



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 11:12 pm BST

PDB ID : 4N76  
Title : Structure of Thermus thermophilus Argonaute bound to guide DNA and cleaved target DNA with Mn<sup>2+</sup>  
Authors : Sheng, G.; Zhao, H.; Wang, J.; Rao, Y.; Wang, Y.  
Deposited on : 2013-10-15  
Resolution : 2.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

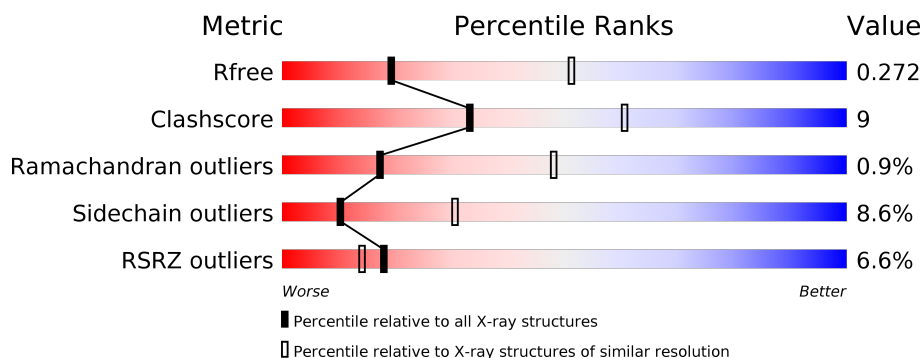
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	685	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>22%</div> <div>• 6%</div> </div> </div>
1	B	685	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>
2	C	21	<div> <div>29%</div> <div>19%</div> <div>52%</div> </div>
2	E	21	<div> <div>33%</div> <div>19%</div> <div>48%</div> </div>
3	D	10	<div> <div>80%</div> <div>20%</div> </div>
3	F	10	<div> <div>60%</div> <div>40%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10818 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 Argonaute.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	641	Total	C	N	O	S	4	0	0
			4803	3069	895	834	5			
1	B	667	Total	C	N	O	S	0	0	0
			5115	3273	959	877	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			212	100	41	61	10			
2	E	11	Total	C	N	O	P	0	0	0
			234	110	46	67	11			

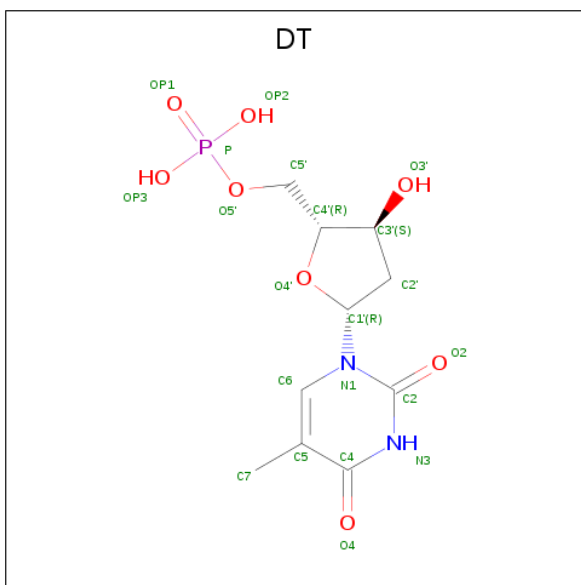
- Molecule 3 is a DNA chain called 5'-D(P\*TP\*AP\*CP\*TP\*AP\*CP\*CP\*TP\*CP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	10	Total	C	N	O	P	0	0	0
			201	96	33	62	10			
3	F	10	Total	C	N	O	P	0	0	0
			201	96	33	62	10			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Mn	0	0
			3	3		
4	C	1	Total	Mn	0	0
			1	1		

- Molecule 5 is THYMIDINE-5'-MONOPHOSPHATE (three-letter code: DT) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>2</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			21	10	2	8	1		

