

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

#### Nov 13, 2023 – 04:24 PM JST

PDB ID	:	5XOU
Title	:	Crystal structure of T. thermophilus Argonaute protein complexed with a
		bulge 7T8 on the guide strand
Authors	:	Sheng, G.; Wang, J.; Zhao, H.; Wang, Y.
Deposited on	:	2017-05-31
Resolution	:	2.63  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
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
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 2.63 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	1426 (2.66-2.62)
Clashscore	141614	1472(2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain				
1	А	685	8%	57%	20%	•• 18%	
1	В	685	7%	59%	18%	5%• 16%	
2	С	22	32%	23%	9%	36%	
2	Е	22	23%	36%	14%	27%	
3	D	19	53	%	32%	16%	
3	F	19	37%		47%	16%	



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# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10096 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 protein called TtAgo (D546N).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	564	Total	С	Ν	0	S	0	0	0
1	A	504	4373	2799	819	751	4	0		0
1	Р	574	Total	С	Ν	0	S	0	0	0
1	D	574	4435	2837	832	762	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	546	ASN	ASP	engineered mutation	UNP $Q746M7$
В	546	ASN	ASP	engineered mutation	UNP $Q746M7$

• Molecule 2 is a DNA chain called DNA (5'-D(P\*TP\*GP\*AP\*GP\*GP\*TP\*AP\*TP\*GP\*G P\*TP\*TP\*GP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	C	14	Total	С	Ν	Ο	Р	0	0	0
		14	295	140	52	89	14	0		0
0	F	16	Total	С	Ν	Ο	Р	0	0	0
	Z E	10	338	160	62	100	16	0	0	0

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

Mol	Chain	Residues		Ate	$\mathbf{oms}$			ZeroOcc	AltConf	Trace
3	Л	16	Total	С	Ν	Ο	Р	0	0	0
0	D	10	317	153	57	92	15	0		0
2	Б	16	Total C N O I	Р	0	0	0			
5	Г	10	317	153	57	92	15	0	0	0

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



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

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	5	$\begin{array}{cc} \text{Total} & \text{O} \\ 5 & 5 \end{array}$	0	0
5	В	11	Total         O           11         11	0	0
5	Е	2	Total O 2 2	0	0
5	$\mathbf{F}$	1	Total O 1 1	0	0



# 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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: TtAgo (D546N)





R96 P97 L98 P100 P100 R101 P102 P102 R104 R105 R105	8100 1100 1100 1110 1111 1111 1111 1111	E125 G126 W127 W128 W128 M128	V134 V135 V135 R136 R136 R137 E138 A12 A12 A12 A12 A12 A12 A12 A12 A12 A12	G144 M145 G150 C153 D154 L153	N156 V157 S157 S156 F162 L164 L165	
D168 P169 A170 A171 1173 L173 C175 C175 C175 CLU	LEU LEU GLU ALLA ALLA ALLA GLN GLY HIS PHIS PHIS PHIS PHIS	ARG VAL ARG ASN ALA ASN TYR ASC ARG	ARG THR TRP GLU GLU LEU LLU GLU GLU	GLU ASP PRO LYS GLU GLU FLEU LEU PRO	GLY GLY LLEU SER LLEU LLEU ASP TTYR HITS	
ALA SER LYS GLY GLY GLN GLN GLY GLV GLV	GLY GLY ARG ARG ARA ARA ASP ASP ASP ASP ASP	L YS PRO PRO PRO PRO FRO HIS THEU CLFU	LEU LEU VAL PRO PRO VAL LEU THR LEU GLU ASP	LEU HIS GLU GLU GLU SER LEU ALA	8280 1281 1281 1281 1284 1288 1288 1288 1288	
1290 8291 1293 1293 1293 8295 1295 1295 1295 1201	C 2002 C 2003 C 2003 C 2009 C 2009 C 2009 C 2009 C 2009 C 2009 C 2003 C 200 C 2003 C 2003	P315 P315 K320 K320 K329 K325 R335	F338 F339 R341 6341 6343 1344 1344 1344 1344 1345 850	L351 D352 Q355 F360 F363 A364	L365 L366 L378 L379 L379 L379 L381 L381	
H384 L389 K399 K399 W415	L425 L426 L426 L426 L430 P431 S433 V437 V437 V437	R444 R449 R449 L451 L451 L455 R455	K457 L460 Q461 V463 V463 L473 L473 C476	A490 A499 H500 L501 L503 W503 T504	L505 R513 R533 K533 R533 R533 R540	
V541 R545 R545 R548 V549 V549 P550 Q551 L556	R603 K675 K675 K675 V681 V681 V681 V583 P583 P583 F583 F583	V594 L604 H607 R611	P614 H621 L628 L631 L631	R640 L641 F649 F649 R651 R651 V677 D678	V685	
• Molecule 2: )	DNA (5'-D(P*T	P*GP*AP	*GP*GP*TP	P*AP*TP*C	P*GP*TP*TP*G	P*T)-:
Chain C:	32%	23%	9%	36%		
T1 G2 G4 DG DG DG DG DG DA						
• Molecule 2: )	DNA (5'-D(P*T	P*GP*AP	*GP*GP*TP	P*AP*TP*C	P*GP*TP*TP*G	P*T)-3
Chain E:	23%	36%	14%	27%		
11 62 64 65 16 76 110 110 110	612 613 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1					
• Molecule 3: 3')	DNA (5'-D(*AP*	CP*AP*AF	P*CP*CP*TP	*AP*CP*T	P*AP*CP*CP*TP*	CP*G
Chain D:	53%		32%		6%	
DT DA DT A4 CS CS CS CS C3 C3 C12 C12	0 10					
• Molecule 3: 3')	DNA (5'-D(*AP*	CP*AP*AF	P*CP*CP*TP	*AP*CP*T	P*AP*CP*CP*TP*	CP*G
Chain F:	37%		47%	16	%	







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	112.75Å $114.98$ Å $160.44$ Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	43.17 - 2.63	Depositor
Resolution (A)	43.17 - 2.63	EDS
% Data completeness	97.3 (43.17-2.63)	Depositor
(in resolution range)	92.0 (43.17-2.63)	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.47 (at 2.61 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
D D.	0.235 , $0.276$	Depositor
$\Pi, \Pi_{free}$	0.240 , $0.279$	DCC
$R_{free}$ test set	3091 reflections $(5.07%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	58.5	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , $25.3$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.46, < L^2>=0.28$	Xtriage
Estimated twinning fraction	0.038 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10096	wwPDB-VP
Average B, all atoms $(Å^2)$	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bo	ond lengths	Bond angles		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.95	23/4474~(0.5%)	1.48	80/6073~(1.3%)	
1	В	0.91	19/4537~(0.4%)	1.40	63/6158~(1.0%)	
2	С	1.18	1/329~(0.3%)	1.25	3/504~(0.6%)	
2	Е	1.13	2/379~(0.5%)	1.14	3/584~(0.5%)	
3	D	0.89	0/354	1.02	1/542~(0.2%)	
3	F	0.84	0/354	1.03	0/542	
All	All	0.95	45/10427~(0.4%)	1.40	150/14403~(1.0%)	

