 182 182 182 182
R97 098 099 1100 E101 E102 1104 E103 1104 K106 S107 ASP			
• Molecule 2: TRP REF	PRESSOR		
Chain B:	50%	26% 9% 15	% .
4504 8505 8505 7507 7507 8506 8510 8511 8515 8513 8515 8513 8515 8513 8515 8515	1522 1526 1526 1526 1526 1533 1533 1538 1538 1538 1543 1543 1543 1543	1551 1551 15554 15554 15555 15555 15556 15556 15553 15570 15571 15571	1579 1581 1581 1581 1582 1582 1583 R584
K550 K550 Q559 Q559 Q559 K555 K663 L664 L664 L665 K605 K605 X605 X605 X605			

4.2.10 Score per residue for model 10

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



Chain E:	70%	30%	
C1 C2 C2 C2 C2 C2 C2 C2 C2 C2 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	117 117 A18 C19 C20		
• Molecule 1: DNA	(5'-D(*CP*GP*TP*AP*C	CP*TP*AP*GP*TP*TP*AP	*AP*CP*

TP*AP*GP *TP*AP*CP*G)-3')

Chain F:	60%		35%	5%
C1 73 62 62 62 73 73 74 71 71 71 71 71 71 715 715 715 715 715 7	C19 C20			
• Molecule 2: TRP REP	RESSOR			
Chain A:	51%	22%	10% 15%	·
94 85 85 85 86 86 81 81 81 81 81 81 81 81 81 81 81 81 81	F22 V23 V23 V23 V23 V23 V23 V23 V23 V23 V	T44 R54 V55 R56 V58 V58	R63 R69 E70 L71 K72 K72	179 480 181 182 183 183 884 884
L96 R97 899 U99 L100 L100 K106 K106 K106 K106 K106 K106 K106 K				
• Molecule 2: TRP REP	PRESSOR			
Chain B:	52%	23%	8% • 15%	•
q504 \$505 \$506 \$506 \$506 \$506 \$506 \$506 \$506 \$506 \$506 \$506 \$506 \$508 \$508 \$509 \$511 \$512 \$513 \$513 \$513 \$513 \$513 \$513 \$514 \$515 \$513 \$514 \$515 \$515 \$515 \$515 \$515 \$516 \$517 \$518 \$517 \$518 \$519 \$510 \$510 \$510 \$510 \$510 \$510 \$510 \$510 \$510 \$510 \$510	F522 L526 L526 A529 A529 A529 L533 L533 L533 L541 M542 L543 L544	L551 1557 V558 E559 E560	R563 R569 E570 L571 K572 G576 A577	G578 1579 A580 1581 1582 L596 R597

Q598 W599 L600 V603 K606 S607 ASP

4.2.11 Score per residue for model 11

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

Chain E:	70%	25%	5%
C1 622 73 73 74 74 75 75 71 71 71 71 71 71 71 71 71 71 71 71 71			

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

Chain F:	80%	15%	5%
C1 73 73 73 73 75 75 71 71 711 711 715 715 715 715 715			

• Molecule 2: TRP REPRESSOR



4.2.12 Score per residue for model 12

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

Chain E:	70%	25%	5%
C1 C1 C2 C3 C5 C5 C5 C5 C5 C5 C10 C13 C13 C13 C13 C13 C13 C13 C13 C13 C13			

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

Chain F:	75%		25%	
C1 C1 C2 C2 C2 C2 C3 C4 C4 C4 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	117 A18 C19 G20			
• Molecule 2: TRP R	EPRESSOR			
Chain A:	52%	23%	8% • 1	5% •
94 55 77 85 88 88 88 811 410 411 4115 4115 4115 4115 4115 4115	R21 F22 V23 V23 V23 V23 V23 V23 V23 V23 V23 V	N40 L41 N42 L43 L43 L43 T44 R48 R48 R48 R48 R54 R54 R54	R57 157 157 157 R63 R69 R69	172 179 181 182 182 K90
R97 098 1199 1100 1100 1100 1100 8107 8107 8107				
• Molecule 2: TRP R	EPRESSOR			
Chain B:	50%	29%	5%•	15% •
		WORLDWIDE PROTEIN DATA BANK		

L589 C604 K590 K506 K599 K506 W599 M511 W599 A510 W599 A510 W599 A511 K606 A512 K606 H516 K614 K519 K614 K519 K614 K530 K614 K644 K64 K644

4.2.13 Score per residue for model 13

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

Chain E:	70%	30%	
C1 C2 C2 C3 C3 C4 A7 A7 C5 C5 C5 C5 C5 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	019 020		
• Molecule 1: DNA (5'-I *TP*AP*CP*G)-3')	D(*CP*GP*TP*AP*CP*	TP*AP*GP*TP*TP	*AP*AP*CP*TP*AP*GP
Chain F:	60%	35%	5%
C1 C2 C2 C5 C5 A7 A7 A11 C13 C13 C13 C13 C13 C13 C13 C13 C13 C	619 620		
• Molecule 2: TRP REP	RESSOR		
Chain A:	52%	26% 5% · 15%	
94 55 77 77 76 77 88 49 10 813 813 814 815 814 815 817 817 817 817 817 817 817 817 817 817	r22 v23 L26 L26 A29 A29 B33 L34 H35 L34 L39 L34 L39 L41 M40 L41 M40 L43 L43	R48 R54 V55 V58 V58 V58 V58 V58 C64 C1 L71 K72	678 179 180 182 182 182
q98 1400 1100 1100 1100 1100 8107 ASP			
• Molecule 2: TRP REP	RESSOR		
Chain B:	52%	27% •• 15%	
q504 q505 p505 p505 p505 p505 p505 p505 p505 p505 p505 p512 p513 p515 p520 p521	F522 V523 V523 A529 A529 A529 A533 L538 L538 L538 L538 L543 L543 L543 T544 T544	8548 1551 1551 1557 1558 8563 8563 8563 8563 8570 1571 1571 1575	1579 A580 1581 1582 1596 R597
4598 1859 1859 1850 1860 1850 1850 1850 1850			

4.2.14 Score per residue for model 14

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



Chain E:	65%	30%	5%

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

Chain F:	70%		20%	10%	•
C1 62 62 62 62 62 71 71 71 71 71 71 71 71 71 71 71 71 71					
• Molecule 2: TRP REPRE	ESSOR				
Chain A: 5	5%	22%	7%	15%	•
94 85 85 85 85 85 86 81 81 81 81 81 81 81 11 81 81 82 11 82 11 82 122 823	L26 L26 A29 K30 B33 H35 L34 H35 L34 L34 L41 L41 L41 L41 L41 C41	R54 V65 I57 V58 V58	R69 E70 K72 K72	179 A80 181 182	K90 R97 W99
V103 K106 S107 ASP					
• Molecule 2: TRP REPRE	ESSOR				
Chain B: 54	1%	25%	5%	15%	•
9604 8505 8505 8506 8506 8508 8508 8611 8611 8611 8613 8614 8614 8614 8614 8614 8614 8614 8614	L526 A529 Y530 D533 L534 H535 L538 L538 L538 L538 L538 L538 L538 L	1557 V558 R569 E570 L571 K572	L575 G578 I579	T581 T581 T582 T583 R584	K590 R597 Q598 W599



4.2.15 Score per residue for model 15

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

Chain E:	65%	30%	5%
C1 G2 G2 A4 A4 A4 A1 C13 C13 C13 C13 C13 C13 C13 C13 C13 C1	A18 G20		

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

Chain F:	75%	20%	5%
C1 73 73 74 75 75 75 76 710 7110 7110 713 713 713 713 713 713 713 713 713 713			



• Molecule 2: TRP REPRESSOR



• Molecule 2: TRP REPRESSOR





5 Refinement protocol and experimental data overview (i)

Of the ? calculated structures, 15 were deposited, based on the following criterion: ?.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	refinement	

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

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 (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol Chain		Bond lengths		Bond angles		
	Ullaili	RMSZ	#Z > 5	RMSZ	#Z > 5	
1	Е	$4.33 {\pm} 0.03$	$115{\pm}2/456~(~25.3{\pm}~0.5\%)$	$4.90 {\pm} 0.03$	$109{\pm}3/702$ ($15.6{\pm}$ $0.5\%)$	
1	F	$4.33 {\pm} 0.03$	$115{\pm}1/456$ ($25.2{\pm}$ 0.3%)	$4.89 {\pm} 0.03$	$107{\pm}3/702~(~15.2{\pm}~0.5\%)$	
2	А	$1.80{\pm}0.01$	$3{\pm}1/720~(~0.4{\pm}~0.1\%)$	1.07 ± 0.02	$5{\pm}1/975$ ($0.5{\pm}$ $0.1\%)$	
2	В	$1.80{\pm}0.02$	$2{\pm}1/720~(~0.3{\pm}~0.1\%)$	1.08 ± 0.02	$5{\pm}2/975~(~0.5{\pm}~0.2\%)$	
All	All	3.04	3537/35280~(~10.0%)	3.27	3388/50310 ($6.7%$)	

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	Planarity
1	Е	1.3 ± 0.5	$1.9{\pm}0.6$
1	F	1.1 ± 0.2	2.3 ± 0.6
2	А	$0.0{\pm}0.0$	2.2 ± 1.3
2	В	$0.0{\pm}0.0$	$1.9{\pm}0.9$
All	All	36	126

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mal	Chain	Dec	Turne	Atoma	7	Z Observed(Å)	Ideal(Å)	Mo	dels
	Unain	nes	s rybe	Atoms		Observed(A)	Ideal(A)	Worst	Total
1	F	7	DA	C4'-C3'	-11.91	1.40	1.52	12	15
1	F	7	DA	C3'-C2'	-11.36	1.38	1.52	14	15
1	F	13	DC	C3'-O3'	11.26	1.58	1.44	6	15
1	Е	13	DC	C3'-O3'	11.06	1.58	1.44	5	15
1	Е	9	DT	C3'-O3'	11.05	1.58	1.44	10	15
1	Е	17	DT	C3'-O3'	11.01	1.58	1.44	9	15
1	F	5	DC	C3'-O3'	10.99	1.58	1.44	15	15
1	Е	8	DG	C3'-O3'	10.98	1.58	1.44	11	15
1	Е	5	DC	C3'-O3'	10.96	1.58	1.44	13	15
1	E	7	DA	C3'-C2'	-10.75	1.39	1.52	12	15



