



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:00 am BST

PDB ID : 5GQ9  
Title : Crystal structure of Thermus thermophilus Argonaute in complex with g1C  
siDNA and DNA target  
Authors : Zhao, H.; Sheng, G.; Wang, Y.  
Deposited on : 2016-08-06  
Resolution : 2.70 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

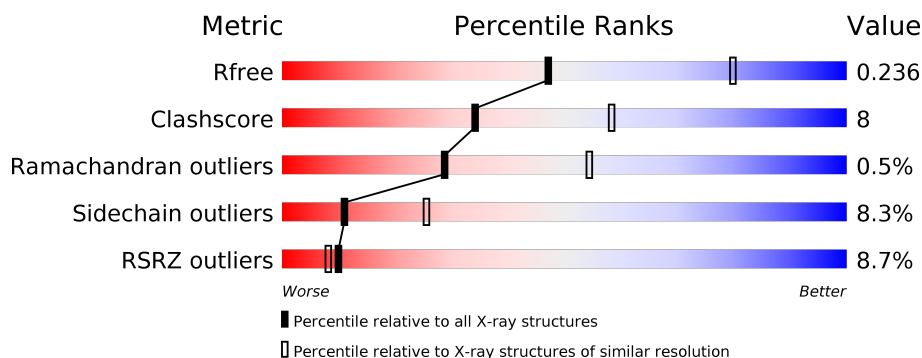
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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>9%</div> <div>68% 22% 7%</div> </div>
1	B	685	<div> <div>9%</div> <div>78% 18% . .</div> </div>
2	C	21	<div> <div>24% 48% 5% 24%</div> </div>
2	E	21	<div> <div>33% 33% 10% 24%</div> </div>
3	D	16	<div> <div>63% 19% 19%</div> </div>
3	F	16	<div> <div>44% 44% 13%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11609 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 *Thermus thermophilus* Argonaute.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	1	0
			5027	3213	946	861	7			
1	B	673	Total	C	N	O	S	0	0	0
			5262	3366	988	902	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	16	Total	C	N	O	P	0	0	0
			337	159	63	99	16			
2	E	16	Total	C	N	O	P	0	0	0
			337	159	63	99	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	16	Total	C	N	O	P	0	5	0
			320	153	57	94	16			
3	F	16	Total	C	N	O	P	0	5	0
			320	153	57	94	16			

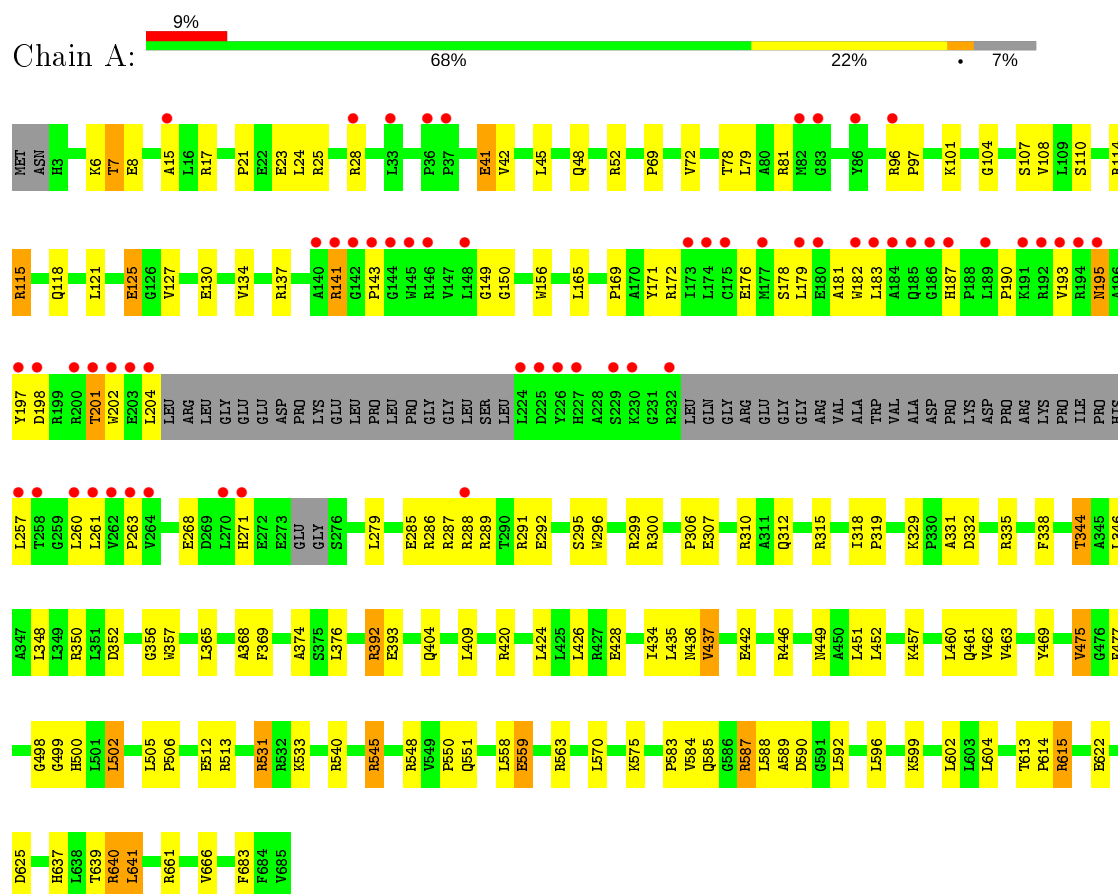
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Mg	0	0
			3	3		
4	A	3	Total	Mg	0	0
			3	3		