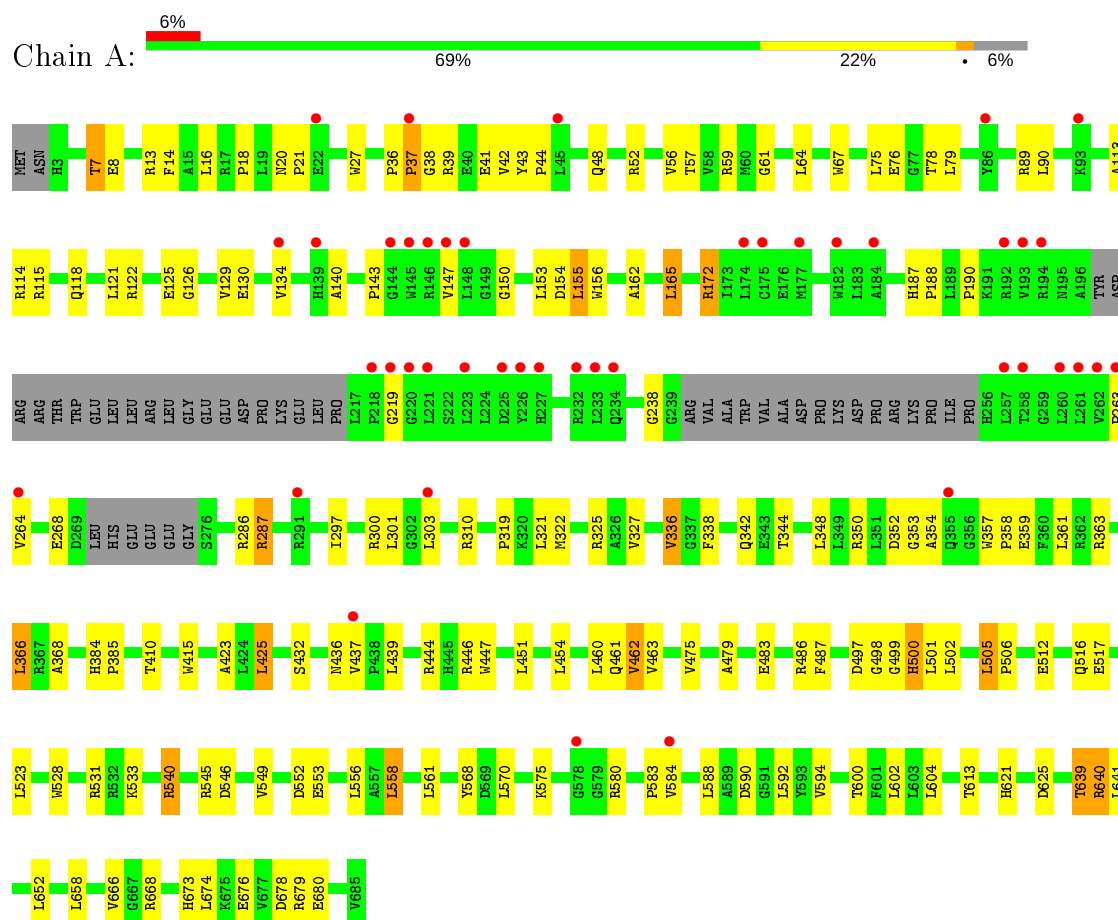
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	14	Total	O	0	0
			14	14		
6	C	1	Total	O	0	0
			1	1		
6	E	3	Total	O	0	0
			3	3		
6	F	1	Total	O	0	0
			1	1		