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	А	0	3
1	В	0	4
All	All	0	7

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	309	VAL	CB-CG1	-14.16	1.23	1.52
1	А	309	VAL	CB-CG2	-10.81	1.30	1.52
1	В	309	VAL	CB-CG2	-9.87	1.32	1.52
1	А	300	ARG	CZ-NH1	-9.60	1.20	1.33
2	С	1	DT	OP3-P	-8.94	1.50	1.61
2	Е	1	DT	OP3-P	-8.72	1.50	1.61
1	А	300	ARG	CB-CG	-8.61	1.29	1.52
1	А	98	LEU	CG-CD2	-8.42	1.20	1.51
1	А	122	ARG	CZ-NH2	-8.41	1.22	1.33
1	В	30	GLU	CB-CG	-8.38	1.36	1.52



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	В	122	ARG	CB-CG	-8.37	1.29	1.52
1	В	23	GLU	CD-OE2	-7.97	1.16	1.25
1	А	335	ARG	CZ-NH1	-7.93	1.22	1.33
1	В	309	VAL	CB-CG1	-7.88	1.36	1.52
1	В	335	ARG	CZ-NH1	-7.85	1.22	1.33
1	А	98	LEU	CG-CD1	-7.68	1.23	1.51
1	В	98	LEU	CG-CD1	-7.68	1.23	1.51
1	А	23	GLU	CD-OE1	-7.64	1.17	1.25
1	А	23	GLU	CD-OE2	-7.64	1.17	1.25
1	В	300	ARG	CZ-NH1	-7.58	1.23	1.33
1	А	52	ARG	CB-CG	-7.20	1.33	1.52
1	А	427	ARG	CZ-NH1	-7.14	1.23	1.33
1	В	98	LEU	CG-CD2	-6.85	1.26	1.51
1	В	79	LEU	CG-CD2	-6.85	1.26	1.51
1	В	23	GLU	CD-OE1	-6.74	1.18	1.25
1	В	363	ARG	CZ-NH1	-6.71	1.24	1.33
1	А	539	SER	CB-OG	-6.41	1.33	1.42
1	А	122	ARG	CB-CG	-6.21	1.35	1.52
1	А	30	GLU	CB-CG	-6.12	1.40	1.52
1	В	442	GLU	CB-CG	-6.11	1.40	1.52
1	В	52	ARG	CB-CG	-6.08	1.36	1.52
1	В	343	GLU	CB-CG	-5.98	1.40	1.52
1	А	42	VAL	CB-CG2	5.97	1.65	1.52
1	А	363	ARG	CZ-NH1	-5.89	1.25	1.33
1	А	291	ARG	CG-CD	-5.77	1.37	1.51
1	А	564	GLU	CB-CG	-5.57	1.41	1.52
1	А	124	LEU	CG-CD1	-5.40	1.31	1.51
1	А	119	GLU	CD-OE2	-5.39	1.19	1.25
1	В	533	LYS	CB-CG	-5.32	1.38	1.52
1	В	427	ARG	CZ-NH1	-5.29	1.26	1.33
1	А	79	LEU	CG-CD1	-5.28	1.32	1.51
1	А	641	LEU	CG-CD2	-5.25	1.32	1.51
2	Е	3	DA	C3'-O3'	-5.15	1.37	1.44
1	В	99	ASP	CA-CB	-5.08	1.42	1.53
1	В	285	GLU	CB-CG	-5.04	1.42	1.52

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	300	ARG	NE-CZ-NH1	-30.68	104.96	120.30
1	А	300	ARG	NE-CZ-NH2	22.17	131.39	120.30
1	В	300	ARG	NE-CZ-NH1	-19.97	110.32	120.30



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JAU	0

Mol	Chain	i previo	Type	Atoms	Z	$Observed(^{o})$	Idoal(0)
11101		225		NE CZ NII1	10.67	110.07	$\frac{1000}{1000}$
1	B	335	ARG	NE-CZ-NHI	-18.07	110.97	120.30
1	A	95	ARG	NE-CZ-NH2	-18.21	111.19	120.30
1	<u>В</u>	303	ARG	NE-CZ-NH2	10.13	128.30	120.30
1	A	427	ARG	NE-CZ-NH2	15.88	128.24	120.30
1	B	335	ARG	NE-CZ-NH2	14.91	127.75	120.30
1	В	52	ARG	CG-CD-NE	14.79	142.85	111.80
1	A	122	ARG	NE-CZ-NHI	14.77	127.68	120.30
1	B	13	ARG	CG-CD-NE	14.58	142.41	111.80
1	B	23	GLU	OEI-CD-OE2	-14.35	106.08	123.30
1	A	101	LYS	CD-CE-NZ	14.15	144.24	111.70
1	В	300	ARG	NE-CZ-NH2	13.88	127.24	120.30
1	A	335	ARG	NE-CZ-NH2	13.60	127.10	120.30
1	В	628	LEU	CB-CG-CD2	-13.40	88.22	111.00
1	А	13	ARG	CG-CD-NE	12.98	139.06	111.80
1	А	52	ARG	CG-CD-NE	12.88	138.84	111.80
1	А	641	LEU	CB-CG-CD1	12.78	132.73	111.00
1	А	23	GLU	OE1-CD-OE2	-12.72	108.04	123.30
1	В	300	ARG	CG-CD-NE	12.60	138.26	111.80
1	А	427	ARG	NE-CZ-NH1	-12.60	114.00	120.30
1	А	95	ARG	NE-CZ-NH1	12.53	126.56	120.30
1	В	628	LEU	CB-CG-CD1	12.01	131.42	111.00
1	В	99	ASP	CB-CG-OD1	11.96	129.07	118.30
1	А	335	ARG	NE-CZ-NH1	-11.61	114.50	120.30
1	А	363	ARG	NE-CZ-NH2	11.35	125.97	120.30
1	В	502	LEU	CB-CG-CD2	-11.16	92.03	111.00
1	В	611	ARG	NE-CZ-NH1	-10.85	114.87	120.30
1	А	300	ARG	CG-CD-NE	10.74	134.36	111.80
1	В	95	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	А	291	ARG	CA-CB-CG	10.66	136.85	113.40
1	В	30	GLU	CA-CB-CG	10.34	136.15	113.40
1	В	300	ARG	CB-CG-CD	-10.19	85.10	111.60
1	А	420	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	В	79	LEU	CB-CG-CD1	10.05	128.09	111.00
1	А	99	ASP	CB-CG-OD2	-9.63	109.63	118.30
1	В	122	ARG	CB-CA-C	-9.38	91.64	110.40
1	В	641	LEU	CD1-CG-CD2	-9.34	82.49	110.50
1	А	25	ARG	NE-CZ-NH1	-9.13	115.74	120.30
1	В	427	ARG	NE-CZ-NH2	9.00	124.80	120.30
1	А	297	ILE	CG1-CB-CG2	-8.82	92.00	111.40
1	А	611	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	В	23	GLU	CG-CD-OE1	8.65	135.60	118.30
1	В	95	ARG	NE-CZ-NH2	-8.56	116.02	120.30