1	R	CS	
-	10	∇D	

		D			7		T1 1(8)	Mod	lels
Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)	Worst	Total
1	F	5	DC	O4'-C1'	10.72	1.55	1.42	7	15
1	F	2	DG	C3'-O3'	10.70	1.57	1.44	2	15
1	F	9	DT	C3'-O3'	10.68	1.57	1.44	6	15
1	Е	5	DC	O4'-C1'	10.67	1.55	1.42	5	15
1	F	7	DA	C3'-O3'	10.55	1.57	1.44	10	15
1	F	14	DT	O4'-C1'	10.55	1.54	1.42	3	15
1	Е	11	DA	C3'-O3'	10.47	1.57	1.44	9	15
1	Е	9	DT	O4'-C1'	10.47	1.54	1.42	12	15
1	Е	10	DT	C3'-O3'	10.44	1.57	1.44	2	15
1	F	1	DC	O4'-C1'	10.44	1.54	1.42	2	15
1	Е	14	DT	O4'-C1'	10.41	1.54	1.42	9	15
1	Е	2	DG	O4'-C1'	10.40	1.54	1.42	15	15
1	F	10	DT	C3'-O3'	10.34	1.57	1.44	1	15
1	F	9	DT	O4'-C1'	10.29	1.54	1.42	3	15
1	F	12	DA	O4'-C1'	10.28	1.54	1.42	2	15
1	Е	3	DT	O4'-C1'	10.26	1.54	1.42	5	15
1	F	3	DT	O4'-C1'	10.26	1.54	1.42	9	15
1	Е	17	DT	O4'-C1'	10.25	1.54	1.42	11	15
1	F	10	DT	O4'-C1'	10.23	1.54	1.42	5	15
1	F	1	DC	C3'-O3'	10.21	1.57	1.44	11	15
1	Е	1	DC	O4'-C1'	10.21	1.54	1.42	7	15
1	F	6	DT	C3'-O3'	10.20	1.57	1.44	13	15
1	Е	14	DT	C3'-O3'	10.18	1.57	1.44	10	15
1	F	19	DC	O4'-C1'	10.18	1.54	1.42	11	15
1	Е	11	DA	O4'-C1'	10.15	1.54	1.42	2	15
1	F	14	DT	C3'-O3'	10.15	1.57	1.44	9	15
1	Е	6	DT	C3'-O3'	10.15	1.57	1.44	11	15
1	Е	12	DA	C3'-O3'	10.13	1.57	1.44	2	15
1	F	6	DT	O4'-C1'	10.11	1.54	1.42	8	15
1	F	17	DT	O4'-C1'	10.07	1.54	1.42	7	15
1	F	2	DG	O4'-C1'	10.06	1.54	1.42	7	15
1	F	11	DA	O4'-C1'	10.04	1.54	1.42	7	15
1	Е	12	DA	O4'-C1'	10.02	1.54	1.42	10	15
1	F	4	DA	O4'-C1'	10.00	1.54	1.42	12	15
1	F	16	DG	O4'-C1'	10.00	1.54	1.42	1	15
1	Е	4	DA	C3'-O3'	9.98	1.56	1.44	1	15
1	F	12	DA	C3'-O3'	9.97	1.56	1.44	8	15
1	F	19	DC	C3'-O3'	9.96	1.56	1.44	15	15
1	Е	19	DC	O4'-C1'	9.95	1.54	1.42	2	15
1	F	6	DT	C3'-C2'	-9.94	1.40	1.52	5	15
1	Е	18	DA	O4'-C1'	9.93	1.54	1.42	2	15



1	\mathbf{D}	ng	
Т	11	OO	

					7		T1 1(8)	Mod	lels
Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)	Worst	Total
1	Е	10	DT	O4'-C1'	9.92	1.54	1.42	11	15
1	Е	6	DT	C3'-C2'	-9.89	1.40	1.52	15	15
1	F	4	DA	C3'-O3'	9.85	1.56	1.44	9	15
1	Е	5	DC	C3'-C2'	-9.83	1.40	1.52	1	15
1	F	11	DA	C3'-O3'	9.82	1.56	1.44	8	15
1	Е	4	DA	O4'-C1'	9.82	1.54	1.42	7	15
1	Е	12	DA	C3'-C2'	-9.79	1.40	1.52	1	15
1	F	18	DA	C3'-O3'	9.76	1.56	1.44	6	15
1	Е	8	DG	O4'-C1'	9.74	1.53	1.42	13	15
1	F	18	DA	O4'-C1'	9.72	1.53	1.42	14	15
1	Е	15	DA	O4'-C1'	9.69	1.53	1.42	13	15
1	F	10	DT	C3'-C2'	-9.69	1.40	1.52	15	15
1	Е	6	DT	O4'-C1'	9.68	1.53	1.42	15	15
1	Е	14	DT	C3'-C2'	-9.67	1.40	1.52	3	15
1	Е	11	DA	C3'-C2'	-9.64	1.40	1.52	10	15
1	F	12	DA	C3'-C2'	-9.64	1.40	1.52	15	15
1	Е	10	DT	C3'-C2'	-9.63	1.40	1.52	2	15
1	F	13	DC	C3'-C2'	-9.60	1.40	1.52	11	15
1	Е	16	DG	O4'-C1'	9.60	1.53	1.42	1	15
1	F	17	DT	C3'-O3'	9.56	1.56	1.44	7	15
1	Е	1	DC	C3'-O3'	9.56	1.56	1.44	11	15
1	F	8	DG	O4'-C1'	9.55	1.53	1.42	13	15
1	F	13	DC	O4'-C1'	9.53	1.53	1.42	13	15
1	F	2	DG	C3'-C2'	-9.53	1.40	1.52	7	15
1	Е	13	DC	O4'-C1'	9.52	1.53	1.42	11	15
1	F	15	DA	O4'-C1'	9.52	1.53	1.42	1	15
1	Е	3	DT	C3'-O3'	9.51	1.56	1.44	14	15
1	F	3	DT	C3'-O3'	9.50	1.56	1.44	9	15
1	Е	7	DA	C3'-O3'	9.47	1.56	1.44	12	15
1	F	14	DT	C3'-C2'	-9.44	1.41	1.52	15	15
1	Е	19	DC	C3'-O3'	9.44	1.56	1.44	12	15
1	Е	2	DG	C3'-O3'	9.43	1.56	1.44	1	15
1	Е	17	DT	N1-C2	9.34	1.45	1.38	3	15
1	F	3	DT	C3'-C2'	-9.31	1.41	1.52	14	15
1	Е	9	DT	C3'-C2'	-9.28	1.41	1.52	4	15
1	F	11	DA	C3'-C2'	-9.27	1.41	1.52	14	15
1	Е	18	DA	C3'-C2'	-9.25	1.41	1.52	12	15
1	Е	13	DC	C3'-C2'	-9.25	1.41	1.52	6	15
1	Е	7	DA	C4'-C3'	-9.22	1.43	1.52	13	15
1	F	5	DC	C3'-C2'	-9.21	1.41	1.52	13	15
1	Е	13	DC	N1-C6	9.19	1.42	1.37	15	5



1	R	CS	
-	10	∇D	

								Mod	lels
Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)	Worst	Total
1	F	19	DC	C3'-C2'	-9.18	1.41	1.52	14	15
1	F	9	DT	C3'-C2'	-9.13	1.41	1.52	4	15
1	Ε	19	DC	C3'-C2'	-9.09	1.41	1.52	11	15
1	Ε	17	DT	C3'-C2'	-9.07	1.41	1.52	9	15
1	F	8	DG	C3'-C2'	-9.05	1.41	1.52	2	15
1	F	14	DT	N1-C2	9.05	1.45	1.38	3	15
1	Ε	16	DG	C3'-O3'	9.04	1.55	1.44	8	15
1	Ε	9	DT	N1-C2	9.02	1.45	1.38	7	15
1	Ε	3	DT	C3'-C2'	-8.99	1.41	1.52	11	15
1	Ε	1	DC	C3'-C2'	-8.96	1.41	1.52	5	15
1	Ε	2	DG	C3'-C2'	-8.93	1.41	1.52	14	15
1	F	16	DG	C3'-O3'	8.92	1.55	1.44	6	15
1	F	9	DT	N1-C2	8.84	1.45	1.38	3	15
1	Е	18	DA	C3'-O3'	8.82	1.55	1.44	10	15
1	Е	4	DA	C3'-C2'	-8.82	1.41	1.52	13	15
1	Е	10	DT	C2'-C1'	8.81	1.61	1.52	15	15
1	F	1	DC	C3'-C2'	-8.81	1.41	1.52	7	15
1	Е	8	DG	C3'-C2'	-8.78	1.41	1.52	5	15
1	Е	16	DG	C3'-C2'	-8.76	1.41	1.52	1	15
1	F	8	DG	C3'-O3'	8.76	1.55	1.44	2	15
1	Е	15	DA	C3'-C2'	-8.75	1.41	1.52	4	15
1	F	16	DG	C3'-C2'	-8.74	1.41	1.52	13	15
1	F	17	DT	C3'-C2'	-8.74	1.41	1.52	13	15
1	F	18	DA	C3'-C2'	-8.73	1.41	1.52	7	15
1	Е	14	DT	N1-C2	8.65	1.45	1.38	11	15
1	F	15	DA	C3'-C2'	-8.63	1.41	1.52	3	15
1	F	4	DA	C3'-C2'	-8.62	1.42	1.52	5	15
1	F	10	DT	C2'-C1'	8.62	1.60	1.52	11	15
1	Е	12	DA	C4'-C3'	-8.62	1.44	1.52	9	14
1	Е	3	DT	C5-C7	8.58	1.55	1.50	11	15
1	F	13	DC	N1-C6	8.58	1.42	1.37	15	1
1	Е	15	DA	C3'-O3'	8.56	1.55	1.44	3	15
1	F	2	DG	C4'-C3'	-8.55	1.44	1.52	11	12
1	Е	3	DT	N1-C2	8.51	1.44	1.38	2	15
1	Е	10	DT	C5-C7	8.49	1.55	1.50	9	15
1	Е	6	DT	C5-C7	8.46	1.55	1.50	7	15
1	Е	10	DT	C4'-C3'	-8.45	1.44	1.52	9	15
1	F	6	DT	C5-C7	8.44	1.55	1.50	1	15
1	F	17	DT	N1-C2	8.43	1.44	1.38	10	15
1	F	15	DA	C3'-O3'	8.40	1.54	1.44	2	15
1	F	3	DT	C5-C7	8.35	1.55	1.50	15	15