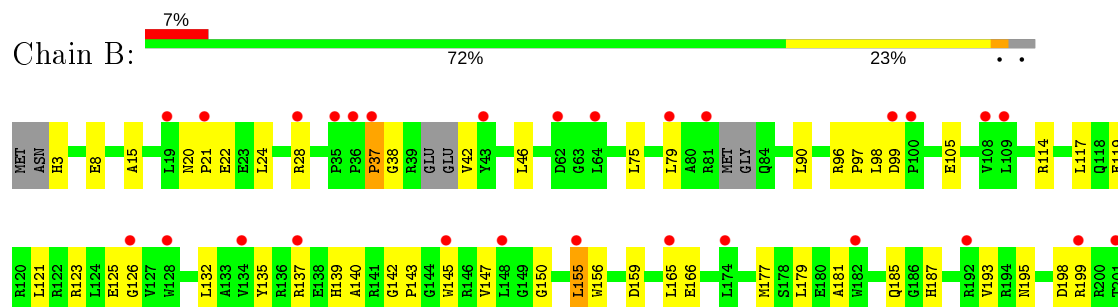
### 3 Residue-property plots

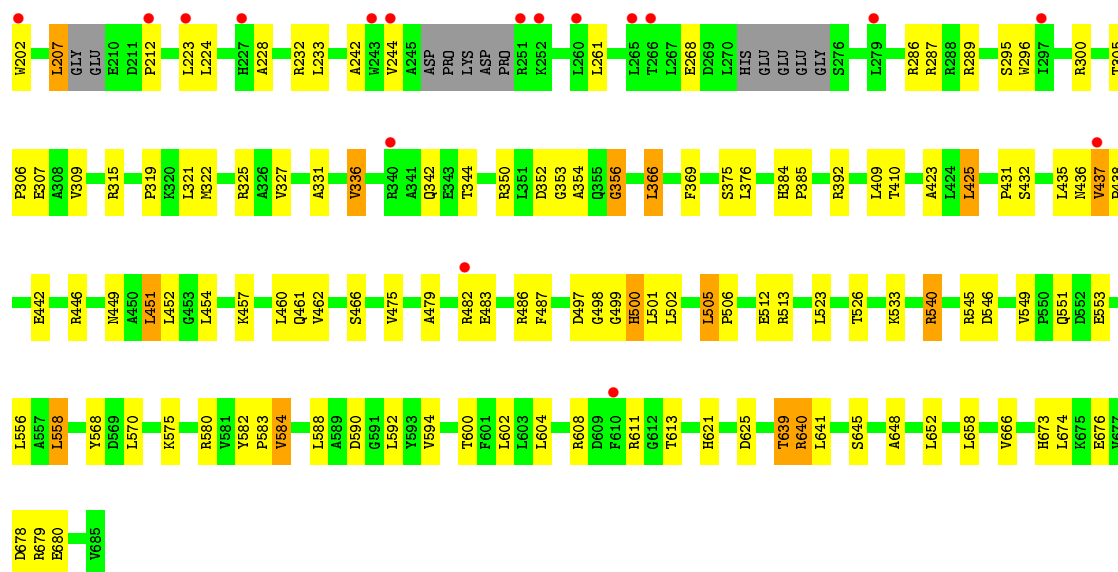
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Argonaute

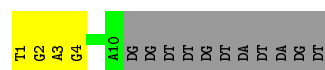
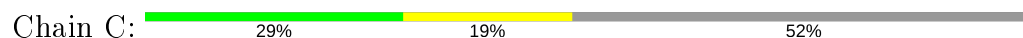


#### • Molecule 1: Argonaute

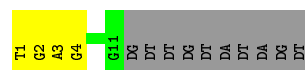
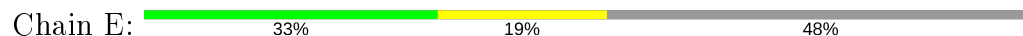




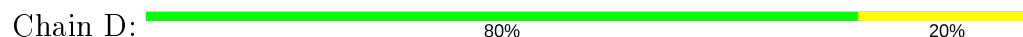
- Molecule 2: 5'-D(P\*TP\*GP\*AP\*GP\*GP\*TP\*AP\*GP\*TP\*AP\*GP\*GP\*TP\*TP\*GP\*TP\*AP\*TP\*AP\*GP\*T)-3'



- Molecule 2: 5'-D(P\*TP\*GP\*AP\*GP\*GP\*TP\*AP\*GP\*TP\*AP\*GP\*GP\*TP\*TP\*GP\*TP\*AP\*TP\*AP\*GP\*T)-3'



- Molecule 3: 5'-D(P\*TP\*AP\*CP\*TP\*AP\*CP\*CP\*TP\*CP\*G)-3'



- Molecule 3: 5'-D(P\*TP\*AP\*CP\*TP\*AP\*CP\*CP\*TP\*CP\*G)-3'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.92Å 117.42Å 160.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 2.89 49.37 – 2.89	Depositor EDS
% Data completeness (in resolution range)	95.0 (49.37-2.89) 94.7 (49.37-2.89)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.219 , 0.269 0.225 , 0.272	Depositor DCC
$R_{free}$ test set	2294 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 8.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	10818	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.26	0/4910	0.46	1/6677 (0.0%)
1	B	0.27	0/5235	0.45	2/7115 (0.0%)
2	C	0.82	1/238 (0.4%)	1.21	1/365 (0.3%)
2	E	0.79	1/263 (0.4%)	1.18	1/404 (0.2%)
3	D	0.86	1/223 (0.4%)	1.18	0/339
3	F	0.92	1/223 (0.4%)	1.22	1/339 (0.3%)
All	All	0.35	4/11092 (0.0%)	0.57	6/15239 (0.0%)

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	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	DT	OP3-P	-10.96	1.48	1.61
2	E	1	DT	OP3-P	-10.72	1.48	1.61
3	F	10	DT	OP3-P	-10.30	1.48	1.61
3	D	10	DT	OP3-P	-10.28	1.48	1.61

