Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:55 PM GMT

PDB ID	:	4N76
Title	:	Structure of Thermus thermophilus Argonaute bound to guide DNA and cleaved target DNA with Mn2+
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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

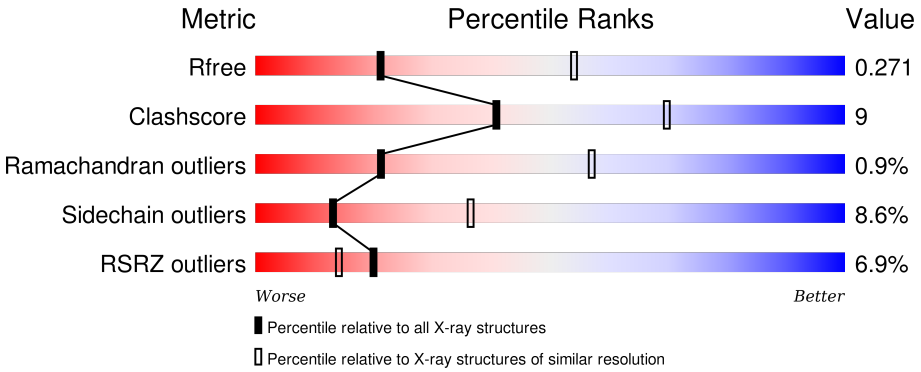
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 >=3, 2, 1 and 0 types of geometric quality criteria. 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	A	685	7%, 69%, 22%, 6%
1	B	685	7%, 72%, 23%
2	C	21	29%, 19%, 52%
2	E	21	33%, 19%, 48%
3	D	10	80%, 20%

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Mol	Chain	Length	Quality of chain
3	F	10	

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			

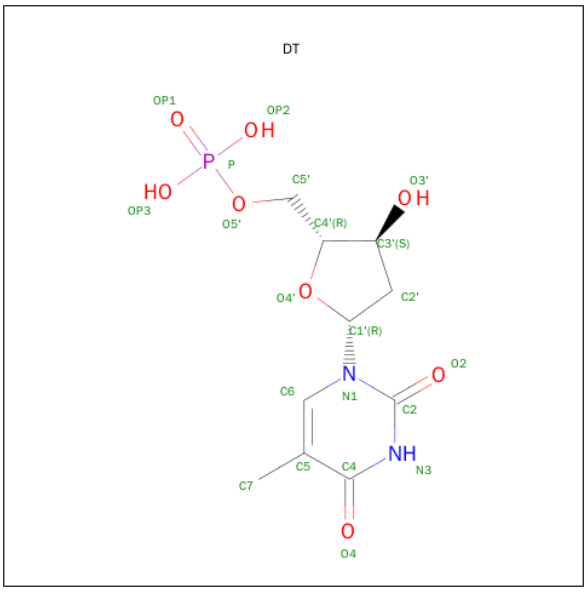
- Molecule 3 is a DNA chain called 5'-D(P*TP*AP*CP*TP*AP*CP*CP*TP*CP*G)-3'.

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: $C_{10}H_{15}N_2O_8P$).



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.