1	\mathbf{D}	ng	
Т	11	OO	

		D	n		7		T 1 1(%)	Mod	lels
Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)	Worst	Total
1	F	10	DT	C5-C7	8.34	1.55	1.50	12	15
1	F	10	DT	N1-C2	8.31	1.44	1.38	5	15
1	F	14	DT	C2'-C1'	8.31	1.60	1.52	8	15
1	Ε	9	DT	C5-C7	8.26	1.55	1.50	5	15
1	F	9	DT	C5-C7	8.25	1.55	1.50	4	15
1	F	11	DA	C4'-C3'	-8.24	1.44	1.52	7	15
1	Ε	5	DC	C2'-C1'	8.24	1.60	1.52	1	15
1	F	17	DT	C5-C7	8.24	1.54	1.50	15	15
1	F	20	DG	O4'-C1'	8.22	1.52	1.42	6	15
1	Ε	6	DT	C4'-C3'	-8.18	1.44	1.52	14	15
1	Ε	7	DA	O4'-C1'	8.14	1.52	1.42	4	15
1	Ε	10	DT	N1-C2	8.12	1.44	1.38	7	15
1	Ε	8	DG	C4'-C3'	-8.11	1.44	1.52	8	15
1	Е	20	DG	O4'-C1'	8.08	1.51	1.42	7	15
1	F	3	DT	N1-C2	8.06	1.44	1.38	4	15
1	F	12	DA	C2'-C1'	8.03	1.60	1.52	15	15
1	Е	18	DA	C4'-C3'	-7.99	1.44	1.52	2	15
1	Е	12	DA	C2'-C1'	7.97	1.60	1.52	11	15
1	Е	11	DA	C4'-C3'	-7.97	1.44	1.52	7	15
1	F	12	DA	N9-C4	7.97	1.42	1.37	15	14
1	Е	17	DT	C5-C7	7.93	1.54	1.50	13	15
1	F	1	DC	C4'-C3'	-7.89	1.44	1.52	3	15
1	F	6	DT	C4'-C3'	-7.87	1.44	1.52	5	15
1	Е	6	DT	N1-C2	7.76	1.44	1.38	7	15
1	Е	14	DT	C2'-C1'	7.75	1.60	1.52	10	15
1	Е	9	DT	C4'-C3'	-7.74	1.44	1.52	7	14
1	F	6	DT	N1-C2	7.69	1.44	1.38	7	15
1	F	6	DT	C2'-C1'	7.68	1.60	1.52	9	15
1	F	5	DC	C2'-C1'	7.67	1.60	1.52	9	15
1	Ε	8	DG	C2'-C1'	7.65	1.59	1.52	5	15
1	F	19	DC	C2'-C1'	7.65	1.59	1.52	7	15
1	F	3	DT	C4'-C3'	-7.64	1.45	1.52	5	15
1	F	7	DA	O4'-C1'	7.62	1.51	1.42	5	15
1	Ε	9	DT	C2'-C1'	7.61	1.59	1.52	5	15
1	F	8	DG	C4'-C3'	-7.54	1.45	1.52	1	15
1	Е	11	DA	C2'-C1'	7.54	1.59	1.52	10	15
1	Е	1	DC	C4'-C3'	-7.47	1.45	1.52	5	15
1	F	1	DC	C2'-C1'	7.46	1.59	1.52	13	15
1	Е	17	DT	C4'-C3'	-7.46	1.45	1.52	3	13
1	Е	5	DC	C4'-C3'	-7.46	1.45	1.52	4	15
1	Е	3	DT	C2'-C1'	7.41	1.59	1.52	5	15



1	\mathbf{D}	ng	
Т	11	OO	

		-			_			Mod	lels
Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)	Worst	Total
1	F	10	DT	C4'-C3'	-7.38	1.45	1.52	7	15
1	F	2	DG	C2'-C1'	7.38	1.59	1.52	1	15
1	F	5	DC	C4'-C3'	-7.33	1.45	1.52	6	15
1	F	9	DT	C2'-C1'	7.31	1.59	1.52	2	15
1	Е	6	DT	C2'-C1'	7.29	1.59	1.52	15	15
1	F	12	DA	C4'-C3'	-7.21	1.45	1.52	5	14
1	Ε	13	DC	C2'-C1'	7.16	1.59	1.52	15	12
1	F	3	DT	C2'-C1'	7.14	1.59	1.52	9	15
1	F	14	DT	C5-C7	7.10	1.54	1.50	5	14
1	Ε	16	DG	C4'-C3'	-7.09	1.45	1.52	11	15
1	F	14	DT	C4'-C3'	-7.09	1.45	1.52	1	15
1	F	4	DA	C2'-C1'	7.09	1.59	1.52	5	15
1	F	17	DT	C4'-C3'	-7.08	1.45	1.52	13	15
1	F	19	DC	C4'-C3'	-7.06	1.45	1.52	5	13
1	F	20	DG	C4'-C3'	7.04	1.60	1.53	8	15
1	Е	14	DT	C5-C7	7.03	1.54	1.50	13	15
1	Е	2	DG	C4'-C3'	-7.00	1.45	1.52	13	15
1	Е	17	DT	C2'-C1'	6.97	1.59	1.52	2	15
1	F	8	DG	C2'-C1'	6.94	1.59	1.52	14	15
1	Е	14	DT	C4'-C3'	-6.92	1.45	1.52	13	15
1	F	16	DG	C4'-C3'	-6.91	1.45	1.52	6	15
1	Е	20	DG	C4'-C3'	6.89	1.60	1.53	9	15
1	F	18	DA	C2'-C1'	6.89	1.59	1.52	7	15
1	F	7	DA	C8-N7	-6.88	1.26	1.31	10	15
1	Е	1	DC	C2'-C1'	6.87	1.59	1.52	5	15
1	Е	3	DT	C4'-C3'	-6.87	1.45	1.52	10	14
1	Е	13	DC	C4'-C3'	-6.85	1.45	1.52	11	11
1	Е	2	DG	C2'-C1'	6.83	1.59	1.52	15	15
1	Е	4	DA	C4'-C3'	-6.80	1.45	1.52	14	15
1	F	9	DT	C4'-C3'	-6.79	1.45	1.52	5	13
1	F	15	DA	C4'-C3'	-6.72	1.45	1.52	12	15
1	F	4	DA	C4'-C3'	-6.72	1.45	1.52	3	14
1	Е	18	DA	C2'-C1'	6.66	1.59	1.52	13	15
1	Е	19	DC	C4'-C3'	-6.60	1.46	1.52	10	15
1	F	17	DT	C2'-C1'	6.57	1.58	1.52	10	15
1	Е	15	DA	C4'-C3'	-6.57	1.46	1.52	14	15
1	Е	4	DA	C2'-C1'	6.56	1.58	1.52	1	15
1	Е	19	DC	C2'-C1'	6.54	1.58	1.52	15	15
1	F	11	DA	C2'-C1'	6.52	1.58	1.52	15	15
1	F	18	DA	C4'-C3'	-6.46	1.46	1.52	15	15
1	F	13	DC	C4'-C3'	-6.45	1.46	1.52	10	12



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Т	11	$\mathcal{O}\mathcal{O}$

		- r			-			Mod	lels
Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)	Worst	Total
1	F	4	DA	N9-C4	6.42	1.41	1.37	3	6
1	E	12	DA	N9-C4	6.41	1.41	1.37	1	7
1	F	20	DG	C2'-C1'	6.39	1.58	1.52	1	15
1	F	7	DA	N9-C4	6.39	1.41	1.37	10	1
1	F	13	DC	C2'-C1'	6.37	1.58	1.52	7	13
1	F	15	DA	C2'-C1'	6.33	1.58	1.52	3	15
2	В	544	THR	N-CA	6.33	1.59	1.46	2	11
1	Ε	15	DA	C2'-C1'	6.27	1.58	1.52	7	15
2	В	576	GLY	N-CA	6.14	1.55	1.46	15	1
1	Ε	16	DG	C2'-C1'	6.12	1.58	1.52	14	15
1	Ε	7	DA	C8-N7	-6.11	1.27	1.31	1	12
1	Ε	7	DA	N9-C4	6.02	1.41	1.37	5	3
1	Ε	15	DA	N7-C5	6.02	1.42	1.39	7	14
2	А	44	THR	N-CA	6.01	1.58	1.46	8	11
2	А	78	GLY	N-CA	5.98	1.55	1.46	13	10
1	F	16	DG	C2'-C1'	5.97	1.58	1.52	1	15
1	F	12	DA	C5'-C4'	5.95	1.57	1.51	8	2
1	Е	14	DT	C5'-C4'	5.93	1.57	1.51	10	5
1	Е	3	DT	C5'-C4'	5.91	1.57	1.51	5	2
2	А	23	VAL	N-CA	5.91	1.58	1.46	12	15
1	F	2	DG	C5'-C4'	5.86	1.57	1.51	9	3
1	Е	5	DC	N1-C2	5.86	1.46	1.40	12	11
2	В	578	GLY	N-CA	5.83	1.54	1.46	11	8
1	Е	20	DG	C2'-C1'	5.80	1.58	1.52	7	15
2	В	523	VAL	N-CA	5.78	1.57	1.46	5	11
1	F	5	DC	N1-C2	5.75	1.46	1.40	3	14
1	F	15	DA	N7-C5	5.69	1.42	1.39	5	7
1	F	19	DC	N1-C2	5.66	1.45	1.40	10	14
1	F	13	DC	N1-C2	5.62	1.45	1.40	4	8
1	Е	19	DC	N1-C2	5.62	1.45	1.40	15	12
1	F	18	DA	N9-C4	5.60	1.41	1.37	12	3
1	Е	6	DT	C5'-C4'	5.56	1.57	1.51	2	2
1	Е	11	DA	N9-C4	5.56	1.41	1.37	5	3
1	Е	13	DC	N1-C2	5.55	1.45	1.40	12	5
1	Е	18	DA	N9-C4	5.54	1.41	1.37	3	2
1	F	13	DC	C5'-C4'	5.50	1.57	1.51	15	3
1	F	11	DA	N9-C4	5.45	1.41	1.37	7	1
1	Е	13	DC	C1'-N1	5.41	1.56	1.49	1	4
1	Е	1	DC	N1-C2	5.38	1.45	1.40	4	10
1	Е	2	DG	C5'-C4'	5.38	1.57	1.51	1	2
1	F	1	DC	N1-C2	5.37	1.45	1.40	13	4