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	DT	OP1-P-OP2	-8.20	107.30	119.60
2	C	1	DT	OP1-P-OP2	-7.34	108.59	119.60
1	B	143	PRO	N-CA-CB	5.92	110.41	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	PRO	N-CA-CB	5.83	110.29	103.30
1	B	356	GLY	N-CA-C	5.35	126.47	113.10
3	F	12	DC	O4'-C1'-N1	5.01	111.51	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	437	VAL	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4803	0	4723	91	0
1	B	5115	0	5099	89	0
2	C	212	0	114	2	0
2	E	234	0	125	3	0
3	D	201	0	114	2	0
3	F	201	0	114	2	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
5	B	21	0	13	5	0
6	A	8	0	0	1	0
6	B	14	0	0	2	0
6	C	1	0	0	0	0
6	E	3	0	0	0	0
6	F	1	0	0	0	0
All	All	10818	0	10302	179	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (179) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:THR:HG22	1:A:640:ARG:HE	1.46	0.81
1:A:344:THR:HG21	1:A:460:LEU:HD11	1.62	0.80
1:B:639:THR:HG22	1:B:640:ARG:HE	1.46	0.80
1:B:608:ARG:HB2	1:B:611:ARG:HG3	1.67	0.76
1:B:99:ASP:N	1:B:105:GLU:OE1	2.18	0.74
1:A:7:THR:OG1	1:A:8:GLU:N	2.17	0.73
1:A:287:ARG:NH2	1:A:583:PRO:O	2.22	0.72
1:A:319:PRO:HG3	1:A:640:ARG:HD3	1.71	0.72
1:B:319:PRO:HG3	1:B:640:ARG:HD3	1.71	0.72
1:A:575:LYS:HD3	1:A:652:LEU:HD11	1.74	0.70
1:B:344:THR:HG21	1:B:460:LEU:HD11	1.72	0.69
1:A:37:PRO:HB2	1:A:42:VAL:HG22	1.74	0.69
1:B:575:LYS:HD3	1:B:652:LEU:HD11	1.75	0.69
1:A:76:GLU:HG2	1:A:89:ARG:HG3	1.76	0.68
1:B:486:ARG:NH1	1:B:512:GLU:OE1	2.28	0.67
1:A:486:ARG:NH1	1:A:512:GLU:OE1	2.28	0.66
1:A:350:ARG:HD3	1:A:354:ALA:HB3	1.78	0.66
1:B:99:ASP:HB3	1:B:105:GLU:OE1	1.96	0.66
1:B:546:ASP:OD1	1:B:575:LYS:NZ	2.29	0.66
1:B:28:ARG:HH21	1:B:96:ARG:HB3	1.62	0.65
1:A:546:ASP:OD1	1:A:575:LYS:NZ	2.30	0.64
1:B:350:ARG:HD3	1:B:354:ALA:HB3	1.79	0.64
1:A:16:LEU:HD13	1:A:303:LEU:HB3	1.80	0.64
1:A:190:PRO:HG2	1:A:263:PRO:HB3	1.79	0.63
1:A:129:VAL:HG22	1:A:134:VAL:HG22	1.81	0.63
1:B:15:ALA:HB3	1:B:307:GLU:HB3	1.83	0.60
1:B:177:MET:HB3	1:B:181:ALA:HB3	1.84	0.60
1:A:59:ARG:NH1	1:A:61:GLY:O	2.35	0.59
1:A:113:ALA:HB1	1:A:155:LEU:HD13	1.84	0.59
1:B:540:ARG:NH2	1:B:625:ASP:OD2	2.36	0.59
1:B:99:ASP:CB	1:B:105:GLU:OE1	2.51	0.58
1:A:8:GLU:OE2	1:A:310:ARG:NH1	2.36	0.58
1:A:540:ARG:NH2	1:A:625:ASP:OD2	2.36	0.58
1:A:359:GLU:HG3	1:A:363:ARG:HE	1.69	0.57
1:B:640:ARG:NH1	6:B:805:HOH:O	2.38	0.57
1:A:39:ARG:HD2	5:B:704:DT:N3	2.19	0.56
1:A:583:PRO:HD3	1:A:588:LEU:HD13	1.88	0.55
1:B:500:HIS:CD2	1:B:502:LEU:HD21	2.41	0.55
1:A:516:GLN:NE2	1:A:552:ASP:O	2.40	0.54
1:B:75:LEU:HD22	1:B:90:LEU:HB2	1.89	0.54
1:A:500:HIS:HD2	1:A:502:LEU:HD21	1.73	0.54
1:A:506:PRO:HG2	1:A:666:VAL:HG11	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:PRO:HD3	1:B:588:LEU:HD13	1.90	0.53
1:A:358:PRO:HG2	1:A:361:LEU:HD12	1.91	0.53
1:A:425:LEU:HD12	1:A:432:SER:HB3	1.90	0.53
1:B:232:ARG:NH1	5:B:704:DT:OP2	2.34	0.53
2:C:3:DA:H2'	2:C:4:DG:C8	2.43	0.53
2:E:3:DA:H2'	2:E:4:DG:C8	2.44	0.52
1:B:425:LEU:HD12	1:B:432:SER:HB3	1.90	0.52