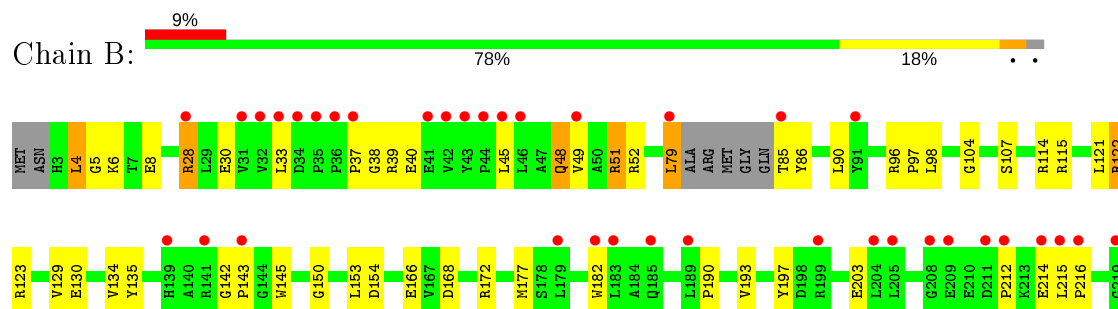
### 3 Residue-property plots

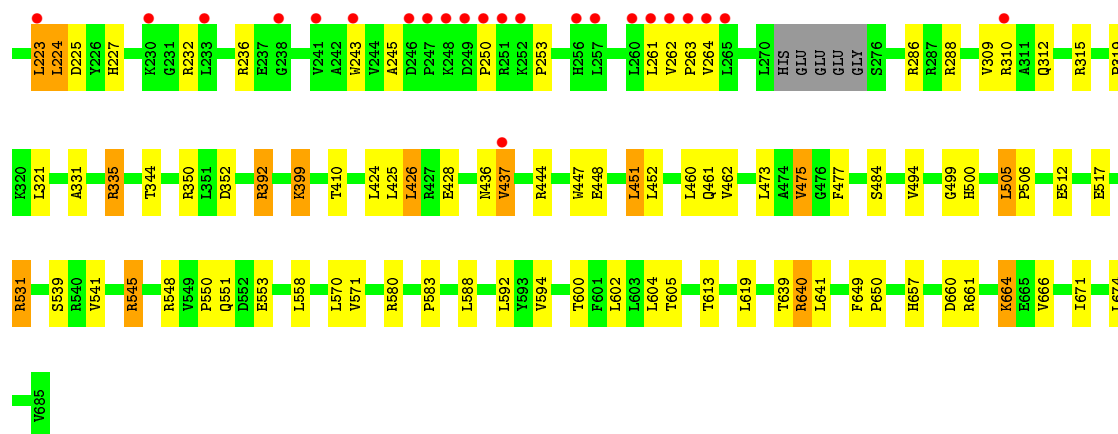
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Thermus thermophilus Argonaute



#### • Molecule 1: Thermus thermophilus Argonaute





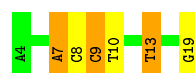
- Molecule 2: DNA (5'-D(P\*CP\*GP\*AP\*GP\*GP\*TP\*AP\*GP\*TP\*AP\*GP\*GP\*TP\*TP\*GP\*T)-3')



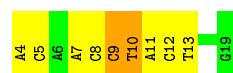
- Molecule 2: DNA (5'-D(P\*CP\*GP\*AP\*GP\*GP\*TP\*AP\*GP\*TP\*AP\*GP\*GP\*TP\*TP\*GP\*T)-3')