Mal	Chain	Dec	Turno	Atoma	7	Observed (Å)	$\mathbf{I}_{\mathbf{d}}$	Mo	dels
	Chain	nes	Type	Atoms	Z	Observed(A)	Ideal(A)	Worst	Total
1	Е	13	DC	C5'-C4'	5.36	1.57	1.51	10	2
1	Е	2	DG	N9-C4	5.32	1.42	1.38	15	1
1	F	14	DT	C5'-C4'	5.24	1.57	1.51	14	3
2	В	564	GLY	N-CA	5.24	1.53	1.46	5	1
1	F	13	DC	C1'-N1	5.22	1.56	1.49	15	1
1	Е	8	DG	P-O5'	5.21	1.65	1.59	11	2
1	Е	4	DA	N9-C4	5.21	1.41	1.37	15	1
2	А	33	ASP	N-CA	5.16	1.56	1.46	2	6
1	Е	15	DA	C5'-C4'	5.15	1.57	1.51	15	2
1	F	10	DT	C5'-C4'	5.10	1.56	1.51	13	1
2	А	39	LEU	N-CA	5.09	1.56	1.46	15	3
1	Е	10	DT	C5'-C4'	5.09	1.56	1.51	10	1
2	В	533	ASP	N-CA	5.07	1.56	1.46	14	4
1	F	20	DG	C3'-C2'	5.05	1.58	1.52	1	1
1	F	4	DA	C5'-C4'	5.04	1.56	1.51	10	1
1	F	11	DA	C8-N7	-5.03	1.28	1.31	7	1
1	F	16	DG	N7-C5	5.03	1.42	1.39	10	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mal	Mol Chain	Dec	Turne	Atoma	7	Observed ⁽⁰⁾		Moo	dels
INIOI	Unam	nes	Type	Atoms		Observed()	Ideal()	Worst	Total
1	F	13	DC	O4'-C1'-N1	23.09	124.17	108.00	15	15
1	Е	13	DC	O4'-C1'-N1	22.40	123.68	108.00	2	15
1	Е	11	DA	O4'-C1'-N9	19.82	121.88	108.00	13	15
1	F	11	DA	O4'-C1'-N9	19.33	121.53	108.00	9	15
1	F	4	DA	O4'-C1'-N9	18.49	120.94	108.00	15	15
1	Е	2	DG	O4'-C1'-N9	18.38	120.86	108.00	3	15
1	Е	18	DA	O4'-C1'-N9	18.26	120.78	108.00	1	15
1	Е	12	DA	O4'-C1'-N9	18.24	120.77	108.00	15	15
1	F	19	DC	O4'-C1'-N1	18.21	120.75	108.00	10	15
1	Е	19	DC	O4'-C1'-N1	18.18	120.73	108.00	11	15
1	F	18	DA	O4'-C1'-N9	18.01	120.61	108.00	3	15
1	Е	4	DA	O4'-C1'-N9	17.95	120.56	108.00	11	15
1	F	3	DT	O4'-C1'-N1	17.90	120.53	108.00	13	15
1	F	9	DT	O4'-C1'-N1	17.82	120.48	108.00	4	15
1	F	12	DA	O4'-C1'-N9	17.82	120.47	108.00	9	15
1	Е	8	DG	O4'-C1'-N9	17.80	120.46	108.00	13	15
1	E	16	DG	O4'-C1'-N9	17.78	120.44	108.00	13	15
1	F	20	DG	O4'-C1'-N9	17.68	120.38	108.00	8	15
1	F	8	DG	O4'-C1'-N9	17.66	120.36	108.00	10	15



			us page					Mo	dels
Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$	Worst	Total
1	E	5	DC	O4'-C1'-N1	17.64	120.35	108.00	1	15
1	E	3	DT	O4'-C1'-N1	17.64	120.35	108.00	6	15
1	Е	17	DT	O4'-C1'-N1	17.62	120.34	108.00	7	15
1	Е	6	DT	O4'-C1'-N1	17.61	120.33	108.00	14	15
1	Ε	15	DA	O4'-C1'-N9	17.56	120.29	108.00	1	15
1	F	6	DT	O4'-C1'-N1	17.49	120.24	108.00	6	15
1	Е	20	DG	O4'-C1'-N9	17.49	120.24	108.00	9	15
1	F	16	DG	O4'-C1'-N9	17.43	120.20	108.00	4	15
1	F	15	DA	O4'-C1'-N9	17.42	120.19	108.00	10	15
1	Е	10	DT	O4'-C1'-N1	17.38	120.17	108.00	3	15
1	Е	9	DT	O4'-C1'-N1	17.35	120.14	108.00	5	15
1	F	14	DT	O4'-C1'-N1	17.29	120.10	108.00	15	15
1	Е	1	DC	O4'-C1'-N1	17.16	120.01	108.00	12	15
1	F	2	DG	O4'-C1'-N9	17.04	119.93	108.00	15	15
1	Е	14	DT	O4'-C1'-N1	16.96	119.87	108.00	1	15
1	F	1	DC	O4'-C1'-N1	16.74	119.72	108.00	4	15
1	F	10	DT	O4'-C1'-N1	16.66	119.66	108.00	2	15
1	F	5	DC	O4'-C1'-N1	16.63	119.64	108.00	13	15
1	F	17	DT	O4'-C1'-N1	16.48	119.54	108.00	7	15
1	Е	3	DT	C4'-C3'-C2'	15.98	117.48	103.10	5	15
1	F	9	DT	C4'-C3'-C2'	15.82	117.34	103.10	2	15
1	F	4	DA	C4'-C3'-C2'	15.79	117.31	103.10	12	15
1	Е	2	DG	C4'-C3'-C2'	15.78	117.30	103.10	15	15
1	Е	9	DT	C4'-C3'-C2'	15.77	117.29	103.10	1	15
1	F	19	DC	C4'-C3'-C2'	15.76	117.28	103.10	7	15
1	Е	1	DC	C4'-C3'-C2'	15.73	117.25	103.10	7	15
1	F	12	DA	C4'-C3'-C2'	15.70	117.23	103.10	1	15
1	Е	12	DA	C4'-C3'-C2'	15.69	117.22	103.10	12	15
1	Е	5	DC	C4'-C3'-C2'	15.65	117.19	103.10	10	15
1	F	7	DA	N7-C8-N9	15.60	121.60	113.80	10	15
1	F	17	DT	C4'-C3'-C2'	15.59	117.13	103.10	7	15
1	Е	14	DT	C4'-C3'-C2'	15.58	117.12	103.10	12	15
1	F	10	DT	C4'-C3'-C2'	15.58	117.12	103.10	4	15
1	F	1	DC	C4'-C3'-C2'	15.54	117.09	103.10	6	15
1	F	14	DT	C4'-C3'-C2'	15.53	117.08	103.10	8	15
1	Е	10	DT	C4'-C3'-C2'	15.50	117.05	103.10	11	15
1	Е	19	DC	C4'-C3'-C2'	15.47	117.02	103.10	12	15
1	Е	11	DA	C4'-C3'-C2'	15.46	117.02	103.10	3	15
1	F	20	DG	N7-C8-N9	15.43	120.82	113.10	11	15
1	F	3	DT	C4'-C3'-C2'	15.40	116.96	103.10	9	15
1	E	2	DG	N7-C8-N9	15.37	120.79	113.10	8	15