1:A:437:VAL:O	1:A:439:LEU:N	2.42	0.52
1:B:500:HIS:CE1	1:B:533:LYS:HE3	2.44	0.52
1:A:676:GLU:OE1	1:B:679:ARG:NH2	2.43	0.52
1:B:331:ALA:HA	1:B:452:LEU:HD11	1.92	0.52
1:A:500:HIS:CD2	1:A:502:LEU:HD21	2.45	0.52
1:A:523:LEU:HD21	1:A:561:LEU:HD11	1.92	0.51
1:A:13:ARG:HD3	1:A:156:TRP:CZ2	2.46	0.51
1:A:38:GLY:O	1:A:39:ARG:C	2.48	0.51
1:A:286:ARG:HD2	1:A:613:THR:HG21	1.92	0.51
1:B:207:LEU:HD23	1:B:242:ALA:HA	1.92	0.51
1:A:75:LEU:HD22	1:A:90:LEU:HB2	1.93	0.51
1:B:20:ASN:HB2	1:B:21:PRO:HD2	1.93	0.50
1:A:500:HIS:NE2	1:A:533:LYS:HE2	2.26	0.50
1:A:497:ASP:OD1	1:A:497:ASP:N	2.44	0.50
1:B:350:ARG:NH2	1:B:352:ASP:OD2	2.45	0.50
1:B:8:GLU:O	1:B:584:VAL:HB	2.12	0.50
1:B:156:TRP:HZ3	1:B:166:GLU:HB2	1.76	0.50
1:A:39:ARG:HD3	5:B:704:DT:C2	2.47	0.50
1:A:679:ARG:NH2	1:B:676:GLU:OE1	2.45	0.50
1:A:410:THR:O	1:A:436:ASN:HA	2.11	0.49
1:A:350:ARG:NH2	1:A:352:ASP:OD2	2.45	0.49
1:A:13:ARG:HD3	1:A:156:TRP:HZ2	1.77	0.49
1:B:558:LEU:HG	1:B:568:TYR:CE2	2.48	0.49
1:A:52:ARG:HG3	1:A:79:LEU:HD13	1.93	0.49
1:B:513:ARG:NH2	1:B:551:GLN:O	2.45	0.49
1:A:20:ASN:HB2	1:A:21:PRO:HD2	1.95	0.49
1:A:558:LEU:HG	1:A:568:TYR:CE2	2.47	0.49
1:B:117:LEU:HD22	1:B:155:LEU:HB2	1.95	0.49
1:B:506:PRO:HG2	1:B:666:VAL:HG11	1.93	0.49
1:A:666:VAL:HG22	1:A:674:LEU:HD11	1.95	0.49
1:B:268:GLU:HA	3:F:14:DA:H5'	1.94	0.49
1:B:446:ARG:HG3	2:E:2:DG:C8	2.47	0.49
1:B:410:THR:O	1:B:436:ASN:HA	2.12	0.49
1:B:295:SER:HA	1:B:306:PRO:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:LEU:HD13	1:B:658:LEU:HD11	1.95	0.48
1:A:140:ALA:HB3	1:A:147:VAL:HB	1.94	0.48
1:B:449:ASN:ND2	2:E:2:DG:H21	2.11	0.48
1:B:125:GLU:HA	1:B:126:GLY:HA2	1.48	0.48
1:B:423:ALA:HB1	1:B:673:HIS:CE1	2.49	0.48
1:A:423:ALA:HB1	1:A:673:HIS:CE1	2.48	0.48
1:A:462:VAL:HG23	1:A:463:VAL:HG13	1.96	0.48
1:A:498:GLY:HA3	1:A:641:LEU:HD11	1.94	0.48
1:A:154:ASP:OD2	1:A:155:LEU:N	2.48	0.47
1:B:498:GLY:HA3	1:B:641:LEU:HD11	1.95	0.47
1:A:501:LEU:HD13	1:A:658:LEU:HD11	1.97	0.47
1:A:56:VAL:HG13	1:A:67:TRP:HB2	1.97	0.47
1:B:135:TYR:HA	1:B:150:GLY:HA3	1.97	0.47
1:B:500:HIS:HD2	1:B:502:LEU:HD21	1.79	0.47
1:B:202:TRP:HB3	1:B:244:VAL:HB	1.96	0.47
1:B:137:ARG:HH21	1:B:139:HIS:CE1	2.33	0.47
1:A:121:LEU:HD11	1:A:153:LEU:HD12	1.97	0.47
1:B:436:ASN:HB2	1:B:446:ARG:HH12	1.80	0.46
1:B:666:VAL:HG22	1:B:674:LEU:HD11	1.96	0.46
1:A:18:PRO:HA	1:A:162:ALA:HA	1.96	0.46
1:A:338:PHE:CZ	1:A:368:ALA:HB1	2.50	0.46
1:B:594:VAL:HB	1:B:602:LEU:HB2	1.98	0.46
1:A:56:VAL:HG23	1:A:115:ARG:HB3	1.96	0.46
1:A:594:VAL:HB	1:A:602:LEU:HB2	1.97	0.46
1:B:119:GLU:OE1	1:B:123:ARG:NH2	2.49	0.46
1:B:545:ARG:NH1	1:B:553:GLU:OE2	2.47	0.46
1:B:287:ARG:HG3	1:B:582:TYR:CG	2.51	0.46
1:A:348:LEU:HB2	1:A:357:TRP:CE2	2.51	0.45
1:A:39:ARG:CD	5:B:704:DT:C2	3.00	0.45
1:A:125:GLU:HA	1:A:126:GLY:HA2	1.60	0.45
1:A:134:VAL:O	1:A:150:GLY:HA3	2.17	0.45
1:A:114:ARG:NH1	1:A:154:ASP:OD1	2.50	0.45
1:A:502:LEU:HD23	1:A:680:GLU:HA	1.99	0.45
1:A:384:HIS:CD2	1:A:385:PRO:HD2	2.52	0.44