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Mol	Chain	l prevu	Type	Atoms	7	Observed <sup>(0)</sup>	$\mathbf{Ideal}^{(0)}$
1		110			<b>2</b>	120.45	111 90
1	A D	410 201	IFU	CA CP CC	0.40	129.40	111.00
1		201		NE CZ NH1	-0.39	90.00	110.00
1	A	291 12	ANG	NE-CZ-NH1	-0.20	110.17	120.30
1	A D	10	ANG	NE-CZ-NH1	-0.20	110.10	120.30
1		20	ANG	CC CD NE	-0.13	04.88	120.30
1	A D	20 12	ANG	CB-CD-NE	-0.00	94.00	111.00
1		10	ARG	CA CP CC	-8.04	90.08	111.00
1	A D	120	ANG	NE CZ NH2	7.90	130.92	110.40
1	D	15	IFU	$\frac{\text{NE-CZ-NH2}}{\text{CP-CC-CD2}}$	-1.89	07.00	120.30 111.00
1		192		CC CD NE	-1.11	97.90	111.00
1	A	123	IFU	CR-CD-NE	7.42	127.09	111.80
1	A	98	CLU	CB-CG-CD2	7.43	123.03	111.00
1	B	119	GLU	UA-UB-UG	-1.43	97.00	113.40
	A	420	ARG	NE-CZ-NHI	7.24	124.00	120.30
1	A	125	GLU	C-N-CA	7.34	137.72	122.30
1	B	42	VAL	CGI-CB-CG2	7.31	122.60	110.90
1	В	30	GLU	N-CA-CB	7.28	123.70	110.60
1	A	533	LYS	CB-CG-CD	7.25	130.44	111.60
1	B	13	ARG	CD-NE-CZ	7.24	133.73	123.60
1	В	611	ARG	NE-CZ-NH2	7.09	123.84	120.30
1	A	124	LEU	CB-CG-CD1	-7.08	98.96	111.00
1	A	123	ARG	N-CA-CB	-6.91	98.17	110.60
1	A	425	LEU	CB-CG-CD1	6.87	122.67	111.00
1	A	288	ARG	NE-CZ-NH1	-6.87	116.87	120.30
1	В	99	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	А	45	LEU	CB-CG-CD2	-6.78	99.48	111.00
1	А	13	ARG	CD-NE-CZ	-6.74	114.16	123.60
1	В	30	GLU	CB-CG-CD	-6.71	96.09	114.20
1	А	13	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	А	356	GLY	N-CA-C	-6.69	96.37	113.10
2	С	4	DG	O4'-C4'-C3'	-6.68	101.83	104.50
1	А	29	LEU	CA-CB-CG	6.55	130.36	115.30
1	А	611	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	В	119	GLU	CB-CG-CD	6.47	131.67	114.20
1	A	122	ARG	NH1-CZ-NH2	-6.44	112.31	119.40
2	Е	12	DG	C1'-O4'-C4'	-6.42	103.68	110.10
1	А	418	ARG	CD-NE-CZ	6.41	132.58	123.60
1	В	25	ARG	CG-CD-NE	-6.41	98.34	111.80
1	В	29	LEU	CA-CB-CG	6.40	130.03	115.30
1	А	25	ARG	NE-CZ-NH2	6.39	123.49	120.30
1	А	99	ASP	CB-CG-OD1	6.37	124.03	118.30
1	В	98	LEU	CB-CG-CD2	6.35	121.79	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed <sup>(o)</sup>	Ideal(°)
1	Δ	420	ARG	CG-CD-NE	-6.29	98.59	111 80
1	Δ	30	GLU	CA-CB-CG	6.26	127.17	113.40
1	B	$\frac{50}{25}$	ARG	NE-CZ-NH2	6.25	123.42	120.30
1	A	539	SER	N-CA-CB	-6.24	101 13	110.50
1	Δ	574	ARG	NE-CZ-NH1	-6.24	101.10	120.30
1	Δ	23	GLU	CG-CD-OE1	6.13	130.55	120.00
1	Δ	<u> </u>	GLU	CA-CB-CG	6.13	126.88	113.00
1	B	513	ARG	CG-CD-NE	-6.12	08.05	111.40
1	Δ	628	LEU	CA-CB-CG	-6.12	101.25	115.30
1	Δ	486	ARG	CA-CB-CG	6.04	101.25	113.00
1	B	363	ARC	NH1 CZ NH2	6.01	112 70	110.40
1	Δ	303	CLU	$\frac{\text{CB} \text{CA} \text{C}}{\text{CB} \text{CA} \text{C}}$	-0.01	08.55	119.40
1		50		CA CB CC	-5.92	98.00	110.40
1	A	- <u>5</u> 2 - 200	ARG	CA-CD-CG	5.80	00.54	113.40
1	A	299	IFU	CB CC CD1	-5.84	99.04	111.00
1	A D	90		CC CD NE	5.04	120.92	111.00
1		291	IFU	CB-CD-NE	5.81	124.01	111.00
1	A	309		CD-CG-CD2	-3.80	101.14	111.00
1	A	124		CR-CD-CG	-0.78	102.00	110.30 111.70
1	B	93		CD-CE-NZ	0.78 E 77	124.99	111.70
1	В	40		CB-CG-CD2	-0.11	101.19	111.00
1	A	$\frac{513}{101}$	AKG	CG-CD-NE	-0.11	99.09	111.80
1	B	101		CD-CE-NZ	5.70	124.90	111.70
1	A	52	ARG	CB-CA-C	5.70	121.92	110.40
1	A	122	ARG	CB-CA-C	-0.74	98.92	110.40
1	A	95	ARG	CD-NE-CZ	-5.72	115.00	123.00
2	E	11	DA	$04^{\circ}-01^{\circ}-N9$	5.69	111.98	108.00
1	В	580	ARG	NE-CZ-NH2	-5.04	117.48	120.30
1	A	123	ARG	NE-CZ-NHI	-5.58	117.51	120.30
1	B	300	LEU	CB-CG-CD2	-5.57	101.53	111.00
1	В	028		$\frac{\text{ODI-UG-UD2}}{\text{OD} \text{ OD} \text{ OD}}$	-5.51	93.98	110.50
1	A	- 52 - 19	ARG	O42 O12 NO	5.50	125.90	111.00
1		12		O4 - O1 - N9	5.49	111.84	108.00
1	A	110		OB-OG-OD2	5.49	120.33	111.00
1	В	285	GLU	UB-UA-U	0.48	121.30	110.40
1	A	080 005	AKG	NE-UZ-NH2	-5.45		120.30
1	В	285	GLU	OEI-OD-OE2	-5.42	110.80	123.30
1	A	309	VAL	UA-UB-UGI	5.38	118.98	110.90
1	A	291	AKG	NE-CZ-NH2	5.38	122.99	120.30
	B	533		CB-CG-CD	5.36	125.53	111.60
	B	98		$\frac{\text{CD1-CG-CD2}}{\text{CD1-CG-CD2}}$	-5.35	94.45	110.50
3		12	DC	$04^{\prime}-04^{\prime}-03^{\prime}$	-5.35	102.36	104.50
1	B	119	GLU	CG-CD-OE2	-5.33	107.63	118.30