Mol Chain		T T	• /	7		T 1 1(0)	Mod	dels	
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Worst	Total
1	F	2	DG	N7-C8-N9	15.35	120.78	113.10	6	15
1	F	15	DA	N7-C8-N9	15.31	121.46	113.80	13	15
1	F	13	DC	C4'-C3'-C2'	15.30	116.87	103.10	12	15
1	Е	20	DG	N7-C8-N9	15.30	120.75	113.10	6	15
1	F	16	DG	N7-C8-N9	15.28	120.74	113.10	1	15
1	Е	4	DA	C4'-C3'-C2'	15.27	116.84	103.10	1	15
1	Е	15	DA	N7-C8-N9	15.25	121.42	113.80	12	15
1	Е	17	DT	C4'-C3'-C2'	15.23	116.81	103.10	8	15
1	F	5	DC	C4'-C3'-C2'	15.22	116.80	103.10	3	15
1	Е	13	DC	C4'-C3'-C2'	15.21	116.79	103.10	11	15
1	Е	6	DT	C4'-C3'-C2'	15.09	116.68	103.10	1	15
1	Е	16	DG	N7-C8-N9	15.08	120.64	113.10	9	15
1	F	18	DA	C4'-C3'-C2'	15.07	116.67	103.10	6	15
1	Е	8	DG	N7-C8-N9	15.06	120.63	113.10	4	15
1	F	11	DA	C4'-C3'-C2'	15.04	116.63	103.10	8	15
1	F	2	DG	C4'-C3'-C2'	14.99	116.59	103.10	14	15
1	Е	7	DA	N7-C8-N9	14.93	121.26	113.80	1	15
1	F	6	DT	C4'-C3'-C2'	14.89	116.50	103.10	1	15
1	F	8	DG	N7-C8-N9	14.73	120.47	113.10	5	15
1	Е	15	DA	C4'-C3'-C2'	14.61	116.25	103.10	3	15
1	Е	18	DA	C4'-C3'-C2'	14.58	116.22	103.10	9	15
1	Е	8	DG	C4'-C3'-C2'	14.55	116.19	103.10	4	15
1	F	16	DG	C4'-C3'-C2'	14.54	116.19	103.10	11	15
1	F	15	DA	C4'-C3'-C2'	14.53	116.18	103.10	15	15
1	F	8	DG	C4'-C3'-C2'	14.53	116.18	103.10	9	15
1	Е	16	DG	C4'-C3'-C2'	14.40	116.06	103.10	12	15
1	F	7	DA	C4'-C3'-C2'	14.06	115.75	103.10	10	15
1	Е	4	DA	N7-C8-N9	14.04	120.82	113.80	14	15
1	Е	12	DA	N7-C8-N9	14.01	120.81	113.80	14	15
1	F	12	DA	N7-C8-N9	14.00	120.80	113.80	15	15
1	Е	11	DA	N7-C8-N9	13.83	120.72	113.80	11	15
1	F	4	DA	N7-C8-N9	13.73	120.67	113.80	12	15
1	Е	18	DA	N7-C8-N9	13.72	120.66	113.80	2	15
1	F	18	DA	N7-C8-N9	13.41	120.50	113.80	2	15
1	F	11	DA	N7-C8-N9	13.31	120.45	113.80	5	15
1	Е	2	DG	C8-N9-C4	-12.62	101.35	106.40	15	15
1	F	20	DG	C8-N9-C4	-12.47	101.41	106.40	11	15
1	Е	7	DA	C4'-C3'-C2'	12.42	114.28	103.10	10	15
1	F	7	DA	N9-C1'-C2'	12.37	136.11	112.60	10	15
1	F	7	DA	C8-N9-C4	-12.15	100.94	105.80	10	15
1	F	16	DG	C8-N9-C4	-12.02	101.59	106.40	1	15



		D	T T	• •	7		T 1 (0)	Mo	dels
Mol	Chain	Res	Type	Atoms		Observed(⁶)	Ideal(°)	Worst	Total
1	F	2	DG	C8-N9-C4	-12.01	101.59	106.40	15	15
1	Е	20	DG	C8-N9-C4	-12.01	101.60	106.40	2	15
1	Е	16	DG	C8-N9-C4	-12.00	101.60	106.40	14	15
1	Е	12	DA	C8-N9-C4	-11.95	101.02	105.80	14	15
1	Е	8	DG	C8-N9-C4	-11.95	101.62	106.40	4	15
1	F	8	DG	C8-N9-C4	-11.92	101.63	106.40	11	15
1	F	12	DA	C8-N9-C4	-11.86	101.06	105.80	15	15
1	Е	18	DA	C8-N9-C4	-11.72	101.11	105.80	3	15
1	Е	7	DA	C8-N9-C4	-11.58	101.17	105.80	5	15
1	F	15	DA	C5-N7-C8	-11.41	98.19	103.90	15	15
1	Е	13	DC	N1-C1'-C2'	11.26	133.98	112.60	15	13
1	Е	11	DA	C8-N9-C4	-11.23	101.31	105.80	9	15
1	Е	15	DA	C5-N7-C8	-11.13	98.33	103.90	3	15
1	F	18	DA	C8-N9-C4	-11.07	101.37	105.80	14	15
1	F	11	DA	C8-N9-C4	-10.99	101.41	105.80	7	15
1	Е	4	DA	C8-N9-C4	-10.94	101.42	105.80	15	15
1	F	15	DA	C8-N9-C4	-10.80	101.48	105.80	12	15
1	F	4	DA	C8-N9-C4	-10.79	101.48	105.80	3	15
1	Е	7	DA	N9-C1'-C2'	10.75	133.02	112.60	1	15
1	Е	15	DA	C8-N9-C4	-10.57	101.57	105.80	14	15
1	F	13	DC	P-O3'-C3'	10.56	132.37	119.70	6	10
1	F	9	DT	P-O3'-C3'	9.94	131.63	119.70	13	11
1	Е	8	DG	P-O3'-C3'	9.76	131.42	119.70	14	13
1	Е	13	DC	P-O3'-C3'	9.70	131.34	119.70	5	12
1	Е	7	DA	O4'-C1'-N9	8.94	114.26	108.00	8	13
1	F	13	DC	N1-C1'-C2'	8.87	129.44	112.60	15	15
1	F	14	DT	C6-C5-C7	-8.83	117.60	122.90	7	15
1	F	2	DG	P-O3'-C3'	8.71	130.16	119.70	9	12
1	Е	10	DT	P-O3'-C3'	8.71	130.16	119.70	2	10
1	Е	14	DT	C6-C5-C7	-8.59	117.74	122.90	1	15
1	Е	2	DG	C5-N7-C8	-8.47	100.06	104.30	1	15
1	F	16	DG	C5-N7-C8	-8.42	100.09	104.30	10	15
1	F	5	DC	P-O3'-C3'	8.40	129.78	119.70	9	11
1	Е	9	DT	C6-C5-C7	-8.40	117.86	122.90	15	15
1	Е	9	DT	P-O3'-C3'	8.23	129.58	119.70	10	13
1	F	10	DT	P-O3'-C3'	8.22	129.56	119.70	9	15
1	Е	5	DC	P-O3'-C3'	8.20	129.53	119.70	13	13
1	F	12	DA	P-O3'-C3'	8.20	129.53	119.70	15	9
1	Е	7	DA	O4'-C1'-C2'	-8.16	99.37	105.90	5	5
1	Е	17	DT	P-O3'-C3'	8.13	129.46	119.70	9	13
1	F	2	DG	C5-N7-C8	-8.11	100.24	104.30	15	15



				• •	7	Ω $1(a)$	T 1 1 (0)	Mo	dels
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Worst	Total
1	Е	4	DA	C5-N7-C8	-7.98	99.91	103.90	12	15
1	E	16	DG	C5-N7-C8	-7.87	100.36	104.30	8	15
1	Е	17	DT	C6-C5-C7	-7.84	118.20	122.90	3	15
2	В	569	ARG	NE-CZ-NH1	7.83	124.21	120.30	3	8
1	F	10	DT	C6-C5-C7	-7.76	118.24	122.90	2	15
1	Е	12	DA	P-O3'-C3'	7.73	128.97	119.70	1	7
1	Е	8	DG	C5-N7-C8	-7.72	100.44	104.30	15	15
1	F	7	DA	O4'-C1'-N9	7.72	113.41	108.00	10	12
1	F	4	DA	P-O3'-C3'	7.64	128.87	119.70	9	4
1	F	17	DT	C6-C5-C7	-7.64	118.32	122.90	11	15
1	F	7	DA	C5-N7-C8	-7.64	100.08	103.90	4	15
1	F	4	DA	C5-N7-C8	-7.63	100.08	103.90	14	15
1	Е	3	DT	C6-C5-C7	-7.58	118.35	122.90	4	15
1	Е	7	DA	C5-N7-C8	-7.56	100.12	103.90	7	15
1	F	3	DT	C6-C5-C7	-7.56	118.36	122.90	11	15
1	Е	6	DT	P-O3'-C3'	7.55	128.76	119.70	12	8
1	F	9	DT	C6-C5-C7	-7.53	118.38	122.90	2	15
1	F	13	DC	N1-C2-O2	7.50	123.40	118.90	4	15
1	Е	4	DA	P-O3'-C3'	7.49	128.68	119.70	1	3
1	F	8	DG	C5-N7-C8	-7.46	100.57	104.30	1	15
1	F	6	DT	P-O3'-C3'	7.45	128.64	119.70	12	10
1	F	20	DG	C5-N7-C8	-7.44	100.58	104.30	12	15
1	Е	20	DG	C5-N7-C8	-7.41	100.60	104.30	3	15
1	F	1	DC	P-O3'-C3'	7.38	128.56	119.70	7	11
1	F	7	DA	O4'-C1'-C2'	-7.38	99.99	105.90	14	2
1	Е	2	DG	P-O3'-C3'	7.35	128.52	119.70	15	2
1	Е	11	DA	C5-N7-C8	-7.32	100.24	103.90	7	15
1	Е	10	DT	C6-C5-C7	-7.31	118.51	122.90	3	15
1	Е	11	DA	P-O3'-C3'	7.29	128.45	119.70	5	7
2	А	21	ARG	NE-CZ-NH1	7.25	123.92	120.30	12	12
1	F	18	DA	C5-N7-C8	-7.22	100.29	103.90	7	15
1	F	11	DA	C5-N7-C8	-7.20	100.30	103.90	12	15
1	F	7	DA	O4'-C4'-C3'	-7.16	101.64	104.50	1	10
1	F	18	DA	P-O3'-C3'	7.14	128.27	119.70	6	1
1	Е	18	DA	C5-N7-C8	-7.13	100.33	103.90	10	15
1	Е	3	DT	P-O3'-C3'	7.02	128.12	119.70	11	4
1	F	19	DC	N1-C2-O2	6.94	123.06	118.90	15	15
1	E	13	DC	C2-N3-C4	6.93	123.37	119.90	15	14
1	E	13	DC	N1-C2-O2	6.92	123.05	118.90	6	15
1	E	12	DA	C5-N7-C8	-6.91	100.45	103.90	7	15
2	B	597	ARG	NE-CZ-NH1	6.90	123.75	120.30	8	11
					0.00				