1:A:461:GLN:HG3	1:A:499:GLY:O	2.17	0.44
1:B:193:VAL:HG21	1:B:261:LEU:HB3	1.99	0.44
1:B:409:LEU:HB3	1:B:437:VAL:HG21	1.99	0.44
1:A:297:ILE:O	1:A:301:LEU:HB2	2.17	0.44
1:B:461:GLN:HG3	1:B:499:GLY:O	2.17	0.44
1:B:645:SER:OG	1:B:648:ALA:O	2.31	0.44
1:B:497:ASP:N	1:B:497:ASP:OD1	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:TRP:HA	1:A:358:PRO:HD2	1.86	0.44
1:B:369:PHE:CE1	1:B:376:LEU:HD13	2.53	0.44
1:A:43:TYR:N	1:A:44:PRO:HD2	2.32	0.44
1:A:444:ARG:HG2	1:A:447:TRP:CZ2	2.53	0.44
1:A:545:ARG:HG2	1:A:549:VAL:HG22	2.00	0.44
1:A:545:ARG:NH1	1:A:553:GLU:OE2	2.48	0.44
1:B:545:ARG:HG2	1:B:549:VAL:HG22	2.00	0.44
1:A:38:GLY:O	1:A:41:GLU:N	2.51	0.43
1:B:228:ALA:HA	1:B:233:LEU:HB2	2.00	0.43
1:B:114:ARG:HD3	1:B:132:LEU:HD11	1.99	0.43
1:B:523:LEU:O	1:B:526:THR:OG1	2.29	0.43
1:A:48:GLN:HG2	1:A:79:LEU:HD11	1.99	0.43
1:A:590:ASP:OD1	3:D:19:DG:N2	2.48	0.43
1:B:366:LEU:HD13	1:B:376:LEU:HD23	1.99	0.43
1:B:321:LEU:HB3	1:B:327:VAL:HG23	2.00	0.43
1:B:608:ARG:O	1:B:611:ARG:HB2	2.18	0.43
1:A:14:PHE:O	1:A:165:LEU:N	2.48	0.43
1:B:142:GLY:N	1:B:145:TRP:O	2.52	0.43
1:B:117:LEU:O	1:B:121:LEU:HG	2.19	0.42
1:A:130:GLU:OE2	1:A:172:ARG:NH1	2.52	0.42
1:A:528:TRP:CE2	1:B:392:ARG:HD3	2.53	0.42
1:B:212:PRO:HB2	1:B:224:LEU:HB2	2.00	0.42
1:A:187:HIS:HA	1:A:188:PRO:HD3	1.91	0.42
1:A:505:LEU:HA	1:A:505:LEU:HD23	1.92	0.42
1:B:195:ASN:HB2	1:B:198:ASP:OD1	2.19	0.42
1:A:325:ARG:HG2	1:A:336:VAL:HG13	2.02	0.42
1:A:366:LEU:HA	1:A:366:LEU:HD13	1.83	0.42
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.74	0.42
1:B:37:PRO:HB2	1:B:38:GLY:H	1.64	0.42
1:B:409:LEU:HD23	1:B:435:LEU:HB3	2.02	0.42
1:B:315:ARG:NH2	6:B:802:HOH:O	2.46	0.42
1:A:321:LEU:HB3	1:A:327:VAL:HG23	2.02	0.42
1:B:296:TRP:CH2	1:B:300:ARG:HG3	2.55	0.42
1:B:505:LEU:HD23	1:B:505:LEU:HA	1.93	0.42
1:A:36:PRO:HA	1:A:37:PRO:HD3	1.82	0.41
1:A:415:TRP:CZ3	1:A:668:ARG:HD2	2.55	0.41
1:B:140:ALA:HB3	1:B:147:VAL:HB	2.01	0.41
1:B:195:ASN:HD21	1:B:202:TRP:HE1	1.67	0.41
1:B:502:LEU:HD23	1:B:680:GLU:HA	2.01	0.41
1:B:590:ASP:OD1	3:F:19:DG:N1	2.51	0.41
1:A:122:ARG:NH1	6:A:704:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:HD2	5:B:704:DT:H3	1.83	0.41
1:A:479:ALA:HA	1:A:487:PHE:O	2.21	0.41
1:A:590:ASP:OD1	3:D:19:DG:N1	2.48	0.41
1:B:286:ARG:HD2	1:B:613:THR:HG21	2.02	0.41
1:A:348:LEU:HB2	1:A:357:TRP:CZ2	2.55	0.41
1:B:185:GLN:HB2	1:B:187:HIS:ND1	2.36	0.41
1:B:431:PRO:HB2	1:B:457:LYS:HB3	2.01	0.41
1:A:446:ARG:HG3	2:C:2:DG:C8	2.56	0.41
1:B:384:HIS:CG	1:B:385:PRO:HD2	2.56	0.41
1:B:24:LEU:O	1:B:97:PRO:HA	2.21	0.40
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.77	0.40
1:B:451:LEU:HA	1:B:451:LEU:HD12	1.88	0.40
1:B:325:ARG:HG2	1:B:336:VAL:HG13	2.03	0.40
1:B:479:ALA:HA	1:B:487:PHE:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	633/685 (92%)	580 (92%)	47 (7%)	6 (1%)	17	48
1	B	655/685 (96%)	613 (94%)	36 (6%)	6 (1%)	17	48
All	All	1288/1370 (94%)	1193 (93%)	83 (6%)	12 (1%)	17	48