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Mol	Chain	$\operatorname{Res}$	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
1	А	25	ARG	CD-NE-CZ	5.32	131.05	123.60
1	А	612	GLY	N-CA-C	-5.30	99.85	113.10
1	А	13	ARG	CB-CG-CD	5.29	125.34	111.60
1	В	52	ARG	CB-CG-CD	5.26	125.27	111.60
1	В	288	ARG	CB-CA-C	-5.24	99.92	110.40
1	В	122	ARG	CA-CB-CG	5.21	124.85	113.40
1	В	384	HIS	C-N-CD	5.20	139.32	128.40
1	В	342	GLN	CB-CA-C	5.19	120.77	110.40
1	А	427	ARG	NH1-CZ-NH2	-5.18	113.70	119.40
1	А	564	GLU	CA-CB-CG	5.18	124.79	113.40
1	В	300	ARG	N-CA-CB	-5.15	101.33	110.60
1	А	25	ARG	CB-CG-CD	5.15	124.98	111.60
2	С	12	DG	O4'-C1'-N9	5.13	111.59	108.00
1	А	384	HIS	C-N-CD	5.11	139.12	128.40
1	В	427	ARG	CG-CD-NE	5.08	122.48	111.80
1	А	164	LEU	CA-CB-CG	-5.05	103.67	115.30
1	В	343	GLU	N-CA-CB	-5.04	101.53	110.60
1	А	392	ARG	NE-CZ-NH1	-5.03	117.79	120.30
1	А	590	ASP	CB-CG-OD2	-5.02	113.78	118.30
2	С	15	DT	N3-C4-O4	5.02	122.91	119.90
1	В	146	ARG	CB-CA-C	-5.01	100.38	110.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	312	GLN	Sidechain
1	А	39	ARG	Mainchain
1	А	99	ASP	Sidechain
1	В	285	GLU	Sidechain
1	В	312	GLN	Sidechain
1	В	533	LYS	Mainchain
1	В	548	ARG	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	А	4373	0	4421	137	0
1	В	4435	0	4461	132	1
2	С	295	0	162	5	0
2	Е	338	0	183	11	0
3	D	317	0	181	7	0
3	F	317	0	181	6	0
4	А	1	0	0	0	0
4	В	1	0	0	0	0
5	А	5	0	0	0	0
5	В	11	0	0	2	0
5	Е	2	0	0	0	0
5	F	1	0	0	0	0
All	All	10096	0	9589	284	1

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 15.

All (284) 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 $(\text{\AA})$	overlap (Å)
1:A:119:GLU:OE2	1:A:122:ARG:NH2	1.87	1.06
1:A:124:LEU:HD23	1:A:300:ARG:HD3	1.35	1.06
1:A:25:ARG:CZ	1:A:95:ARG:HH22	1.72	1.03
1:A:513:ARG:NH2	1:A:551:GLN:O	1.94	1.00
1:B:119:GLU:OE2	1:B:122:ARG:NH2	1.96	0.97
1:A:124:LEU:CD2	1:A:300:ARG:HD3	2.01	0.91
1:A:128:TRP:HD1	1:A:135:TYR:HD2	1.16	0.91
1:B:513:ARG:NH2	1:B:551:GLN:O	2.02	0.90
1:A:124:LEU:N	1:A:124:LEU:HD12	1.83	0.90
1:B:128:TRP:HD1	1:B:135:TYR:HD2	1.10	0.90
1:B:100:PRO:O	1:B:106:ARG:HG3	1.74	0.88
1:B:128:TRP:HD1	1:B:135:TYR:CD2	1.92	0.88
1:A:101:LYS:HA	1:A:159:ASP:OD1	1.75	0.86
1:A:99:ASP:OD2	1:A:101:LYS:HE3	1.77	0.84
1:A:119:GLU:CD	1:A:122:ARG:HH21	1.80	0.84
1:A:128:TRP:HD1	1:A:135:TYR:CD2	1.99	0.81
1:A:119:GLU:HG3	1:A:122:ARG:HH21	1.46	0.80
1:A:119:GLU:CG	1:A:122:ARG:HH21	1.95	0.79
1:B:27:TRP:HA	1:B:95:ARG:HG2	1.62	0.79
1:B:128:TRP:CD1	1:B:135:TYR:HD2	1.98	0.79
1:A:53:ALA:HA	1:A:74:VAL:HG23	1.63	0.79
1:B:35:PRO:HD2	1:B:86:TYR:HD1	1.49	0.77



	A L O	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:590:ASP:OD2	3:D:19:DG:N1	2.16	0.77	
2:E:9:DG:H2"	2:E:10:DT:H5"	1.65	0.76	
1:A:604:LEU:HD11	1:A:614:PRO:HB2	1.68	0.76	
1:A:500:HIS:CE1	1:A:533:LYS:HE2	2.21	0.75	
1:B:145:TRP:HA	1:B:175:CYS:HA	1.68	0.75	
1:B:158:SER:HB3	1:B:164:LEU:HD21	1.68	0.74	
1:A:128:TRP:CD1	1:A:135:TYR:HD2	2.04	0.72	
1:B:580:ARG:NH2	2:E:7:DA:OP2	2.22	0.72	
1:B:583:PRO:HD3	1:B:588:LEU:HD13	1.71	0.72	
1:A:598:ASP:O	1:A:599:LYS:HB2	1.89	0.71	
1:B:171:TYR:OH	1:B:289:ARG:NH1	2.22	0.71	
2:E:11:DA:H1'	2:E:12:DG:H5'	1.73	0.71	
1:A:583:PRO:HD3	1:A:588:LEU:HD13	1.72	0.70	
1:B:128:TRP:CD1	1:B:135:TYR:CD2	2.76	0.70	
1:A:129:VAL:HG22	1:A:134:VAL:HG12	1.75	0.69	
1:B:25:ARG:NH2	1:B:95:ARG:HH22	1.90	0.69	
1:B:427:ARG:CB	1:B:427:ARG:HH11	2.04	0.69	
1:B:102:ASP:HB3	1:B:105:GLU:HG3	1.75	0.69	
1:A:45:LEU:HD21	1:A:86:TYR:CE2	2.28	0.69	
1:A:35:PRO:HG2	1:A:86:TYR:HE1	1.58	0.68	
1:B:25:ARG:CZ	1:B:95:ARG:HH22	2.06	0.68	
1:A:25:ARG:CZ	1:A:95:ARG:NH2	2.53	0.68	
1:B:45:LEU:HD21	1:B:86:TYR:CE2	2.30	0.67	
1:B:461:GLN:HG3	1:B:499:GLY:O	1.95	0.67	
1:A:128:TRP:CD1	1:A:135:TYR:CD2	2.81	0.67	
1:B:136:ARG:NH2	1:B:293:ILE:HG23	2.10	0.67	
1:B:129:VAL:HG22	1:B:134:VAL:HG12	1.76	0.66	
1:B:35:PRO:HD2	1:B:86:TYR:CD1	2.30	0.66	
1:A:109:LEU:HB3	1:A:157:VAL:HG21	1.76	0.66	
1:B:49:VAL:HG22	1:B:79:LEU:HD21	1.76	0.66	
1:A:41:GLU:O	1:A:45:LEU:HB2	1.96	0.65	
1:A:82:MET:O	1:A:84:GLN:N	2.30	0.65	
1:B:640:ARG:NH1	1:B:649:PHE:CD2	2.62	0.65	
1:A:124:LEU:HD23	1:A:300:ARG:CD	2.22	0.65	
1:B:427:ARG:O	5:B:801:HOH:O	2.15	0.65	
1:A:295:SER:HA	1:A:306:PRO:HG3	1.79	0.64	
1:B:101:LYS:O	1:B:103:PRO:HD3	1.97	0.64	
1:B:35:PRO:HG2	1:B:86:TYR:HE1	1.63	0.63	
1:A:27:TRP:HA	1:A:95:ARG:HG2	1.79	0.63	
1:B:607:HIS:ND1	1:B:614:PRO:HG3	2.13	0.63	
1:B:44:PRO:HB3	3:F:4:DA:C8	2.33	0.63	