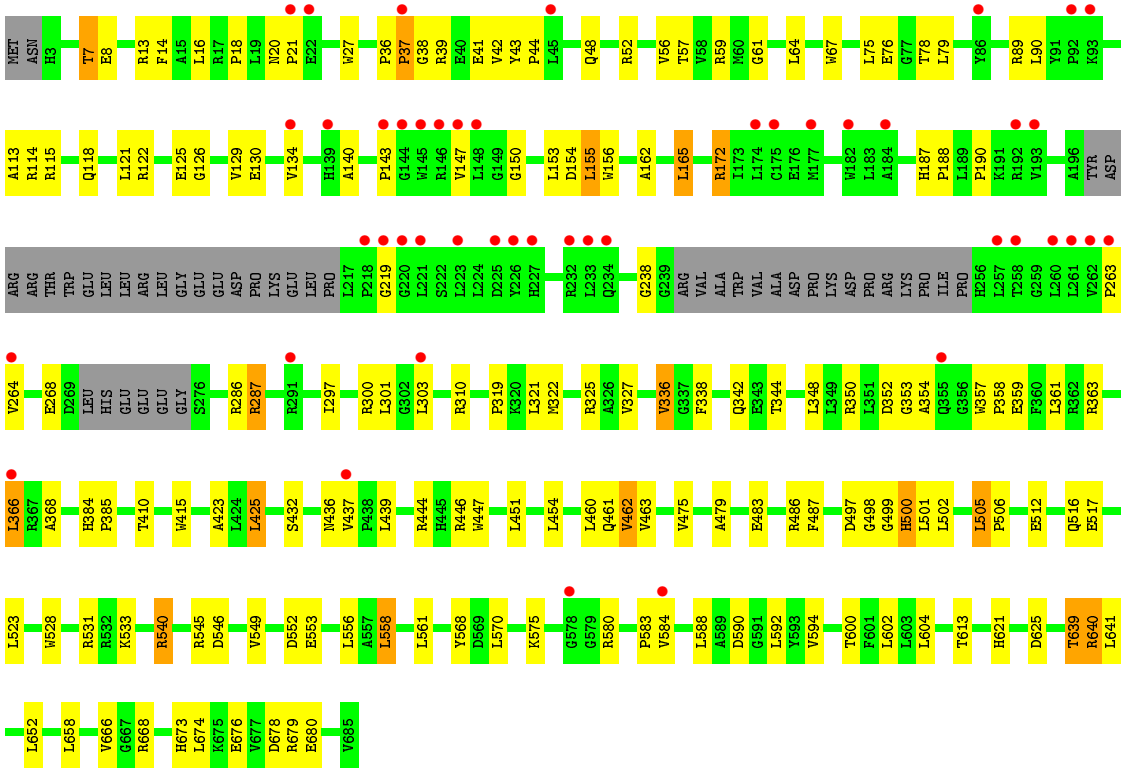
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	14	Total	O	0	0
			14	14		
6	C	1	Total	O	0	0
			1	1		
6	E	3	Total	O	0	0
			3	3		
6	F	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

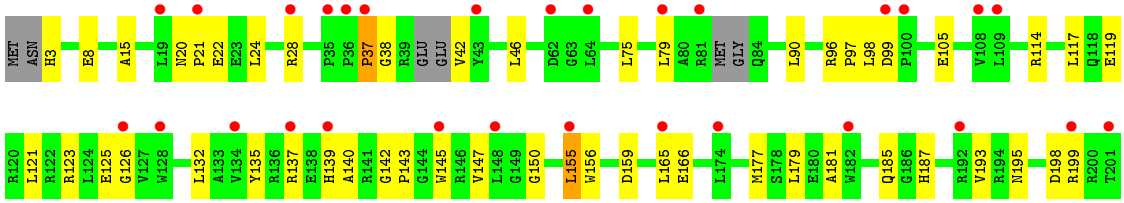
- Molecule 1: Argonaute

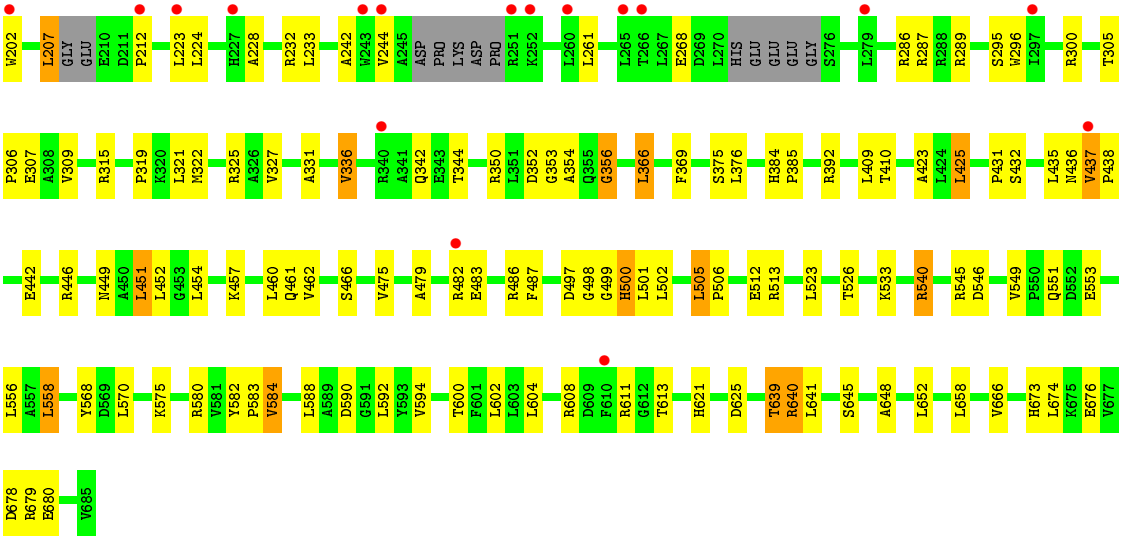
Chain A:



- Molecule 1: Argonaute

Chain B:





• 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'

Chain C:

• 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'

Chain E:

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

Chain D:

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

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.44 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.219 , 0.269 0.222 , 0.271	Depositor DCC
R_{free} test set	2294 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	42.6	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 8.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 45264 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	10818	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (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	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:B:500:HIS:CE1	1:B:533:LYS:HE3	2.44	0.52
1:A:437:VAL:O	1:A:439:LEU:N	2.42	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:38:GLY:O	1:A:39:ARG:C	2.48	0.51
1:A:13:ARG:HD3	1:A:156:TRP:CZ2	2.46	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:501:LEU:HD13	1:B:658:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:SER:HA	1:B:306:PRO:HG3	1.95	0.48
1:B:449:ASN:ND2	2:E:2:DG:H21	2.11	0.48
1:A:140:ALA:HB3	1:A:147:VAL:HB	1.94	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:498:GLY:HA3	1:A:641:LEU:HD11	1.94	0.48
1:A:462:VAL:HG23	1:A:463:VAL:HG13	1.96	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:338:PHE:CZ	1:A:368:ALA:HB1	2.50	0.46
1:A:18:PRO:HA	1:A:162:ALA:HA	1.96	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:287:ARG:HG3	1:B:582:TYR:CG	2.51	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: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:B:193:VAL:HG21	1:B:261:LEU:HB3	1.99	0.44
1:A:461:GLN:HG3	1:A:499:GLY:O	2.17	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:B:545:ARG:HG2	1:B:549:VAL:HG22	2.00	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:A:43:TYR:N	1:A:44:PRO:HD2	2.32	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:B:366:LEU:HD13	1:B:376:LEU:HD23	1.99	0.43
1:A:590:ASP:OD1	3:D:19:DG:N2	2.48	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:B:142:GLY:N	1:B:145:TRP:O	2.52	0.43
1:A:14:PHE:O	1:A:165:LEU:N	2.48	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:B:212:PRO:HB2	1:B:224:LEU:HB2	2.00	0.42
1:A:528:TRP:CE2	1:B:392:ARG:HD3	2.53	0.42
1:B:195:ASN:HB2	1:B:198:ASP:OD1	2.19	0.42
1:A:505:LEU:HA	1:A:505:LEU:HD23	1.92	0.42
1:A:187:HIS:HA	1:A:188:PRO:HD3	1.91	0.42
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.74	0.42
1:A:366:LEU:HA	1:A:366:LEU:HD13	1.83	0.42
1:A:325:ARG:HG2	1:A:336:VAL:HG13	2.02	0.42
1:B:409:LEU:HD23	1:B:435:LEU:HB3	2.02	0.42
1:B:37:PRO:HB2	1:B:38:GLY:H	1.64	0.42
1:B:315:ARG:NH2	6:B:802:HOH:O	2.46	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:321:LEU:HB3	1:A:327:VAL:HG23	2.02	0.42
1:A:36:PRO:HA	1:A:37:PRO:HD3	1.82	0.41
1:B:195:ASN:HD21	1:B:202:TRP:HE1	1.67	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: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:431:PRO:HB2	1:B:457:LYS:HB3	2.01	0.41
1:B:185:GLN:HB2	1:B:187:HIS:ND1	2.36	0.41
1:B:384:HIS:CG	1:B:385:PRO:HD2	2.56	0.41
1:A:446:ARG:HG3	2:C:2:DG:C8	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%)	21	57
1	B	655/685 (96%)	613 (94%)	36 (6%)	6 (1%)	21	57
All	All	1288/1370 (94%)	1193 (93%)	83 (6%)	12 (1%)	21	57

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	447/549 (81%)	409 (92%)	38 (8%)	13	37
1	B	492/549 (90%)	449 (91%)	43 (9%)	13	36
All	All	939/1098 (86%)	858 (91%)	81 (9%)	13	36