Mal	Chain	Dec	Turne	Atoma	7	Observed(0)		Mod	dels
IVIOI	Chain	nes	туре	Atoms		Observed(*)	Ideal(*)	Worst	Total
1	Е	19	DC	N1-C2-O2	6.88	123.03	118.90	14	15
1	F	1	DC	N1-C2-O2	6.88	123.03	118.90	2	15
1	F	5	DC	N1-C2-O2	6.88	123.03	118.90	8	15
1	F	13	DC	C2-N3-C4	6.86	123.33	119.90	15	15
1	F	14	DT	P-O3'-C3'	6.83	127.90	119.70	14	9
1	F	11	DA	P-O3'-C3'	6.82	127.89	119.70	14	2
1	Е	1	DC	N1-C2-O2	6.79	122.97	118.90	6	15
1	Е	14	DT	P-O3'-C3'	6.78	127.84	119.70	2	7
1	F	12	DA	C5-N7-C8	-6.77	100.51	103.90	10	15
1	F	19	DC	P-O3'-C3'	6.77	127.83	119.70	7	4
1	Е	1	DC	P-O3'-C3'	6.75	127.80	119.70	1	3
1	F	3	DT	P-O3'-C3'	6.69	127.73	119.70	9	1
2	А	69	ARG	NE-CZ-NH1	6.65	123.62	120.30	7	8
2	В	521	ARG	NE-CZ-NH1	6.59	123.60	120.30	6	11
1	Е	5	DC	N1-C2-O2	6.54	122.83	118.90	5	15
1	F	5	DC	N1-C1'-C2'	6.49	124.94	112.60	12	9
1	F	7	DA	P-O3'-C3'	6.49	127.49	119.70	10	1
1	F	6	DT	C6-C5-C7	-6.47	119.02	122.90	9	15
2	А	30	TYR	CB-CG-CD2	-6.42	117.15	121.00	5	1
1	Е	20	DG	C4'-C3'-O3'	6.41	125.73	109.70	3	15
1	Е	5	DC	C2-N3-C4	6.41	123.10	119.90	3	15
1	Е	10	DT	N1-C1'-C2'	6.40	124.76	112.60	15	3
1	F	6	DT	O4'-C4'-C3'	-6.40	101.94	104.50	11	5
1	F	17	DT	P-O3'-C3'	6.39	127.37	119.70	7	1
1	F	20	DG	C4'-C3'-O3'	6.36	125.60	109.70	8	15
1	F	5	DC	C2-N3-C4	6.35	123.08	119.90	9	15
1	F	10	DT	N1-C1'-C2'	6.34	124.64	112.60	9	6
2	А	56	ARG	NE-CZ-NH1	6.32	123.46	120.30	14	11
1	Е	7	DA	O4'-C4'-C3'	-6.32	101.97	104.50	2	11
2	В	569	ARG	NE-CZ-NH2	-6.23	117.18	120.30	3	2
1	Е	19	DC	P-O3'-C3'	6.23	127.18	119.70	12	1
1	F	18	DA	N9-C1'-C2'	6.20	124.38	112.60	7	1
2	В	548	ARG	NE-CZ-NH1	6.20	123.40	120.30	13	8
2	В	554	ARG	NE-CZ-NH1	6.16	123.38	120.30	9	8
2	А	48	ARG	NE-CZ-NH1	6.16	123.38	120.30	11	9
2	А	54	ARG	NE-CZ-NH1	6.12	123.36	120.30	8	8
1	F	19	DC	C2-N3-C4	6.05	122.93	119.90	11	15
1	Е	6	DT	O4'-C4'-C3'	-6.05	102.08	104.50	4	3
1	Е	5	DC	N1-C1'-C2'	5.98	123.97	112.60	7	9
1	Е	6	DT	C6-C5-C7	-5.98	119.31	122.90	8	15
2	В	563	ARG	NE-CZ-NH1	5.96	123.28	120.30	15	9



		prees		• ·	-		T 1 (a)	Mod	dels
Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$	Worst	Total
1	Е	13	DC	C6-N1-C2	-5.96	117.92	120.30	1	3
1	Е	8	DG	N9-C1'-C2'	5.94	123.88	112.60	10	2
2	В	556	ARG	NE-CZ-NH1	5.93	123.27	120.30	8	8
2	А	97	ARG	NE-CZ-NH1	5.93	123.26	120.30	4	9
1	Е	9	DT	N1-C1'-C2'	5.92	123.85	112.60	11	7
1	Е	15	DA	C6-N1-C2	5.92	122.15	118.60	12	15
1	F	15	DA	C6-N1-C2	5.91	122.14	118.60	11	15
1	Е	19	DC	C2-N3-C4	5.90	122.85	119.90	2	15
2	А	63	ARG	NE-CZ-NH1	5.89	123.25	120.30	9	9
1	F	8	DG	N9-C1'-C2'	5.89	123.79	112.60	14	2
1	F	1	DC	C2-N3-C4	5.87	122.83	119.90	15	15
1	Е	1	DC	C2-N3-C4	5.80	122.80	119.90	5	15
1	F	14	DT	C4-C5-C6	5.77	121.47	118.00	4	15
1	F	10	DT	O4'-C4'-C3'	-5.70	102.22	104.50	7	1
1	Е	8	DG	C4'-C3'-O3'	-5.70	95.46	109.70	3	10
1	Е	5	DC	C2'-C3'-O3'	-5.69	93.81	112.60	1	2
1	F	19	DC	N1-C1'-C2'	5.67	123.37	112.60	6	1
1	Е	9	DT	C4-C5-C6	5.65	121.39	118.00	8	15
1	Е	6	DT	N1-C1'-C2'	5.64	123.31	112.60	10	9
1	Е	7	DA	C6-N1-C2	5.60	121.96	118.60	8	11
1	Е	15	DA	N1-C2-N3	-5.60	126.50	129.30	2	13
1	Е	17	DT	C4-C5-C6	5.58	121.35	118.00	5	15
1	F	9	DT	N1-C1'-C2'	5.58	123.20	112.60	1	5
1	Е	14	DT	C4-C5-C6	5.55	121.33	118.00	11	15
1	F	17	DT	C4-C5-C6	5.55	121.33	118.00	12	14
1	F	7	DA	C6-N1-C2	5.53	121.92	118.60	5	15
1	F	9	DT	C4-C5-C6	5.53	121.31	118.00	1	15
2	В	584	ARG	NE-CZ-NH1	5.51	123.06	120.30	4	7
1	Е	8	DG	O4'-C4'-C3'	-5.50	102.30	104.50	6	4
1	F	11	DA	N1-C2-N3	-5.49	126.56	129.30	4	3
1	F	10	DT	C4'-C3'-O3'	-5.47	96.03	109.70	7	1
1	Е	7	DA	N1-C2-N3	-5.46	126.57	129.30	8	9
1	Е	3	DT	C4-C5-C6	5.46	121.28	118.00	3	12
1	F	9	DT	C2'-C3'-O3'	-5.44	94.64	112.60	4	2
1	F	6	DT	N1-C1'-C2'	5.44	122.94	112.60	11	4
1	F	16	DG	N9-C1'-C2'	5.43	122.92	112.60	12	5
1	F	10	DT	C2'-C3'-O3'	-5.40	94.78	112.60	9	3
1	Е	11	DA	C4'-C3'-O3'	-5.39	96.22	109.70	13	1
1	Е	4	DA	N1-C2-N3	-5.39	126.61	129.30	12	10
1	Е	11	DA	C2'-C3'-O3'	-5.39	94.83	112.60	10	1
1	F	3	DT	C4-C5-C6	5.38	121.23	118.00	11	11



			T T	• · ·	7		T 1 (0)	Mo	dels
Mol	Chain	Res	Type	Atoms		Observed(⁶)	Ideal(°)	Worst	Total
1	F	15	DA	N1-C2-N3	-5.36	126.62	129.30	8	11
1	F	13	DC	C6-N1-C2	-5.36	118.16	120.30	15	1
1	F	10	DT	C4-C5-C6	5.34	121.20	118.00	2	10
1	Е	7	DA	C1'-O4'-C4'	-5.34	104.76	110.10	5	1
1	Е	9	DT	C2'-C3'-O3'	-5.31	95.07	112.60	5	3
2	А	30	TYR	CB-CG-CD1	5.30	124.18	121.00	5	1
1	Е	11	DA	N1-C2-N3	-5.29	126.66	129.30	10	2
1	F	4	DA	N1-C2-N3	-5.29	126.66	129.30	15	6
1	Е	8	DG	C2'-C3'-O3'	-5.29	95.16	112.60	10	2
1	F	15	DA	N9-C1'-C2'	5.28	122.64	112.60	3	4
1	Е	18	DA	O4'-C4'-C3'	-5.27	102.39	104.50	13	3
1	F	19	DC	C2'-C3'-O3'	-5.25	95.27	112.60	8	4
1	F	20	DG	C3'-C2'-C1'	5.25	108.79	102.50	13	3
1	F	11	DA	C6-N1-C2	5.24	121.74	118.60	4	3
1	Е	15	DA	P-O3'-C3'	5.23	125.98	119.70	12	4
1	Е	20	DG	C3'-C2'-C1'	5.23	108.77	102.50	2	6
1	Е	10	DT	O4'-C4'-C3'	-5.21	102.42	104.50	9	3
1	Е	16	DG	N9-C1'-C2'	5.21	122.50	112.60	11	1
1	Е	6	DT	C4-C5-C6	5.21	121.12	118.00	1	2
1	F	12	DA	N1-C2-N3	-5.21	126.70	129.30	7	1
1	F	5	DC	C2'-C3'-O3'	-5.20	95.43	112.60	12	1
1	Е	12	DA	N1-C2-N3	-5.18	126.71	129.30	3	6
1	Е	11	DA	C6-N1-C2	5.18	121.71	118.60	13	2
2	А	84	ARG	NE-CZ-NH1	5.18	122.89	120.30	6	3
1	Е	12	DA	N9-C1'-C2'	5.17	122.43	112.60	2	1
1	F	14	DT	O4'-C4'-C3'	-5.17	102.43	104.50	13	1
1	Е	12	DA	C4'-C3'-O3'	-5.16	96.80	109.70	2	1
1	Е	14	DT	N1-C1'-C2'	5.16	122.40	112.60	15	1
1	Е	18	DA	C4'-C3'-O3'	-5.16	96.81	109.70	10	1
1	Е	10	DT	C4-C5-C6	5.15	121.09	118.00	5	7
1	F	18	DA	N1-C2-N3	-5.15	126.73	129.30	1	3
1	F	11	DA	O4'-C4'-C3'	-5.15	102.44	104.50	15	2
1	F	3	DT	O4'-C4'-C3'	-5.13	102.45	104.50	5	2
1	Е	20	DG	O4'-C4'-C3'	5.12	109.08	106.00	12	4
1	F	6	DT	C4-C5-C6	5.12	121.07	118.00	7	5
1	F	12	DA	N9-C1'-C2'	5.10	122.29	112.60	3	1
1	Е	15	DA	N9-C1'-C2'	5.07	122.23	112.60	2	1
1	F	7	DA	N1-C2-N3	-5.05	126.77	129.30	12	1
2	А	21	ARG	NE-CZ-NH2	-5.05	117.78	120.30	12	1
1	Е	10	DT	C4'-C3'-O3'	-5.04	97.10	109.70	5	1
1	Е	17	DT	N1-C1'-C2'	5.04	122.17	112.60	3	1