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



- Molecule 3: DNA (5'-D(P\*AP\*CP\*AP\*AP\*CP\*CP\*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, $\alpha$ , $\beta$ , $\gamma$	111.83Å 116.50Å 161.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.13 – 2.70 45.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.13-2.70) 98.0 (45.93-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.2 _1309	Depositor
R, $R_{free}$	0.189 , 0.237 0.189 , 0.236	Depositor DCC
$R_{free}$ test set	3022 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.6	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11609	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: 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	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.43	0/5147	0.62	1/6980 (0.0%)
1	B	0.42	0/5388	0.61	1/7317 (0.0%)
2	C	0.98	1/378 (0.3%)	1.50	10/582 (1.7%)
2	E	0.99	1/378 (0.3%)	1.47	5/582 (0.9%)
3	D	0.79	0/357	1.50	5/546 (0.9%)
3	F	0.93	0/357	1.52	5/546 (0.9%)
All	All	0.52	2/12005 (0.0%)	0.79	27/16553 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	DC	OP3-P	-10.26	1.48	1.61
2	E	1	DC	OP3-P	-9.85	1.49	1.61

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	7[A]	DA	O4'-C1'-N9	8.42	113.90	108.00
3	F	13	DT	O4'-C1'-N1	7.78	113.45	108.00
3	D	9[A]	DC	O4'-C1'-N1	7.26	113.08	108.00
3	F	9[A]	DC	O4'-C1'-N1	7.09	112.96	108.00
3	F	7[A]	DA	O4'-C1'-N9	6.54	112.58	108.00
2	E	16	DT	O4'-C1'-N1	6.53	112.57	108.00
2	C	11	DG	O4'-C1'-N9	6.50	112.55	108.00
2	C	16	DT	N3-C4-O4	6.48	123.79	119.90
3	F	8[A]	DC	C4'-C3'-C2'	-6.42	97.32	103.10
3	F	10	DT	O5'-P-OP2	-6.30	100.03	105.70
2	E	13	DT	C5-C4-O4	-6.00	120.70	124.90
1	A	502	LEU	CA-CB-CG	5.96	129.02	115.30
2	E	13	DT	N3-C4-O4	5.86	123.42	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	9[A]	DC	C4'-C3'-C2'	-5.64	98.03	103.10
2	C	10	DA	O4'-C1'-N9	5.57	111.90	108.00
2	C	14	DT	N3-C4-O4	5.57	123.25	119.90
2	C	13	DT	C5-C4-O4	-5.46	121.08	124.90
2	C	13	DT	N3-C4-O4	5.46	123.17	119.90
2	C	6	DT	N3-C4-O4	5.44	123.16	119.90
2	E	10	DA	O4'-C4'-C3'	-5.35	102.36	104.50
2	C	9	DT	O4'-C1'-N1	5.34	111.74	108.00
3	D	13	DT	N3-C4-O4	5.34	123.11	119.90
3	D	8[A]	DC	C4'-C3'-C2'	-5.31	98.32	103.10
1	B	437	VAL	C-N-CD	5.27	139.47	128.40
2	C	16	DT	C5-C4-O4	-5.26	121.22	124.90
2	E	16	DT	C5-C4-O4	-5.23	121.24	124.90
2	C	9	DT	N3-C4-O4	5.12	122.97	119.90

There are no chirality outliers.

There are no planarity outliers.

## 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	5027	0	5115	106	0
1	B	5262	0	5333	76	0
2	C	337	0	182	5	0
2	E	337	0	182	5	0
3	D	320	0	180	6	0
3	F	320	0	180	5	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
All	All	11609	0	11172	190	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 8.