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Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:340:ARG:HH22	1:B:500:HIS:HD2	1.46	0.62	
1:B:641:LEU:O	1:B:641:LEU:HD23	2.00	0.62	
1:B:25:ARG:HG3	1:B:25:ARG:O	2.00	0.62	
1:A:640:ARG:NH1	1:A:649:PHE:CD2	2.67	0.62	
2:E:4:DG:H2'	2:E:5:DG:C8	2.35	0.62	
1:B:98:LEU:HD22	1:B:105:GLU:HB3	1.80	0.61	
1:B:340:ARG:NH2	1:B:500:HIS:HD2	1.99	0.61	
1:B:426:LEU:HD22	1:B:677:VAL:HG21	1.81	0.61	
1:B:136:ARG:NH2	1:B:297:ILE:HD12	2.16	0.61	
1:A:461:GLN:HG3	1:A:499:GLY:O	2.01	0.60	
1:A:44:PRO:HB3	3:D:4:DA:C8	2.36	0.60	
1:B:106:ARG:HD2	1:B:157:VAL:O	2.01	0.60	
1:A:35:PRO:HD2	1:A:86:TYR:HD1	1.66	0.59	
1:B:499:GLY:O	1:B:500:HIS:CD2	2.55	0.59	
1:A:35:PRO:HG2	1:A:86:TYR:CE1	2.38	0.59	
1:A:531:ARG:HD2	1:A:531:ARG:O	2.03	0.59	
1:A:45:LEU:HD21	1:A:86:TYR:CD2	2.38	0.59	
1:A:82:MET:C	1:A:84:GLN:H	2.06	0.59	
1:B:155:LEU:HD13	1:B:165:LEU:HD13	1.85	0.58	
1:A:119:GLU:HG3	1:A:122:ARG:NH2	2.16	0.58	
1:A:102:ASP:OD1	1:A:103:PRO:HD2	2.03	0.58	
1:B:121:LEU:HD11	1:B:153:LEU:HD12	1.84	0.58	
1:A:426:LEU:HD22	1:A:677:VAL:HG21	1.86	0.57	
1:B:340:ARG:NH2	1:B:500:HIS:CD2	2.72	0.57	
1:A:465:LEU:HG	1:A:641:LEU:CD1	2.35	0.56	
1:A:155:LEU:HD13	1:A:165:LEU:HD13	1.87	0.56	
1:B:295:SER:HA	1:B:306:PRO:HG3	1.87	0.56	
1:A:502:LEU:CD2	1:A:680:GLU:HG3	2.36	0.56	
1:A:502:LEU:HD21	1:A:680:GLU:HG3	1.88	0.56	
1:A:531:ARG:HD2	1:A:531:ARG:C	2.25	0.56	
1:B:25:ARG:NH2	1:B:95:ARG:NH2	2.53	0.55	
1:B:31:VAL:HG22	1:B:90:LEU:HD22	1.88	0.55	
1:B:117:LEU:O	1:B:121:LEU:HG	2.06	0.55	
1:A:120:ARG:O	1:A:124:LEU:CD1	2.54	0.55	
1:A:329:LYS:HD3	3:D:19:DG:H3'	1.88	0.55	
1:B:120:ARG:HB3	1:B:301:LEU:CD2	2.36	0.55	
1:B:291:ARG:HH11	1:B:291:ARG:HG2	1.71	0.55	
1:A:151:ALA:HB2	1:A:293:ILE:HD13	1.88	0.55	
1:B:502:LEU:HD21	1:B:680:GLU:HG3	1.88	0.55	
1:A:119:GLU:HA	1:A:122:ARG:HE	1.72	0.55	
1:B:500:HIS:ND1	1:B:533:LYS:HG2	2.21	0.54	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:377:ARG:NH2	1:B:379:HIS:NE2	2.55	0.54	
1:A:580:ARG:NH2	2:C:7:DA:OP2	2.41	0.54	
1:B:20:ASN:OD1	1:B:22:GLU:HB2	2.06	0.54	
1:B:35:PRO:HG2	1:B:86:TYR:CE1	2.43	0.53	
1:A:598:ASP:O	1:A:599:LYS:CB	2.55	0.53	
1:A:120:ARG:O	1:A:124:LEU:HD11	2.09	0.53	
1:A:135:TYR:HA	1:A:150:GLY:HA3	1.90	0.53	
1:A:499:GLY:C	1:A:500:HIS:CD2	2.82	0.53	
1:B:500:HIS:CE1	1:B:533:LYS:HG2	2.43	0.53	
1:A:121:LEU:HA	1:A:124:LEU:HD13	1.91	0.52	
2:E:12:DG:H2"	2:E:13:DG:H8	1.74	0.52	
1:A:335:ARG:HH11	1:A:335:ARG:CG	2.21	0.52	
1:B:109:LEU:HB2	1:B:157:VAL:HG21	1.91	0.52	
1:B:449:ASN:ND2	2:E:3:DA:O4'	2.43	0.52	
1:B:18:PRO:HA	1:B:162:ALA:HA	1.92	0.51	
1:B:350:ARG:HD2	1:B:352:ASP:OD1	2.10	0.51	
1:A:431:PRO:HB2	1:A:457:LYS:HB3	1.92	0.51	
1:A:22:GLU:OE1	1:A:25:ARG:NH1	2.43	0.51	
1:A:25:ARG:O	1:A:25:ARG:HG3	2.09	0.51	
1:A:575:LYS:HB3	1:A:651:ARG:NH2	2.25	0.51	
1:A:119:GLU:CD	1:A:122:ARG:NH2	2.49	0.51	
1:B:335:ARG:HH21	1:B:444:ARG:NH1	2.09	0.51	
1:B:575:LYS:HB3	1:B:651:ARG:NH2	2.26	0.50	
1:A:350:ARG:HD2	1:A:352:ASP:OD1	2.11	0.50	
1:B:171:TYR:OH	1:B:281:LEU:HD21	2.11	0.50	
1:A:27:TRP:CZ2	1:A:95:ARG:NH1	2.80	0.50	
1:B:106:ARG:HD2	1:B:157:VAL:HG23	1.93	0.50	
1:B:427:ARG:HH11	1:B:427:ARG:HB3	1.74	0.50	
1:B:621:HIS:CE1	1:B:631:LEU:HD11	2.47	0.50	
1:A:27:TRP:CE2	1:A:95:ARG:NE	2.79	0.50	
1:B:432:SER:O	1:B:457:LYS:HE3	2.12	0.50	
1:B:377:ARG:NH2	1:B:379:HIS:CE1	2.80	0.49	
1:A:500:HIS:HE1	1:A:533:LYS:HE2	1.72	0.49	
1:B:45:LEU:HD21	1:B:86:TYR:CD2	2.47	0.49	
1:A:26:PRO:O	1:A:95:ARG:HB3	2.11	0.49	
1:A:427:ARG:HD3	1:A:673:HIS:ND1	2.27	0.49	
1:B:29:LEU:HD13	1:B:92:PRO:HA	1.94	0.49	
1:B:117:LEU:HB2	1:B:155:LEU:HD22	1.95	0.49	
1:B:531:ARG:HD2	1:B:531:ARG:O	2.13	0.49	
1:B:297:ILE:O	1:B:301:LEU:HB2	2.13	0.48	