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	483	GLU
1	B	438	PRO
1	B	37	PRO
1	B	356	GLY

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Mol	Chain	Res	Type
1	B	482	ARG
1	B	483	GLU
1	A	268	GLU
1	A	37	PRO
1	A	353	GLY
1	B	353	GLY
1	A	219	GLY
1	A	238	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	447/549 (81%)	409 (92%)	38 (8%)	10	31
1	B	492/549 (90%)	449 (91%)	43 (9%)	10	30
All	All	939/1098 (86%)	858 (91%)	81 (9%)	10	30

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	27	TRP
1	A	57	THR
1	A	64	LEU
1	A	78	THR
1	A	118	GLN
1	A	155	LEU
1	A	165	LEU
1	A	172	ARG
1	A	264	VAL
1	A	287	ARG
1	A	300	ARG
1	A	322	MET
1	A	336	VAL
1	A	342	GLN

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Mol	Chain	Res	Type
1	A	366	LEU
1	A	425	LEU
1	A	451	LEU
1	A	454	LEU
1	A	462	VAL
1	A	475	VAL
1	A	500	HIS
1	A	505	LEU
1	A	517	GLU
1	A	531	ARG
1	A	540	ARG
1	A	556	LEU
1	A	558	LEU
1	A	570	LEU
1	A	580	ARG
1	A	584	VAL
1	A	592	LEU
1	A	600	THR
1	A	604	LEU
1	A	621	HIS
1	A	639	THR
1	A	640	ARG
1	A	678	ASP
1	B	3	HIS
1	B	22	GLU
1	B	42	VAL
1	B	46	LEU
1	B	79	LEU
1	B	98	LEU
1	B	155	LEU
1	B	159	ASP
1	B	165	LEU
1	B	179	LEU
1	B	199	ARG
1	B	207	LEU
1	B	223	LEU
1	B	289	ARG
1	B	305	THR
1	B	309	VAL
1	B	322	MET
1	B	336	VAL
1	B	342	GLN

