W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:13 AM GMT

PDB ID	:	3HM9
Title	:	Crystal structure of T. thermophilus Argonaute complexed with DNA guide strand and 19-nt RNA target strand
Authors	:	Wang, Y.; Li, H.; Sheng, G.; Patel, D.J.
Deposited on	:	2009-05-28
Resolution	:	3.30 Å(reported)

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

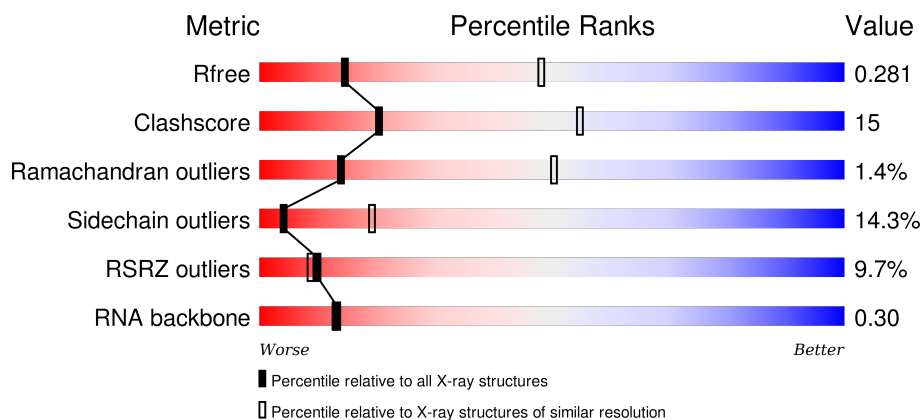|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.30 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	Percentile Ranks	Value
Rfree		0.281
Clashscore		15
Ramachandran outliers		1.4%
Sidechain outliers		14.3%
RSRZ outliers		9.7%
RNA backbone		0.30

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)
RNA backbone	2183	1005 (3.82-2.78)

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	10% 67% 24% 5% 5%
2	X	21	24% 29% 24% 24%
3	Y	19	5% 32% 26% 5% 32%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	A	687	-	-	-	X

Full wwPDB X-ray Structure Validation Report

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5239 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	654	Total 4631	C 2946	N 862	O 817	S 6	0	0	0

- 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	X	16	Total 338	C 160	N 62	O 100	P 16	0	0	0

- Molecule 3 is a RNA chain called 5'-R(*UP*AP*UP*AP*CP*AP*AP*CP*CP*UP*AP*CP *UP*AP*CP*CP*UP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	13	Total 268	C 121	N 44	O 90	P 13	0	0	0

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

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Mg 2	0	0

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 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

• 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'
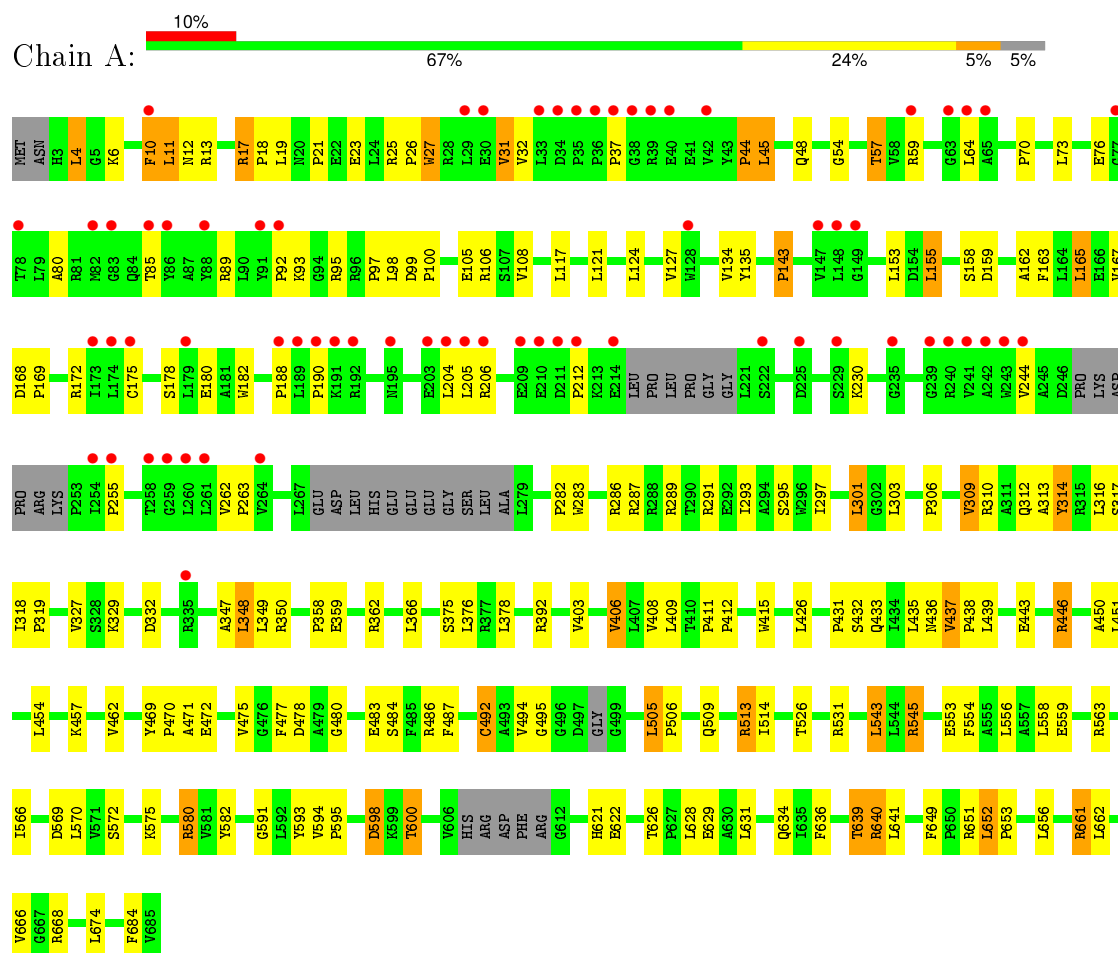
● Molecule 3: 5'-R(*UP*AP*UP*AP*CP*AP*AP*CP*CP*UP*AP*CP*UP*AP*CP*CP*UP*C P*G)-3'