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.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	DT	B	704	-	17,22,22	1.24	3 (17%)	22,33,33	3.51	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DT	B	704	-	-	0/6/22/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	704	DT	C6-C5	-2.18	1.34	1.40
5	B	704	DT	C6-N1	2.15	1.38	1.35
5	B	704	DT	C4-N3	2.84	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	704	DT	C5-C4-N3	-8.72	115.42	125.14
5	B	704	DT	OP2-P-OP3	2.98	118.74	107.38
5	B	704	DT	C4-N3-C2	13.24	126.69	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	704	DT	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{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	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	641/685 (93%)	0.54	47 (7%) 18 12	3, 25, 103, 143	1 (0%)
1	B	667/685 (97%)	0.51	46 (6%) 20 14	1, 27, 82, 113	0
2	C	10/21 (47%)	-0.15	0 100 100	22, 26, 65, 83	0
2	E	11/21 (52%)	-0.07	0 100 100	16, 24, 73, 100	0
3	D	10/10 (100%)	-0.11	0 100 100	27, 66, 90, 91	0
3	F	10/10 (100%)	-0.27	0 100 100	26, 56, 76, 78	0
All	All	1349/1432 (94%)	0.51	93 (6%) 20 14	1, 26, 92, 143	1 (0%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	LEU	10.4
1	A	232	ARG	8.6
1	B	19	LEU	6.3
1	A	220	GLY	6.2
1	A	258	THR	6.0
1	B	37	PRO	6.0
1	A	145	TRP	5.9
1	A	219	GLY	5.9
1	A	226	TYR	5.6
1	A	263	PRO	5.5
1	B	145	TRP	4.9
1	A	260	LEU	4.5
1	B	202	TRP	4.4
1	B	260	LEU	4.4
1	B	610	PHE	4.3
1	A	174	LEU	4.3
1	A	37	PRO	4.1
1	A	584	VAL	4.0
1	A	193	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	251	ARG	3.7
1	A	261	LEU	3.7
1	B	266	THR	3.7
1	A	227	HIS	3.5
1	B	182	TRP	3.5
1	B	279	LEU	3.4
1	A	22	GLU	3.4
1	B	243	TRP	3.3
1	A	146	ARG	3.2
1	B	126	GLY	3.2
1	B	192	ARG	3.2
1	B	100	PRO	3.2
1	A	144	GLY	3.1
1	A	225	ASP	3.1
1	B	165	LEU	3.1
1	B	212	PRO	3.1
1	B	21	PRO	3.0
1	B	81	ARG	3.0
1	B	134	VAL	3.0
1	A	139	HIS	3.0
1	B	109	LEU	2.9
1	A	257	LEU	2.9
1	B	108	VAL	2.8
1	A	175	CYS	2.8
1	A	437	VAL	2.8
1	B	62	ASP	2.7
1	A	182	TRP	2.7
1	A	148	LEU	2.7
1	B	297	ILE	2.6
1	A	578	GLY	2.6
1	B	43	TYR	2.6
1	A	223	LEU	2.6
1	B	28	ARG	2.5
1	B	482	ARG	2.5
1	A	234	GLN	2.4
1	B	35	PRO	2.4
1	A	192	ARG	2.4
1	A	262	VAL	2.4
1	A	45	LEU	2.4
1	B	79	LEU	2.4
1	A	355	GLN	2.4
1	B	437	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	199	ARG	2.3
1	B	128	TRP	2.3
1	A	147	VAL	2.3
1	B	99	ASP	2.3
1	B	252	LYS	2.2
1	B	201	THR	2.2
1	B	227	HIS	2.2
1	A	184	ALA	2.2
1	A	86	TYR	2.2
1	A	177	MET	2.2
1	A	221	LEU	2.2
1	B	64	LEU	2.2
1	B	340	ARG	2.2
1	A	218	PRO	2.2
1	A	134	VAL	2.2
1	B	137	ARG	2.1
1	B	155	LEU	2.1
1	B	244	VAL	2.1
1	A	291	ARG	2.1
1	B	36	PRO	2.1
1	A	264	VAL	2.1
1	B	148	LEU	2.1
1	B	174	LEU	2.1
1	A	93	LYS	2.1
1	B	223	LEU	2.1
1	A	92	PRO	2.1
1	A	143	PRO	2.1
1	A	303	LEU	2.0
1	B	265	LEU	2.0
1	B	139	HIS	2.0
1	A	366	LEU	2.0
1	A	21	PRO	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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
5	DT	B	704	21/21	0.95	0.28	-0.13	47,64,75,84	0
4	MN	B	701	1/1	0.96	0.14	-2.08	50,50,50,50	0
4	MN	B	702	1/1	0.79	0.08	-2.10	63,63,63,63	1
4	MN	B	703	1/1	0.79	0.09	-2.19	81,81,81,81	0
4	MN	C	101	1/1	0.98	0.15	-2.23	53,53,53,53	0

6.5 Other polymers

There are no such residues in this entry.