1:A:300:ARG:HG3	1:A:300:ARG:O	2.08	0.48	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:465:LEU:HG	1:A:641:LEU:HD13	1.95	0.48	
1:A:115:ARG:HG3	1:A:119:GLU:OE1	2.13	0.48	
1:A:20:ASN:HB2	1:A:21:PRO:HD2	1.95	0.48	
1:B:120:ARG:HB3	1:B:301:LEU:HD21	1.95	0.48	
1:A:79:LEU:HD12	1:A:88:TYR:HD2	1.79	0.48	
1:B:119:GLU:HG2	1:B:122:ARG:HH21	1.79	0.48	
1:B:115:ARG:O	1:B:119:GLU:HG3	2.14	0.47	
1:B:52:ARG:HG3	1:B:79:LEU:CD1	2.43	0.47	
1:A:321:LEU:HD22	1:A:463:VAL:HB	1.96	0.47	
1:A:449:ASN:ND2	2:C:2:DG:H21	2.12	0.47	
1:A:636:PHE:HE1	1:A:640:ARG:HH21	1.60	0.47	
1:B:99:ASP:OD1	1:B:101:LYS:HG3	2.14	0.47	
1:A:501:LEU:HD21	1:A:641:LEU:CD2	2.45	0.47	
1:A:13:ARG:HA	1:A:165:LEU:O	2.14	0.47	
3:F:4:DA:H2"	3:F:5:DC:H5'	1.97	0.47	
1:B:345:ALA:HA	1:B:377:ARG:O	2.15	0.47	
2:E:10:DT:H2'	2:E:11:DA:C8	2.49	0.47	
1:B:321:LEU:HD22	1:B:463:VAL:HB	1.95	0.47	
1:B:399:LYS:HG2	1:B:430:LEU:HD21	1.96	0.47	
1:A:16:LEU:HD11	1:A:165:LEU:HD22	1.97	0.46	
1:B:545:ARG:HG2	1:B:549:VAL:HG22	1.96	0.46	
1:B:19:LEU:HD11	1:B:157:VAL:HG12	1.98	0.46	
1:A:340:ARG:HH22	1:A:461:GLN:HG3	1.81	0.46	
1:B:319:PRO:HG3	1:B:640:ARG:HG3	1.98	0.46	
1:B:102:ASP:CB	1:B:105:GLU:HG3	2.43	0.45	
1:A:25:ARG:NH2	1:A:95:ARG:HH22	2.11	0.45	
1:A:99:ASP:CG	1:A:101:LYS:HG3	2.36	0.45	
1:B:25:ARG:CZ	1:B:95:ARG:NH2	2.75	0.45	
1:B:53:ALA:O	1:B:74:VAL:HG23	2.17	0.45	
1:B:679:ARG:NH2	5:B:802:HOH:O	2.27	0.45	
1:A:104:GLY:O	1:A:107:SER:N	2.50	0.45	
1:A:465:LEU:HG	1:A:641:LEU:HD12	1.98	0.45	
1:B:98:LEU:HA	1:B:105:GLU:OE2	2.17	0.45	
1:B:89:ARG:HD3	1:B:91:TYR:CZ	2.52	0.45	
1:A:35:PRO:HD2	1:A:86:TYR:CD1	2.49	0.45	
1:A:473:LEU:HB3	1:A:541:VAL:HG12	1.99	0.45	
1:B:99:ASP:OD2	1:B:101:LYS:HE2	2.16	0.45	
1:A:26:PRO:HD2	1:A:96:ARG:O	2.17	0.45	
1:A:284:GLU:H	1:A:284:GLU:HG2	1.39	0.45	
1:B:41:GLU:O	1:B:44:PRO:HG2	2.17	0.45	
1:B:145:TRP:O	1:B:146:ARG:HB2	2.17	0.45	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:158:SER:HB3	1:A:164:LEU:CD1	2.46	0.45	
1:B:462:VAL:HG12	1:B:463:VAL:HG13	1.98	0.45	
1:A:476:GLY:O	1:A:490:ALA:HA	2.17	0.44	
1:A:499:GLY:O	1:A:500:HIS:CD2	2.70	0.44	
1:A:98:LEU:HD23	1:A:105:GLU:O	2.16	0.44	
2:C:3:DA:H2'	2:C:4:DG:C8	2.53	0.44	
1:B:381:LEU:HD21	1:B:398:ALA:HB2	1.98	0.44	
1:B:128:TRP:HB3	1:B:135:TYR:HB2	2.00	0.44	
1:A:31:VAL:HG22	1:A:90:LEU:HD22	1.99	0.44	
1:B:89:ARG:HD3	1:B:91:TYR:OH	2.17	0.44	
1:B:154:ASP:O	1:B:165:LEU:HD12	2.17	0.44	
1:A:576:SER:O	3:D:8:DC:H5'	2.17	0.44	
1:B:319:PRO:HB3	1:B:637:HIS:CG	2.53	0.44	
1:B:431:PRO:HB2	1:B:457:LYS:HB3	2.00	0.44	
1:B:27:TRP:CZ2	1:B:95:ARG:NH1	2.78	0.44	
3:D:9:DC:H2"	3:D:10:DT:H5'	1.99	0.44	
1:A:327:VAL:HB	1:A:332:ASP:HB2	2.00	0.43	
1:A:621:HIS:CE1	1:A:631:LEU:HD11	2.53	0.43	
1:A:79:LEU:CD1	1:A:88:TYR:CD2	3.01	0.43	
1:A:82:MET:C	1:A:84:GLN:N	2.72	0.43	
1:A:446:ARG:HG3	2:C:2:DG:C8	2.53	0.43	
1:A:329:LYS:HB3	3:D:19:DG:H3'	2.00	0.43	
1:B:473:LEU:HB3	1:B:541:VAL:HG12	2.00	0.43	
1:A:656:LEU:HD23	1:A:656:LEU:HA	1.80	0.43	
1:B:457:LYS:HZ3	1:B:685:VAL:HG22	1.83	0.43	
1:A:22:GLU:CD	1:A:25:ARG:NH1	2.72	0.43	
1:A:27:TRP:CZ2	1:A:69:PRO:HB3	2.53	0.43	
1:A:432:SER:O	1:A:457:LYS:HE3	2.18	0.43	
1:A:44:PRO:HB3	3:D:4:DA:N7	2.34	0.43	
1:B:60:MET:HE2	1:B:65:ALA:HB2	2.01	0.43	
1:B:98:LEU:CD2	1:B:105:GLU:HB3	2.49	0.43	
1:B:136:ARG:NH2	1:B:297:ILE:CD1	2.81	0.43	
1:B:313:ALA:HB1	1:B:592:LEU:HD22	2.01	0.43	
1:A:124:LEU:HD21	1:A:300:ARG:HD3	1.97	0.43	
1:B:106:ARG:CD	1:B:157:VAL:O	2.66	0.43	
1:A:640:ARG:HD3	1:A:649:PHE:CD2	2.54	0.43	
3:F:9:DC:H2"	3:F:10:DT:H5'	2.01	0.43	
1:A:300:ARG:HH11	1:A:300:ARG:HD2	1.36	0.42	
1:B:20:ASN:HB2	1:B:21:PRO:HD2	2.01	0.42	
1:B:73:LEU:HA	1:B:73:LEU:HD23	1.73	0.42	
2:E:3:DA:H2'	2:E:4:DG:C8	2.55	0.42	