All (190) 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:583:PRO:HD3	1:A:588:LEU:HD13	1.60	0.83
1:A:190:PRO:HG3	1:A:263:PRO:HB3	1.61	0.81
1:A:587:ARG:HD2	1:A:588:LEU:H	1.51	0.76
1:B:45:LEU:HD21	1:B:85:THR:HB	1.67	0.75
1:B:344:THR:HG21	1:B:460:LEU:HD11	1.68	0.74
1:B:4:LEU:HD23	1:B:5:GLY:H	1.50	0.74
1:A:319:PRO:HG3	1:A:640:ARG:HD3	1.68	0.74
1:A:15:ALA:HB3	1:A:307:GLU:HB3	1.70	0.72
1:A:513:ARG:NH2	1:A:551:GLN:O	2.24	0.71
1:A:461:GLN:NE2	1:A:498:GLY:O	2.26	0.69
2:C:3:DA:H2'	2:C:4:DG:C8	2.28	0.69
1:A:7:THR:OG1	1:A:8:GLU:N	2.19	0.69
2:E:6:DT:H2''	2:E:7:DA:H5''	1.75	0.69
1:B:122:ARG:O	1:B:122:ARG:NH1	2.26	0.69
1:A:584:VAL:HG12	1:A:585:GLN:HG3	1.76	0.67
1:B:48:GLN:HB3	1:B:79:LEU:HD11	1.76	0.66
1:A:315[B]:ARG:NH2	1:A:590:ASP:O	2.29	0.66
1:B:121:LEU:HD22	1:B:134:VAL:HG21	1.78	0.65
1:B:212:PRO:HB2	1:B:224:LEU:HD12	1.80	0.64
1:A:461:GLN:HG3	1:A:499:GLY:O	1.97	0.64
1:B:8:GLU:OE1	1:B:310:ARG:NH1	2.32	0.62
1:B:286:ARG:HD2	1:B:613:THR:HG21	1.80	0.62
1:A:575:LYS:O	1:A:615:ARG:NH2	2.33	0.62
1:B:33:LEU:HB3	1:B:85:THR:HG21	1.82	0.61
1:B:506:PRO:HG2	1:B:666:VAL:HG21	1.81	0.61
1:A:506:PRO:HG2	1:A:666:VAL:HG21	1.81	0.61
3:F:11:DA:H2'	3:F:12:DC:C6	2.36	0.61
1:B:517:GLU:H	1:B:517:GLU:CD	2.05	0.60
1:B:215:LEU:HD13	1:B:223:LEU:HD12	1.83	0.60
1:A:115:ARG:HH21	1:A:118:GLN:HG2	1.66	0.59
1:B:335:ARG:NH1	1:B:448:GLU:OE2	2.36	0.59
1:B:461:GLN:HG3	1:B:499:GLY:O	2.03	0.58
1:A:28:ARG:HE	1:A:96:ARG:HB2	1.69	0.57
1:A:575:LYS:HZ3	3:D:9[A]:DC:H5''	1.69	0.57
1:A:25:ARG:HH21	1:A:97:PRO:HG3	1.70	0.57
1:A:344:THR:HG21	1:A:460:LEU:HD21	1.85	0.57
1:B:130:GLU:OE1	1:B:172:ARG:NH1	2.37	0.57
1:A:195:ASN:N	1:A:195:ASN:OD1	2.36	0.56
1:A:104:GLY:O	1:A:107:SER:OG	2.22	0.56
1:A:260:LEU:HG	1:A:261:LEU:HD23	1.86	0.56
1:B:392:ARG:HD3	1:B:428:GLU:OE2	2.05	0.56
1:B:473:LEU:HB3	1:B:541:VAL:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ARG:NH2	3:D:7[A]:DA:OP2	2.39	0.55
1:B:475:VAL:HG22	1:B:477:PHE:CE1	2.42	0.55
1:A:318:ILE:HD12	1:A:318:ILE:H	1.72	0.55
1:A:446:ARG:HG3	2:C:2:DG:C8	2.42	0.54
1:A:604:LEU:HD11	1:A:614:PRO:HB2	1.89	0.54
1:B:225:ASP:N	1:B:225:ASP:OD2	2.40	0.54
1:B:135:TYR:HA	1:B:150:GLY:HA3	1.88	0.54
1:A:461:GLN:HE21	1:A:499:GLY:C	2.11	0.54
1:B:28:ARG:HH22	1:B:96:ARG:CZ	2.21	0.54
3:F:11:DA:H2'	3:F:12:DC:H6	1.71	0.54
1:A:436:ASN:O	1:A:446:ARG:NH2	2.40	0.54
1:B:594:VAL:HB	1:B:602:LEU:HB2	1.89	0.53
1:A:331:ALA:HA	1:A:452:LEU:HD11	1.91	0.53
1:B:190:PRO:HG3	1:B:263:PRO:HB3	1.91	0.53
1:B:264:VAL:HG11	2:E:10:DA:H5'	1.90	0.53
1:A:590:ASP:OD2	3:D:19:DG:N1	2.38	0.52
1:A:130:GLU:OE2	1:A:172:ARG:NE	2.38	0.52
1:A:292:GLU:O	1:A:295:SER:OG	2.28	0.52
1:B:203:GLU:HB3	1:B:245:ALA:HB3	1.91	0.52
1:B:392:ARG:HG3	1:B:424:LEU:HD11	1.92	0.52
1:A:295:SER:HA	1:A:306:PRO:HG3	1.91	0.52
1:A:498:GLY:HA3	1:A:641:LEU:HD11	1.91	0.52
1:B:51:ARG:NH2	3:F:5[A]:DC:OP1	2.42	0.52
3:F:4:DA:H2''	3:F:5[A]:DC:H5'	1.91	0.52