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Mol	Chain	Res	Type
1	B	366	LEU
1	B	375	SER
1	B	425	LEU
1	B	442	GLU
1	B	451	LEU
1	B	454	LEU
1	B	462	VAL
1	B	466	SER
1	B	475	VAL
1	B	500	HIS
1	B	505	LEU
1	B	540	ARG
1	B	556	LEU
1	B	558	LEU
1	B	570	LEU
1	B	580	ARG
1	B	584	VAL
1	B	592	LEU
1	B	600	THR
1	B	604	LEU
1	B	621	HIS
1	B	639	THR
1	B	640	ARG
1	B	678	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	500	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	641/685 (93%)	0.53	44 (6%)	16 13	3, 25, 103, 143	1 (0%)
1	B	667/685 (97%)	0.50	45 (6%)	17 13	1, 27, 82, 113	0
2	C	10/21 (47%)	-0.20	0	100 100	22, 26, 65, 83	0
2	E	11/21 (52%)	-0.12	0	100 100	16, 24, 73, 100	0
3	D	10/10 (100%)	-0.17	0	100 100	27, 66, 90, 91	0
3	F	10/10 (100%)	-0.32	0	100 100	26, 56, 76, 78	0
All	All	1349/1432 (94%)	0.49	89 (6%)	18 14	1, 26, 92, 143	1 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	LEU	10.2
1	A	232	ARG	8.9
1	B	19	LEU	6.2
1	A	220	GLY	6.2
1	A	258	THR	5.8
1	A	219	GLY	5.8
1	B	37	PRO	5.8
1	A	145	TRP	5.7
1	A	226	TYR	5.4
1	A	263	PRO	5.4
1	B	145	TRP	4.7
1	A	260	LEU	4.4
1	B	202	TRP	4.3
1	B	260	LEU	4.3
1	B	610	PHE	4.2
1	A	174	LEU	4.2
1	A	37	PRO	3.9
1	A	584	VAL	3.9
1	B	251	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	193	VAL	3.8
1	A	261	LEU	3.6
1	B	266	THR	3.6
1	A	227	HIS	3.5
1	B	279	LEU	3.4
1	B	182	TRP	3.4
1	A	146	ARG	3.3
1	B	192	ARG	3.3
1	A	22	GLU	3.3
1	B	126	GLY	3.2
1	B	243	TRP	3.2
1	B	81	ARG	3.1
1	A	144	GLY	3.1
1	B	100	PRO	3.1
1	B	165	LEU	3.0
1	A	225	ASP	3.0
1	B	134	VAL	3.0
1	B	212	PRO	3.0
1	B	21	PRO	2.9
1	A	139	HIS	2.9
1	B	109	LEU	2.9
1	B	108	VAL	2.8
1	A	257	LEU	2.8
1	A	437	VAL	2.8
1	A	175	CYS	2.7
1	A	148	LEU	2.6
1	B	28	ARG	2.6
1	B	62	ASP	2.6
1	B	297	ILE	2.6
1	B	482	ARG	2.6
1	A	182	TRP	2.6
1	A	578	GLY	2.6
1	A	223	LEU	2.5
1	A	192	ARG	2.5
1	B	43	TYR	2.5
1	B	199	ARG	2.4
1	A	262	VAL	2.4
1	A	45	LEU	2.4
1	B	437	VAL	2.3
1	B	79	LEU	2.3
1	A	234	GLN	2.3
1	B	35	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	355	GLN	2.3
1	A	147	VAL	2.3
1	B	340	ARG	2.3
1	B	128	TRP	2.2
1	B	137	ARG	2.2
1	A	184	ALA	2.2
1	B	99	ASP	2.2
1	A	291	ARG	2.2
1	B	252	LYS	2.2
1	B	227	HIS	2.2
1	A	221	LEU	2.1
1	B	64	LEU	2.1
1	B	201	THR	2.1
1	A	134	VAL	2.1
1	A	86	TYR	2.1
1	A	177	MET	2.1
1	B	244	VAL	2.1
1	A	218	PRO	2.1
1	B	155	LEU	2.1
1	A	194	ARG	2.1
1	A	264	VAL	2.1
1	B	148	LEU	2.1
1	B	174	LEU	2.1
1	B	223	LEU	2.0
1	A	93	LYS	2.0
1	A	303	LEU	2.0
1	B	36	PRO	2.0
1	B	265	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MN	B	703	1/1	0.79	0.09	81,81,81,81	0
4	MN	B	702	1/1	0.79	0.08	63,63,63,63	1
5	DT	B	704	21/21	0.95	0.28	47,64,75,84	0
4	MN	B	701	1/1	0.96	0.14	50,50,50,50	0
4	MN	C	101	1/1	0.98	0.15	53,53,53,53	0

## 6.5 Other polymers

There are no such residues in this entry.