	louo pugom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:104:GLY:C	1:A:106:ARG:N	2.72	0.42	
1:A:537:LEU:HD13	1:A:566:ILE:HD11	2.00	0.42	
1:A:119:GLU:O	1:A:122:ARG:HG3	2.19	0.42	
1:A:410:THR:O	1:A:436:ASN:HA	2.20	0.42	
1:B:150:GLY:O	1:B:169:PRO:HA	2.20	0.42	
1:B:329:LYS:HD3	3:F:19:DG:H3'	2.01	0.42	
1:B:427:ARG:HH11	1:B:427:ARG:HB2	1.84	0.42	
1:A:285:GLU:HG3	1:A:288:ARG:HH21	1.84	0.42	
2:C:1:DT:H5'	2:C:2:DG:H3'	2.01	0.42	
1:A:117:LEU:O	1:A:121:LEU:HG	2.20	0.41	
1:A:473:LEU:HD23	1:A:541:VAL:CG1	2.50	0.41	
1:A:607:HIS:ND1	1:A:614:PRO:HD3	2.35	0.41	
1:B:136:ARG:CZ	1:B:296:TRP:CE3	3.03	0.41	
1:B:119:GLU:CD	1:B:122:ARG:NH2	2.71	0.41	
1:B:96:ARG:HE	1:B:96:ARG:HB2	1.68	0.41	
1:B:425:LEU:HD22	1:B:432:SER:HB3	2.02	0.41	
1:B:505:LEU:HD12	1:B:505:LEU:HA	1.91	0.41	
2:E:10:DT:O4	2:E:11:DA:N6	2.54	0.41	
3:F:15:DC:H2'	3:F:16:DC:C6	2.55	0.41	
1:A:345:ALA:HA	1:A:377:ARG:O	2.20	0.41	
1:A:486:ARG:HH11	1:A:486:ARG:HG3	1.85	0.41	
1:B:25:ARG:O	1:B:95:ARG:HD3	2.20	0.41	
1:A:338:PHE:CZ	1:A:455:LEU:HD13	2.55	0.41	
1:B:503:TRP:CE2	1:B:679:ARG:HA	2.55	0.41	
1:B:604:LEU:HD11	1:B:614:PRO:CB	2.51	0.41	
1:A:29:LEU:HD13	1:A:92:PRO:HA	2.01	0.41	
1:A:385:PRO:HA	1:A:391:PHE:CG	2.55	0.41	
1:B:651:ARG:HB2	2:E:5:DG:H5"	2.03	0.41	
1:A:60:MET:HE2	1:A:60:MET:HB3	1.87	0.41	
1:A:79:LEU:CD1	1:A:88:TYR:HD2	2.33	0.41	
1:A:115:ARG:O	1:A:119:GLU:HB2	2.20	0.41	
1:A:121:LEU:HD11	1:A:153:LEU:HD12	2.03	0.41	
1:A:312:GLN:HE21	1:A:312:GLN:HB2	1.26	0.41	
1:A:479:ALA:HA	1:A:487:PHE:O	2.21	0.41	
1:B:20:ASN:HB2	1:B:21:PRO:CD	2.51	0.41	
1:B:110:SER:OG	1:B:156:TRP:HB2	2.20	0.41	
1:B:134:VAL:O	1:B:150:GLY:HA3	2.21	0.41	
1:B:155:LEU:HD13	1:B:165:LEU:CD1	2.50	0.41	
1:B:318:ILE:H	1:B:318:ILE:HD12	1.86	0.41	
1:B:410:THR:O	1:B:436:ASN:HA	2.20	0.41	
3:F:12:DC:H2'	3:F:13:DT:H6	1.86	0.41	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:651:ARG:HH11	1:A:651:ARG:HD2	1.66	0.40
1:B:120:ARG:HB3	1:B:301:LEU:HD22	2.02	0.40
1:B:338:PHE:CZ	1:B:455:LEU:HD13	2.55	0.40
2:E:6:DT:H2"	2:E:7:DA:C8	2.56	0.40
1:A:8:GLU:O	1:A:584:VAL:HG23	2.21	0.40
1:A:350:ARG:HD3	1:A:409:LEU:HD12	2.02	0.40
1:A:503:TRP:CE2	1:A:679:ARG:HA	2.57	0.40
1:A:164:LEU:HA	1:A:164:LEU:HD23	1.73	0.40
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.39	0.40
1:B:13:ARG:O	1:B:309:VAL:HG23	2.21	0.40
1:B:168:ASP:OD2	1:B:580:ARG:NH1	2.51	0.40
1:A:425:LEU:HD22	1:A:432:SER:HB3	2.03	0.40
1:A:545:ARG:HG2	1:A:549:VAL:HG22	2.03	0.40
1:A:604:LEU:HD12	1:A:604:LEU:HA	1.88	0.40
1:B:31:VAL:HG22	1:B:90:LEU:CD2	2.52	0.40
1:B:476:GLY:O	1:B:490:ALA:HA	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ARG:NH1	$1:B:563:ARG:O[4_455]$	1.93	0.27