1:A:178:SER:O	1:A:182:TRP:N	2.38	0.51
1:B:79:LEU:N	1:B:86:TYR:O	2.41	0.51
1:B:243:TRP:CE3	1:B:253:PRO:HB2	2.46	0.51
1:A:195:ASN:ND2	1:A:198:ASP:OD1	2.41	0.51
1:A:201:THR:OG1	1:A:202:TRP:N	2.42	0.51
1:B:505:LEU:HD22	1:B:671:ILE:HD11	1.93	0.51
1:B:104:GLY:O	1:B:107:SER:HB3	2.11	0.51
1:A:475:VAL:HG22	1:A:477:PHE:CE1	2.46	0.50
1:B:331:ALA:HA	1:B:452:LEU:HD11	1.91	0.50
1:B:494:VAL:HG22	1:B:500:HIS:HB2	1.93	0.50
1:B:37:PRO:HB3	1:B:45:LEU:HD23	1.94	0.50
1:B:512:GLU:OE2	1:B:545:ARG:NH2	2.44	0.50
1:A:559:GLU:OE2	1:A:563:ARG:NE	2.45	0.50
1:A:286:ARG:HD2	1:A:613:THR:HG21	1.93	0.50
1:B:548:ARG:O	1:B:550:PRO:HD3	2.12	0.50
1:A:350:ARG:HB3	1:A:352:ASP:OD1	2.11	0.50
1:B:319:PRO:CG	1:B:640:ARG:HD2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3:DA:H2'	2:E:4:DG:C8	2.47	0.49
1:B:142:GLY:HA3	1:B:145:TRP:CE2	2.48	0.49
1:A:182:TRP:NE1	1:A:187:HIS:HB2	2.27	0.49
1:B:640:ARG:HG3	1:B:649:PHE:CD1	2.47	0.49
1:A:110:SER:OG	1:A:156:TRP:HB2	2.12	0.49
1:A:500:HIS:CD2	1:A:533:LYS:HZ3	2.30	0.49
1:B:319:PRO:HG3	1:B:640:ARG:HD2	1.94	0.48
1:A:575:LYS:NZ	3:D:9[A]:DC:H5''	2.28	0.48
1:B:350:ARG:NH1	1:B:352:ASP:OD2	2.34	0.48
1:A:462:VAL:HG23	1:A:463:VAL:HG13	1.95	0.48
1:A:69:PRO:HG2	1:A:72:VAL:HG22	1.94	0.48
1:B:243:TRP:HE3	1:B:253:PRO:HB2	1.79	0.48
1:B:129:VAL:HG22	1:B:134:VAL:HG22	1.95	0.48
1:A:449:ASN:ND2	2:C:2:DG:H21	2.12	0.47
1:A:149:GLY:HA2	1:A:171:TYR:CD2	2.50	0.47
1:B:168:ASP:OD1	1:B:286:ARG:NH1	2.47	0.47
1:A:338:PHE:CZ	1:A:368:ALA:HB1	2.50	0.47
1:B:172:ARG:HD2	1:B:172:ARG:HA	1.69	0.47
1:B:28:ARG:HH22	1:B:96:ARG:NE	2.12	0.47
1:A:8:GLU:OE2	1:A:310:ARG:NH2	2.48	0.47
1:B:193:VAL:CG2	1:B:261:LEU:HB3	2.45	0.47
1:A:52:ARG:NH1	1:A:78:THR:O	2.48	0.46
1:B:197:TYR:CE2	1:B:232:ARG:HD3	2.50	0.46
1:A:285:GLU:HA	1:A:288:ARG:HG2	1.96	0.46
1:A:287:ARG:NH2	1:A:583:PRO:O	2.47	0.46
1:B:38:GLY:O	1:B:40:GLU:N	2.42	0.46
1:A:512:GLU:OE2	1:A:545:ARG:NH2	2.48	0.46
1:A:434:ILE:O	2:C:1:DC:H4'	2.15	0.46
1:B:49:VAL:HG11	1:B:90:LEU:HD21	1.97	0.46
1:B:227:HIS:ND1	1:B:232:ARG:HD2	2.31	0.46
1:A:457:LYS:HE2	1:A:683:PHE:O	2.16	0.46
1:B:605:THR:O	1:B:640:ARG:NH2	2.49	0.46
2:E:12:DG:H2'	2:E:13:DT:H72	1.98	0.45
1:A:45:LEU:HD13	1:A:81:ARG:HD3	1.99	0.45
1:B:399:LYS:HG3	1:B:428:GLU:O	2.16	0.45
1:B:661:ARG:HD3	1:B:661:ARG:HA	1.70	0.45
1:A:352:ASP:OD2	1:A:437:VAL:HG21	2.16	0.45
1:B:583:PRO:HD3	1:B:588:LEU:HD13	1.99	0.45
1:B:650:PRO:HB3	1:B:657:HIS:CE1	2.51	0.45
1:A:41:GLU:O	1:A:45:LEU:HB2	2.18	0.44
1:A:287:ARG:HD3	1:A:291:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:ASP:OD2	1:B:664:LYS:NZ	2.48	0.44
1:A:179:LEU:O	1:A:183:LEU:HG	2.17	0.44
1:B:177:MET:CE	1:B:182:TRP:HA	2.47	0.44
3:F:9[A]:DC:H2'	3:F:10:DT:H71	2.00	0.44
1:A:179:LEU:HD22	1:A:261:LEU:HB2	1.98	0.44
1:A:531:ARG:HE	1:A:531:ARG:C	2.20	0.44
1:A:369:PHE:CD2	1:A:376:LEU:HD22	2.53	0.44
1:A:21:PRO:HA	1:A:24:LEU:HD12	2.00	0.44