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Mal	Chain	Dog	Tuno	Type Atoms	7	$Observed(^{o})$	Ideal(0)	Moo	dels				
	Ullalli	nes	s Type			Observed()	iueai()	Worst	Total				
1	Е	11	DA	O4'-C4'-C3'	-5.04	102.49	104.50	15	1				
1	F	18	DA	C6-N1-C2	5.01	121.60	118.60	8	1				

All unique chiral outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	Е	7	DA	C1'	15
1	F	7	DA	C1'	15
1	Е	13	DC	C1'	5
1	F	13	DC	C1'	1

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	Е	16	DG	Sidechain	15
1	F	16	DG	Sidechain	15
2	А	69	ARG	Sidechain	11
2	В	569	ARG	Sidechain	10
1	F	4	DA	Sidechain	9
2	А	54	ARG	Sidechain	7
2	А	63	ARG	Sidechain	6
1	Е	4	DA	Sidechain	6
1	F	13	DC	Sidechain	5
2	В	554	ARG	Sidechain	5
2	В	563	ARG	Sidechain	5
1	F	7	DA	Sidechain	5
1	Е	13	DC	Sidechain	4
1	Е	7	DA	Sidechain	4
2	В	597	ARG	Sidechain	4
2	А	21	ARG	Sidechain	4
2	А	56	ARG	Sidechain	3
2	В	548	ARG	Sidechain	2
2	В	521	ARG	Sidechain	2
2	А	48	ARG	Sidechain	1
2	А	97	ARG	Sidechain	1
2	В	556	ARG	Sidechain	1
1	F	2	DG	Sidechain	1



6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	Е	407	228	228	6 ± 1
1	F	407	228	228	5 ± 1
2	А	710	734	734	$19{\pm}2$
2	В	710	734	734	22 ± 3
3	В	15	12	9	0 ± 1
3	А	15	12	9	0 ± 1
All	All	33960	29220	29130	522

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 8.

Atom 1	Atom 2	$Clach(\lambda)$	Distance(Å)	Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
2:A:19:TRP:CE3	2:B:551:LEU:HD22	0.82	2.09	6	7	
1:E:15:DA:H62	2:A:80:ALA:HB2	0.80	1.37	5	15	
1:F:15:DA:H62	2:B:580:ALA:HB2	0.79	1.38	12	15	
1:E:4:DA:H62	2:B:579:ILE:HG21	0.78	1.38	15	2	
1:F:14:DT:H72	2:B:580:ALA:HB3	0.74	1.60	2	13	
2:B:571:LEU:HD23	2:B:582:ILE:HD11	0.74	1.59	9	11	
1:E:14:DT:H72	2:A:80:ALA:HB3	0.73	1.60	14	14	
1:E:4:DA:N6	2:B:579:ILE:HG21	0.71	2.00	5	11	
1:F:7:DA:H2"	1:F:8:DG:H5"	0.68	1.65	10	3	
2:A:19:TRP:O	2:A:23:VAL:HG23	0.65	1.92	2	3	
2:A:39:LEU:HD22	2:B:519:TRP:CE2	0.65	2.27	6	9	
2:A:39:LEU:HD11	2:B:519:TRP:CE2	0.64	2.27	14	5	
2:A:96:LEU:HD21	2:B:534:LEU:HD22	0.63	1.71	11	2	
2:A:36:LEU:HA	2:A:39:LEU:HD23	0.60	1.74	9	8	
2:A:41:LEU:HD11	2:B:592:ALA:HB2	0.60	1.71	15	1	
2:A:39:LEU:HD21	2:B:519:TRP:CZ2	0.59	2.32	13	1	
2:A:19:TRP:N	2:B:551:LEU:HD11	0.59	2.13	1	3	
1:E:7:DA:H2"	1:E:8:DG:C5'	0.59	2.27	2	14	
1:E:7:DA:H2"	1:E:8:DG:H5'	0.59	1.75	2	13	
2:A:19:TRP:CZ3	2:B:551:LEU:HD22	0.59	2.32	10	10	
2:B:534:LEU:O	2:B:538:LEU:HD13	0.58	1.97	5	1	
2:B:551:LEU:HD13	2:B:552:GLY:N	0.58	2.14	1	3	

All unique clashes are listed below, sorted by their clash magnitude.



Continued from preu	vious page			ЪЛ	1 1
Atom-1	Atom-2	$\operatorname{Clash}(\operatorname{\AA})$	Distance(Å)	Worst Total	
2. A. 202. TDD. HD2	2.B.544.THD.HC22	0.58	1 75	worst	10tai 2
2.A.090.1 hf .HD2	2.D.344.1 III.IIG23	0.58	1.70	2 6	้อ 1
2:A:22:PIE:ODI	$2:D:301:LEU:\Pi D21$	0.58	2.34	10	11
$\frac{1:F:10:DA:N0}{0:A:44:TUD:UC02}$	2:D:080:ALA:HB2	0.57	2.14	12	11
2:A:44:1HK:HG23	3:D:998:TRP:HB2	0.57	1.70	<u> </u>	4
2:A:71:LEU:HD23	2:A:82:ILE:HG21	0.57	1.70	15	11
2:A:39:LEU:HD11	2:B:519:TRP:NET	0.57	2.14	10	4
2:B:541:LEU:HD13	2:B:542:MET:N	0.57	2.14	15	10
2:A:29:ALA:HB2	2:B:599:TRP:CZ2	0.57	2.35	9	14
1:F:14:DT:C7	2:B:580:ALA:HB3	0.56	2.31	15	9
2:A:99:TRP:CH2	2:B:529:ALA:HB2	0.56	2.35	8	10
1:F:4:DA:N6	2:A:79:ILE:HG21	0.56	2.15	12	15
2:A:39:LEU:HD22	2:B:519:TRP:NE1	0.56	2.16	7	7
2:A:96:LEU:CD2	2:B:534:LEU:HD22	0.56	2.31	11	8
2:A:99:TRP:CZ2	2:B:529:ALA:HB2	0.56	2.36	15	14
2:B:543:LEU:O	2:B:544:THR:HG23	0.55	2.01	1	4
2:B:579:ILE:HD13	2:B:582:ILE:CG2	0.55	2.31	1	2
2:B:520:LEU:HD22	2:B:520:LEU:N	0.55	2.17	2	14
2:A:41:LEU:HD13	2:A:42:MET:N	0.55	2.16	6	6
2:A:58:VAL:HG11	2:B:541:LEU:HD21	0.54	1.78	5	1
2:A:41:LEU:O	2:A:41:LEU:HD22	0.54	2.02	12	2
1:F:4:DA:H62	2:A:79:ILE:HG21	0.53	1.62	12	1
2:B:571:LEU:CD2	2:B:582:ILE:HD11	0.53	2.32	11	4
2:A:99:TRP:CZ3	2:B:538:LEU:HD21	0.53	2.38	5	1
1:E:14:DT:C7	2:A:80:ALA:HB3	0.53	2.34	1	10
1:F:7:DA:H2"	1:F:8:DG:C5'	0.53	2.34	10	2
2:B:529:ALA:HB1	2:B:535:HIS:N	0.52	2.18	8	14
2:A:99:TRP:CZ3	2:B:538:LEU:HD11	0.52	2.40	5	1
2:B:551:LEU:HD22	2:B:551:LEU:O	0.51	2.05	2	3
2:A:22:PHE:CG	2:B:551:LEU:HD21	0.51	2.40	6	6
1:E:15:DA:N6	2:A:80:ALA:HB2	0.51	2.21	13	8
2:A:34:LEU:HD22	2:B:596:LEU:CD2	0.51	2.36	10	7
2:B:551:LEU:HD22	2:B:551:LEU:C	0.49	2.27	7	3
2:A:20:LEU:HD22	2:A:20:LEU:N	0.49	2.22	1	9
1:E:4:DA:H62	2:B:579:ILE:CG2	0.49	2.18	15	1
2:B:572:LYS:NZ	2:B:579:ILE:HD13	0.49	2.22	10	1
2:A:99:TRP:CH2	2:B:538:LEU:HD21	0.48	2.43	5	1
2:B:527:LYS:HA	$2 \cdot B \cdot 530 \cdot TYB \cdot HB2$	0.48	1.85	6	1
2:A:58:VAL:HG11	2.B.541.LEU.HD11	0.48	1.85	15	2
2.B.510.TRP.HA	2.B.522.PHE.CD2	0.48	2.43	5	13
$2 \cdot \Delta \cdot 10 \cdot \text{TRP} \cdot \text{CE}^3$	$2 \cdot B \cdot 551 \cdot L E I \cdot H C$	0.40	2.40 9 AA	7	10
2.A.13.1111.0E3	2.D.001.LEU.IIG	0.40	L.44	1	T