## 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	Perce	ntiles
1	А	558/685~(82%)	541 (97%)	14 (2%)	3 (0%)	29	43
1	В	568/685~(83%)	554 (98%)	12 (2%)	2(0%)	34	48
All	All	1126/1370 (82%)	1095 (97%)	26~(2%)	5 (0%)	34	48



All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	355	GLN
1	В	355	GLN
1	А	83	GLY
1	В	146	ARG
1	А	597	GLU

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	А	427/549~(78%)	396~(93%)	31 (7%)	14 21		
1	В	429/549~(78%)	400 (93%)	29 (7%)	16 24		
All	All	856/1098~(78%)	796~(93%)	60 (7%)	15 23		

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	6	LYS
1	А	28	ARG
1	А	52	ARG
1	А	74	VAL
1	А	78	THR
1	А	96	ARG
1	А	101	LYS
1	А	115	ARG
1	А	119	GLU
1	А	123	ARG
1	А	125	GLU
1	А	284	GLU
1	А	285	GLU
1	А	288	ARG
1	А	295	SER
1	А	297	ILE
1	А	300	ARG
1	А	307	GLU



R L D W I D E PDB TEIN DATA BANK

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Mol	Chain	Res	Type				
1	А	312	GLN				
1	А	335	ARG				
1	А	342	GLN				
1	А	377	ARG				
1	А	418	ARG				
1	А	425	LEU				
1	А	427	ARG				
1	А	531	ARG				
1	А	548	ARG				
1	А	570	LEU				
1	А	580	ARG				
1	А	628	LEU				
1	А	641	LEU				
1	В	13	ARG				
1	В	41	GLU				
1	В	42	VAL				
1	В	74	VAL				
1	В	78	THR				
1	В	79	LEU				
1	В	96	ARG				
1	В	101	LYS				
1	В	102	ASP				
1	В	106	ARG				
1	В	115	ARG				
1	В	284	GLU				
1	В	295	SER				
1	В	297	ILE				
1	В	300	ARG				
1	В	312	GLN				
1	В	321	LEU				
1	В	355	GLN				
1	В	377	ARG				
1	В	399	LYS				
1	В	427	ARG				
1	В	437	VAL				
1	В	442	GLU				
1	В	460	LEU				
1	В	504	THR				
1	В	540	ARG				
1	В	556	LEU				
1	В	628	LEU				
1	В	641	LEU				

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	312	GLN
1	А	500	HIS
1	В	500	HIS

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers (i)

There are no such residues in this entry.

### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	564/685~(82%)	0.59	56 (9%) 7 5	36, 65, 118, 151	0
1	В	574/685~(83%)	0.54	46 (8%) 12 9	37, 67, 116, 137	0
2	С	14/22~(63%)	-0.35	0 100 100	58, 67, 104, 116	0
2	Е	16/22~(72%)	-0.32	0 100 100	58, 73, 124, 131	0
3	D	16/19~(84%)	-0.58	0 100 100	66, 90, 110, 117	0
3	F	16/19~(84%)	-0.39	0 100 100	61, 93, 111, 116	0
All	All	1200/1452~(82%)	0.52	102 (8%) 10 8	36, 67, 117, 151	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	82	MET	8.8
1	В	81	ARG	7.4
1	В	103	PRO	6.3
1	В	136	ARG	6.2
1	А	86	TYR	5.4
1	А	300	ARG	5.2
1	В	79	LEU	5.1
1	А	98	LEU	5.0
1	А	39	ARG	4.9
1	А	82	MET	4.7
1	А	33	LEU	4.7
1	В	125	GLU	4.6
1	В	127	VAL	4.5
1	А	100	PRO	4.4
1	А	31	VAL	4.2
1	В	80	ALA	3.9
1	А	128	TRP	3.9
1	В	156	TRP	3.8
1	В	30	GLU	3.8



Mol	Chain	Res	Type	RSRZ
1	А	295	SER	3.6
1	А	79	LEU	3.6
1	А	37	PRO	3.6
1	В	107	SER	3.6
1	В	173	ILE	3.6
1	В	56	VAL	3.5
1	В	389	LEU	3.5
1	В	93	LYS	3.5
1	А	5	GLY	3.3
1	А	29	LEU	3.3
1	А	36	PRO	3.3
1	В	21	PRO	3.2
1	А	78	THR	3.2
1	В	451	LEU	3.2
1	А	307	GLU	3.1
1	А	604	LEU	3.1
1	В	108	VAL	3.1
1	А	64	LEU	3.1
1	А	408	VAL	3.1
1	В	144	GLY	3.1
1	А	147	VAL	3.1
1	А	301	LEU	3.0
1	А	677	VAL	3.0
1	А	303	LEU	3.0
1	А	592	LEU	2.9
1	В	164	LEU	2.8
1	А	49	VAL	2.8
1	А	87	ALA	2.8
1	В	19	LEU	2.8
1	В	288	ARG	2.8
1	А	108	VAL	2.8
1	В	315	ARG	2.6
1	A	38	GLY	2.6
1	В	146	ARG	2.6
1	А	389	LEU	2.5
1	В	133	ALA	2.5
1	А	451	LEU	2.5
1	A	10	PHE	2.5
1	А	69	PRO	2.5
1	A	297	ILE	2.5
1	В	134	VAL	2.4
1	А	123	ARG	2.4



Mol	Chain	Res	Type	RSRZ
1	В	45	LEU	2.4
1	В	415	TRP	2.4
1	В	109	LEU	2.4
1	А	127	VAL	2.4
1	В	588	LEU	2.3
1	В	101	LYS	2.3
1	А	281	LEU	2.3
1	В	341	ALA	2.3
1	А	67	TRP	2.3
1	А	28	ARG	2.3
1	В	279	LEU	2.3
1	А	296	TRP	2.3
1	А	45	LEU	2.3
1	А	161	GLY	2.2
1	В	128	TRP	2.2
1	А	155	LEU	2.2
1	А	596	LEU	2.2
1	В	594	VAL	2.2
1	В	592	LEU	2.2
1	В	360	PHE	2.2
1	А	409	LEU	2.2
1	А	395	LEU	2.2
1	В	581	VAL	2.2
1	А	148	LEU	2.2
1	А	346	LEU	2.2
1	В	75	LEU	2.1
1	В	303	LEU	2.1
1	А	541	VAL	2.1
1	А	90	LEU	2.1
1	А	430	LEU	2.1
1	А	132	LEU	2.1
1	В	455	LEU	2.1
1	В	296	TRP	2.1
1	А	109	LEU	2.1
1	В	29	LEU	2.1
1	А	35	PRO	2.1
1	В	285	GLU	2.1
1	В	365	LEU	2.0
1	В	126	GLY	2.0
1	А	134	VAL	2.0
1	А	85	THR	2.0

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
4	MG	А	701	1/1	0.97	0.25	$63,\!63,\!63,\!63$	0
4	MG	В	701	1/1	0.97	0.18	$57,\!57,\!57,\!57$	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