1:A:45:LEU:HD12	1:A:45:LEU:HA	1.78	0.44
1:A:296:TRP:HH2	1:A:300:ARG:HH11	1.65	0.43
1:A:548:ARG:O	1:A:550:PRO:HD3	2.17	0.43
1:A:392:ARG:HD3	1:A:428:GLU:OE2	2.18	0.43
1:A:179:LEU:H	1:A:179:LEU:HD23	1.82	0.43
1:A:115:ARG:HH21	1:A:118:GLN:CG	2.30	0.43
1:A:101:LYS:N	1:A:101:LYS:HD2	2.33	0.43
1:A:149:GLY:HA2	1:A:171:TYR:HD2	1.83	0.43
1:A:661:ARG:HA	1:A:661:ARG:HD3	1.90	0.43
1:A:178:SER:H	1:A:181:ALA:HB3	1.84	0.43
1:B:232:ARG:O	1:B:236:ARG:HD2	2.19	0.43
1:B:4:LEU:HD23	1:B:5:GLY:N	2.26	0.43
1:A:17:ARG:NH2	1:A:23:GLU:OE1	2.46	0.43
1:A:350:ARG:NH2	1:A:356:GLY:O	2.42	0.43
1:B:52:ARG:HD3	1:B:79:LEU:HD13	2.01	0.43
1:A:137:ARG:CZ	1:A:289:ARG:HH22	2.32	0.42
1:A:393:GLU:OE1	1:B:531:ARG:NH2	2.44	0.42
1:A:344:THR:HB	1:A:404:GLN:OE1	2.18	0.42
1:A:319:PRO:CG	1:A:640:ARG:HD3	2.45	0.42
1:A:409:LEU:HD23	1:A:435:LEU:HB3	2.00	0.42
1:A:48:GLN:HG2	1:A:79:LEU:HD11	2.02	0.42
1:A:171:TYR:HD1	1:A:279:LEU:HD23	1.84	0.42
1:A:195:ASN:HB3	1:A:197:TYR:CE1	2.54	0.42
1:A:469:TYR:OH	1:A:637:HIS:ND1	2.49	0.42
1:A:442:GLU:HG3	1:A:442:GLU:H	1.65	0.42
1:A:288:ARG:NH1	1:A:292:GLU:OE2	2.53	0.42
1:B:153:LEU:HA	1:B:166:GLU:O	2.20	0.42
1:A:596:LEU:HD11	1:A:602:LEU:HG	2.01	0.42
1:B:447:TRP:HE3	1:B:451:LEU:HD22	1.85	0.42
3:D:9[A]:DC:H2'	3:D:10:DT:H6	1.84	0.42
1:A:392:ARG:HG3	1:A:424:LEU:HD11	2.00	0.41
1:B:545:ARG:NH1	1:B:553:GLU:OE2	2.46	0.41
1:A:268:GLU:CD	3:D:13:DT:H4'	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ARG:NE	1:A:96:ARG:HB2	2.33	0.41
1:B:666:VAL:HG22	1:B:674:LEU:HD11	2.02	0.41
1:A:625:ASP:N	1:A:625:ASP:OD1	2.51	0.41
1:B:571:VAL:HG11	1:B:619:LEU:HD23	2.03	0.41
1:A:125:GLU:HA	1:A:127:VAL:H	1.86	0.41
1:A:369:PHE:HD1	1:A:374:ALA:HB3	1.86	0.41
1:A:171:TYR:CD1	1:A:279:LEU:HD23	2.56	0.41
1:A:365:LEU:HA	1:A:365:LEU:HD23	1.92	0.41
1:A:393:GLU:CD	1:B:531:ARG:HH21	2.23	0.41
1:A:171:TYR:CB	1:A:279:LEU:HD23	2.51	0.41
1:A:446:ARG:HG3	2:C:2:DG:N7	2.36	0.41
1:A:141:ARG:NH1	1:A:176:GLU:OE1	2.53	0.41
1:A:6:LYS:HG2	1:A:312:GLN:NE2	2.35	0.41
1:A:329:LYS:NZ	1:A:332:ASP:OD1	2.46	0.41
1:B:426:LEU:HA	1:B:426:LEU:HD12	1.82	0.41
1:A:348:LEU:HB2	1:A:357:TRP:CE2	2.55	0.41
2:E:3:DA:H2''	2:E:4:DG:H5'	2.02	0.40
1:A:150:GLY:O	1:A:169:PRO:HA	2.21	0.40
1:B:114:ARG:NE	1:B:154:ASP:OD1	2.50	0.40
1:A:315[B]:ARG:NH1	1:A:589:ALA:HB3	2.37	0.40
1:B:410:THR:O	1:B:436:ASN:HA	2.21	0.40
1:B:97:PRO:O	1:B:98:LEU:HD12	2.22	0.40
1:B:197:TYR:CD2	1:B:232:ARG:HD3	2.57	0.40
1:B:4:LEU:HB3	1:B:315:ARG:O	2.22	0.40
1:B:350:ARG:HB3	1:B:352:ASP:OD1	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	631/685 (92%)	601 (95%)	28 (4%)	2 (0%)	41 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	667/685 (97%)	631 (95%)	32 (5%)	4 (1%)	25 50
All	All	1298/1370 (95%)	1232 (95%)	60 (5%)	6 (0%)	29 54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	250	PRO
1	A	143	PRO
1	B	39	ARG
1	B	143	PRO
1	A	42	VAL
1	B	216	PRO