Contin

2:B:571:LEU:HD23

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3

1.86



0.48

2:B:582:ILE:HG21

	lous page	0	0	Models		
Atom-1	Atom-2	$\operatorname{Clash}(\operatorname{\AA})$	Distance(Å)	Worst	Total	
1:F:5:DC:H41	2:A:80:ALA:HA	0.47	1.69	6	2	
2:B:599:TRP:O	2:B:603:VAL:HG22	0.47	2.09	7	15	
2:A:29:ALA:HB1	2:A:35:HIS:N	0.47	2.24	1	11	
2:A:39:LEU:HD21	2:B:519:TRP:CH2	0.47	2.45	13	1	
1:F:14:DT:OP2	2:B:581:THR:HG21	0.47	2.09	5	1	
2:B:520:LEU:H	2:B:520:LEU:HD13	0.47	1.70	7	1	
2:A:99:TRP:O	2:A:103:VAL:HG22	0.47	2.10	5	15	
2:A:27:LYS:HA	2:A:30:TYR:HB2	0.46	1.86	3	1	
2:A:50:ALA:HB1	2:A:54:ARG:NH1	0.46	2.25	4	1	
2:B:522:PHE:O	2:B:526:LEU:HD23	0.46	2.10	8	6	
2:B:557:ILE:O	2:B:561:LEU:HD13	0.46	2.11	3	1	
1:E:5:DC:H41	2:B:580:ALA:HA	0.46	1.71	7	2	
2:B:551:LEU:O	2:B:555:VAL:HG23	0.46	2.11	14	3	
2:A:23:VAL:HG11	2:B:535:HIS:NE2	0.45	2.26	8	1	
2:A:22:PHE:CZ	2:A:26:LEU:HD21	0.44	2.48	5	1	
2:B:557:ILE:HD13	2:B:558:VAL:N	0.44	2.28	5	2	
2:A:29:ALA:HB2	2:B:599:TRP:CH2	0.44	2.48	2	3	
2:B:579:ILE:HD13	2:B:582:ILE:HG21	0.44	1.90	3	2	
2:B:557:ILE:HB	2:B:582:ILE:HG22	0.44	1.90	14	1	
2:B:553:THR:O	2:B:557:ILE:HG23	0.43	2.13	1	1	
2:A:51:LEU:HD23	2:B:519:TRP:CE3	0.43	2.48	7	1	
2:A:41:LEU:HD21	2:B:558:VAL:CG1	0.43	2.43	12	1	
2:B:571:LEU:CG	2:B:582:ILE:HD11	0.43	2.43	10	1	
2:A:55:VAL:HG22	2:B:542:MET:CE	0.43	2.44	12	1	
2:A:81:THR:HG22	3:A:898:TRP:CZ2	0.43	2.49	12	1	
2:A:22:PHE:O	2:A:26:LEU:HB2	0.43	2.14	15	1	
1:E:13:DC:H2"	1:E:14:DT:O5'	0.43	2.13	4	3	
2:A:35:HIS:HA	2:A:38:LEU:HB3	0.43	1.91	10	1	
2:A:38:LEU:HD21	2:A:42:MET:CE	0.43	2.44	11	1	
2:B:582:ILE:CG2	2:B:583:THR:HG23	0.43	2.44	11	1	
1:E:14:DT:OP2	2:A:81:THR:HG21	0.43	2.13	14	1	
2:A:43:LEU:O	2:A:44:THR:HG23	0.43	2.13	6	3	
2:A:18:GLU:O	2:B:551:LEU:HD21	0.42	2.13	2	1	
2:A:58:VAL:CG1	2:B:541:LEU:HD21	0.42	2.44	5	1	
2:B:557:ILE:HD11	3:B:998:TRP:CZ3	0.42	2.49	8	1	
2:B:520:LEU:N	2:B:520:LEU:CD2	0.42	2.83	1	10	
2:A:34:LEU:HD22	2:B:596:LEU:HD21	0.42	1.91	10	1	
1:F:9:DT:H4'	1:F:10:DT:OP1	0.42	2.15	13	1	
1:E:14:DT:H71	2:A:80:ALA:HB3	0.42	1.91	2	1	
2:A:51:LEU:HG	2:B:522:PHE:CD2	0.41	2.50	1	3	
1:F:14:DT:H71	2:B:580:ALA:HB3	0.41	1.92	13	1	

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Atom 1	Atom 2	$Cleah(\lambda)$	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:F:16:DG:O6	2:B:579:ILE:HB	0.41	2.16	15	1
2:B:519:TRP:O	2:B:523:VAL:HG23	0.41	2.16	2	1
2:B:541:LEU:HD22	2:B:541:LEU:O	0.41	2.15	5	1
2:A:57:ILE:HB	2:A:82:ILE:HG22	0.41	1.93	9	1
2:A:20:LEU:N	2:A:20:LEU:CD2	0.40	2.84	6	1
2:B:579:ILE:HA	2:B:582:ILE:HG22	0.40	1.94	5	1
2:A:19:TRP:CA	2:B:551:LEU:HD11	0.40	2.46	7	1
2:A:19:TRP:CE3	2:B:551:LEU:CD2	0.40	3.03	9	1
2:A:51:LEU:O	2:A:55:VAL:HG23	0.40	2.16	12	1

6.3 Torsion angles (i)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	Perce	entiles
2	А	88/105 (84%)	73 ± 3 (83 $\pm3\%$)	$12\pm3~(14\pm3\%)$	3 ± 1 ($3\pm1\%$)	6	37
2	В	88/105~(84%)	$73 \pm 1 \ (83 \pm 2\%)$	$12\pm2~(13\pm2\%)$	3 ± 1 (4±1%)	6	34
All	All	2640/3150~(84%)	2189 (83%)	359 (14%)	92~(3%)	6	35

All 18 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	А	33	ASP	15
2	В	533	ASP	15
2	А	44	THR	14
2	В	544	THR	10
2	В	578	GLY	9
2	А	78	GLY	9
2	В	565	GLU	4
2	В	547	GLU	2
2	А	66	MET	2
2	В	576	GLY	2
2	В	564	GLY	2
2	В	572	LYS	2



Mol	Chain	Res	Type	Models (Total)
2	В	519	TRP	1
2	В	543	LEU	1
2	В	566	MET	1
2	А	64	GLY	1
2	А	43	LEU	1
2	А	76	GLY	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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		
2	А	77/91~(85%)	61 ± 2 (79 $\pm3\%$)	$16\pm2~(21\pm3\%)$	3	32	
2	В	77/91~(85%)	62 ± 2 (80 $\pm3\%$)	$15\pm2~(20\pm3\%)$	4	34	
All	All	2310/2730 (85%)	1838 (80%)	472 (20%)	3	33	

All 72 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	А	57	ILE	15
2	А	58	VAL	15
2	А	72	LYS	15
2	А	97	ARG	15
2	А	103	VAL	15
2	В	557	ILE	15
2	В	558	VAL	15
2	В	572	LYS	15
2	В	597	ARG	15
2	В	603	VAL	15
2	А	26	LEU	14
2	А	39	LEU	13
2	А	41	LEU	12
2	В	530	TYR	12
2	В	541	LEU	12
2	В	538	LEU	12
2	А	100	LEU	11
2	А	30	TYR	11



Mol	Chain	Res	Type	Models (Total)
2	А	22	PHE	11
2	А	90	LYS	10
2	А	38	LEU	10
2	В	569	ARG	10
2	А	79	ILE	9
2	В	579	ILE	9
2	В	590	LYS	8
2	В	600	LEU	8
2	В	602	GLU	8
2	В	526	LEU	8
2	А	82	ILE	8
2	В	605	LEU	8
2	А	104	LEU	7
2	А	75	LEU	6
2	В	604	LEU	6
2	А	102	GLU	5
2	А	25	LEU	5
2	А	44	THR	5
2	А	45	PRO	5
2	В	543	LEU	5
2	В	575	LEU	5
2	В	581	THR	5
2	В	544	THR	4
2	В	582	ILE	4
2	А	81	THR	4
2	В	521	ARG	4
2	А	43	LEU	3
2	А	56	ARG	3
2	А	63	ARG	3
2	В	551	LEU	3
2	А	21	ARG	3
2	В	563	ARG	2
2	В	588	SER	2
2	В	598	GLN	2
2	В	525	LEU	2
2	В	568	GLN	2
2	А	42	MET	2
2	В	556	ARG	2
2	А	98	GLN	2
2	В	561	LEU	2
2	В	547	GLU	2
2	А	35	HIS	1

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Mol	Chain	Res	Type	Models (Total)
2	А	62	LEU	1
2	В	554	ARG	1
2	А	40	ASN	1
2	А	88	SER	1
2	А	60	GLU	1
2	В	520	LEU	1
2	В	527	LYS	1
2	В	522	PHE	1
2	А	69	ARG	1
2	В	560	GLU	1
2	А	54	ARG	1
2	В	574	GLU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mal	Tuno	Chain	Dog	Link		Bond leng	ths
	Type	Ullaili	nes		Counts	RMSZ	$\#Z{>}2$
3	TRP	В	998	-	$12,\!16,\!16$	$0.86 {\pm} 0.04$	0±0 (0±0%)
3	TRP	А	898	-	12,16,16	$0.91{\pm}0.02$	0±0 (0±0%)



In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mal	Type Chain		Dec	Tinle	Bond angles						
	туре	Chain	nes	nes	nes	nes		nes Link	Counts	RMSZ	#Z>2
3	TRP	В	998	-	12,22,22	$1.83 {\pm} 0.23$	2 ± 0 (16 $\pm0\%$)				
3	TRP	А	898	-	12,22,22	$1.92{\pm}0.26$	2 ± 0 (16 $\pm2\%$)				

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
3	TRP	А	898	-	-	$0\pm 0,3,8,8$	$0\pm 0,2,2,2$
3	TRP	В	998	-	-	$0\pm 0,3,8,8$	$0\pm 0,2,2,2$

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol Chain				Atoma	7	Observed ⁽⁰⁾		Models		
IVIOI	Unam	nes	Type	Atoms	Z		Observed()	Ideal()	Worst	Total
3	В	998	TRP	CB-CG-CD1	5.71	120.92	127.97	13	15	
3	А	898	TRP	CB-CG-CD1	5.58	121.08	127.97	8	15	
3	В	998	TRP	CB-CG-CD2	4.44	133.16	126.25	13	15	
3	A	898	TRP	CB-CG-CD2	4.38	133.07	126.25	2	14	

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers (i)

There are no such molecules in this entry.



6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



7 Chemical shift validation (i)

No chemical shift data were provided