### 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	501/549 (91%)	460 (92%)	41 (8%)	11 26
1	B	522/549 (95%)	478 (92%)	44 (8%)	11 25
All	All	1023/1098 (93%)	938 (92%)	85 (8%)	11 25

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	41	GLU
1	A	108	VAL
1	A	115	ARG
1	A	121	LEU
1	A	125	GLU
1	A	134	VAL
1	A	141	ARG
1	A	165	LEU
1	A	193	VAL

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Mol	Chain	Res	Type
1	A	195	ASN
1	A	201	THR
1	A	204	LEU
1	A	257	LEU
1	A	271	HIS
1	A	299	ARG
1	A	335	ARG
1	A	344	THR
1	A	346	LEU
1	A	392	ARG
1	A	420	ARG
1	A	426	LEU
1	A	437	VAL
1	A	451	LEU
1	A	475	VAL
1	A	502	LEU
1	A	505	LEU
1	A	531	ARG
1	A	540	ARG
1	A	545	ARG
1	A	558	LEU
1	A	559	GLU
1	A	570	LEU
1	A	587	ARG
1	A	592	LEU
1	A	599	LYS
1	A	615	ARG
1	A	622	GLU
1	A	639	THR
1	A	640	ARG
1	A	641	LEU
1	B	4	LEU
1	B	6	LYS
1	B	28	ARG
1	B	30	GLU
1	B	48	GLN
1	B	51	ARG
1	B	79	LEU
1	B	115	ARG
1	B	122	ARG
1	B	123	ARG
1	B	214	GLU

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Mol	Chain	Res	Type
1	B	223	LEU
1	B	224	LEU
1	B	262	VAL
1	B	288	ARG
1	B	309	VAL
1	B	312	GLN
1	B	321	LEU
1	B	335	ARG
1	B	392	ARG
1	B	399	LYS
1	B	425	LEU
1	B	426	LEU
1	B	437	VAL
1	B	444	ARG
1	B	451	LEU
1	B	462	VAL
1	B	475	VAL
1	B	484	SER
1	B	505	LEU
1	B	531	ARG
1	B	539	SER
1	B	545	ARG
1	B	551	GLN
1	B	558	LEU
1	B	570	LEU
1	B	580	ARG
1	B	592	LEU
1	B	600	THR
1	B	604	LEU
1	B	639	THR
1	B	640	ARG
1	B	641	LEU
1	B	664	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	312	GLN
1	A	461	GLN
1	B	312	GLN
1	B	436	ASN



### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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

### 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	638/685 (93%)	0.37	59 (9%)  	45, 67, 135, 152	0
1	B	673/685 (98%)	0.37	60 (8%)  	44, 67, 113, 152	0
2	C	16/21 (76%)	-0.31	0  	58, 82, 96, 105	0
2	E	16/21 (76%)	-0.34	0  	53, 73, 82, 91	0
3	D	16/16 (100%)	-0.48	0  	60, 85, 102, 107	1 (6%)
3	F	16/16 (100%)	-0.50	0  	56, 75, 91, 101	0
All	All	1375/1444 (95%)	0.34	119 (8%)  	44, 68, 119, 152	1 (0%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	LEU	8.5
1	A	186	GLY	8.0
1	B	85	THR	7.6
1	A	203	GLU	7.3
1	A	182	TRP	7.3
1	A	227	HIS	6.9
1	B	43	TYR	6.4
1	B	249	ASP	6.2
1	B	33	LEU	6.0
1	A	200	ARG	5.8
1	A	192	ARG	5.7
1	A	145	TRP	5.6
1	A	232	ARG	5.5
1	A	226	TYR	5.4
1	B	251	ARG	5.4
1	B	45	LEU	5.4
1	A	177	MET	5.2
1	B	212	PRO	5.0
1	A	179	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	194	ARG	4.6
1	A	185	GLN	4.6
1	A	197	TYR	4.6
1	B	31	VAL	4.5
1	A	193	VAL	4.4
1	A	204	LEU	4.3
1	A	187	HIS	4.3
1	B	41	GLU	4.3
1	B	248	LYS	4.2
1	B	182	TRP	4.2
1	B	183	LEU	4.2
1	B	261	LEU	4.2
1	B	243	TRP	4.1
1	B	247	PRO	4.1
1	B	246	ASP	4.1
1	B	219	GLY	4.0
1	B	37	PRO	4.0
1	A	140	ALA	4.0
1	A	183	LEU	3.9
1	A	258	THR	3.8
1	A	15	ALA	3.8
1	B	79	LEU	3.8
1	A	225	ASP	3.8
1	B	223	LEU	3.8
1	A	262	VAL	3.7
1	A	261	LEU	3.7
1	A	175	CYS	3.6
1	B	214	GLU	3.6
1	A	82	MET	3.6
1	A	198	ASP	3.6
1	A	202	TRP	3.5
1	A	184	ALA	3.5
1	A	33	LEU	3.5
1	A	260	LEU	3.5
1	B	250	PRO	3.5
1	A	191	LYS	3.5
1	B	205	LEU	3.4
1	B	204	LEU	3.4
1	B	437	VAL	3.3
1	B	35	PRO	3.2
1	B	44	PRO	3.2
1	B	143	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	260	LEU	3.2
1	A	257	LEU	3.1
1	B	36	PRO	3.1
1	A	270	LEU	3.0
1	A	146	ARG	3.0
1	B	179	LEU	3.0
1	A	96	ARG	3.0
1	B	241	VAL	3.0
1	A	180	GLU	3.0
1	B	216	PRO	3.0
1	B	238	GLY	2.9
1	A	143	PRO	2.9
1	A	201	THR	2.8
1	B	211	ASP	2.8
1	B	263	PRO	2.8
1	A	144	GLY	2.8
1	B	209	GLU	2.8
1	A	174	LEU	2.8
1	B	262	VAL	2.7
1	A	141	ARG	2.7
1	B	215	LEU	2.7
1	B	199	ARG	2.7
1	A	37	PRO	2.6
1	B	34	ASP	2.6
1	A	148	LEU	2.6
1	B	141	ARG	2.6
1	A	229	SER	2.6
1	B	28	ARG	2.5
1	B	230	LYS	2.5
1	B	32	VAL	2.5
1	A	230	LYS	2.5
1	A	224	LEU	2.5
1	A	288	ARG	2.4
1	A	264	VAL	2.4
1	B	256	HIS	2.4
1	B	185	GLN	2.4
1	B	310	ARG	2.4
1	B	252	LYS	2.3
1	A	263	PRO	2.3
1	B	208	GLY	2.3
1	B	265	LEU	2.2
1	B	264	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	86	TYR	2.2
1	B	91	TYR	2.2
1	A	173	ILE	2.2
1	B	189	LEU	2.2
1	B	42	VAL	2.2
1	B	49	VAL	2.1
1	A	271	HIS	2.1
1	B	233	LEU	2.1
1	A	195	ASN	2.1
1	A	83	GLY	2.1
1	A	36	PRO	2.1
1	B	46	LEU	2.0
1	A	142	GLY	2.0
1	A	28	ARG	2.0
1	B	257	LEU	2.0
1	B	139	HIS	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	MG	A	701	1/1	0.83	0.21	65,65,65,65	0
4	MG	A	703	1/1	0.94	0.25	54,54,54,54	0
4	MG	B	701	1/1	0.96	0.23	51,51,51,51	0
4	MG	B	702	1/1	0.97	0.28	67,67,67,67	0
4	MG	B	703	1/1	0.97	0.29	67,67,67,67	0
4	MG	A	702	1/1	0.98	0.22	79,79,79,79	0

## 6.5 Other polymers

There are no such residues in this entry.