Chain Y:
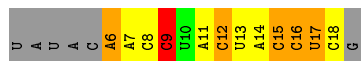
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	111.92Å 111.92Å 175.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 43.48 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-3.30) 99.6 (43.48-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.237 , 0.289 0.233 , 0.281	Depositor DCC
R_{free} test set	871 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	113.2	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 93.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 17386 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5239	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: 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	0.51	3/4727 (0.1%)	0.71	8/6445 (0.1%)
2	X	1.10	2/379 (0.5%)	1.83	15/584 (2.6%)
3	Y	1.38	3/297 (1.0%)	1.86	11/458 (2.4%)
All	All	0.64	8/5403 (0.1%)	0.95	34/7487 (0.5%)

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	A	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	6	A	O3'-P	-17.13	1.40	1.61
2	X	1	DT	OP3-P	-10.98	1.48	1.61
2	X	6	DT	O3'-P	-9.89	1.49	1.61
1	A	204	LEU	C-N	7.40	1.51	1.34
3	Y	9	C	C3'-O3'	6.03	1.50	1.42
1	A	492	CYS	CB-SG	-5.60	1.72	1.81
3	Y	7	A	O3'-P	-5.22	1.54	1.61
1	A	206	ARG	C-N	-5.21	1.22	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	7	DA	P-O3'-C3'	-10.02	107.67	119.70
2	X	7	DA	OP2-P-O3'	9.86	126.90	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	17	U	P-O3'-C3'	-9.75	108.00	119.70
3	Y	12	C	P-O3'-C3'	-9.65	108.11	119.70
2	X	1	DT	OP1-P-OP2	-9.34	105.59	119.60
2	X	15	DG	C3'-C2'-C1'	-8.75	92.00	102.50
2	X	15	DG	P-O3'-C3'	8.56	129.97	119.70
3	Y	7	A	P-O3'-C3'	7.98	129.28	119.70
2	X	15	DG	O4'-C1'-N9	7.91	113.53	108.00
2	X	5	DG	O4'-C4'-C3'	-7.40	101.54	104.50
3	Y	9	C	C4'-C3'-C2'	-7.21	95.39	102.60
3	Y	9	C	P-O3'-C3'	6.76	127.82	119.70
3	Y	12	C	OP2-P-O3'	6.70	119.94	105.20
2	X	15	DG	C1'-O4'-C4'	-6.54	103.56	110.10
1	A	143	PRO	N-CA-CB	6.04	110.55	103.30
1	A	282	PRO	N-CA-CB	5.92	110.41	103.30
1	A	212	PRO	N-CA-CB	5.87	110.34	103.30
1	A	255	PRO	N-CA-CB	5.83	110.29	103.30
1	A	188	PRO	N-CA-CB	5.73	110.17	103.30
3	Y	11	A	C4'-C3'-C2'	-5.68	96.92	102.60
1	A	92	PRO	N-CA-CB	5.67	110.11	103.30
2	X	7	DA	OP1-P-O3'	-5.65	92.77	105.20
1	A	190	PRO	N-CA-CB	5.62	110.04	103.30
1	A	263	PRO	N-CA-CB	5.46	109.86	103.30
2	X	9	DT	C4'-C3'-C2'	-5.46	98.19	103.10
3	Y	13	U	P-O3'-C3'	5.44	126.23	119.70
3	Y	17	U	O4'-C1'-N1	5.42	112.54	108.20
3	Y	9	C	O4'-C1'-N1	5.38	112.50	108.20
2	X	11	DG	O4'-C1'-N9	5.24	111.67	108.00
2	X	5	DG	O4'-C1'-N9	5.19	111.63	108.00
2	X	9	DT	C4-C5-C7	5.18	122.11	119.00
2	X	3	DA	O4'-C1'-N9	5.13	111.59	108.00
3	Y	12	C	O3'-P-O5'	-5.13	94.24	104.00
2	X	15	DG	N9-C1'-C2'	5.01	122.11	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	436	ASN	Peptide
1	A	494	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	4631	0	4271	131	0
2	X	338	0	183	8	0
3	Y	268	0	141	10	0
4	A	2	0	0	0	0
All	All	5239	0	4595	144	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 15.

All (144) 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:11:LEU:HD13	1:A:13:ARG:HG3	1.37	1.06
1:A:513:ARG:HH11	1:A:513:ARG:HG3	1.17	1.05
1:A:11:LEU:CD1	1:A:13:ARG:HG3	1.87	1.04
1:A:17:ARG:HE	1:A:303:LEU:HD23	1.28	0.96
1:A:327:VAL:CG2	1:A:332:ASP:HB2	1.98	0.93
1:A:327:VAL:HG23	1:A:332:ASP:HB2	1.56	0.87
1:A:640:ARG:HG3	1:A:640:ARG:HH11	1.36	0.87
1:A:513:ARG:HH11	1:A:513:ARG:CG	1.89	0.85
1:A:70:PRO:HA	1:A:73:LEU:HG	1.61	0.83
1:A:661:ARG:HH21	1:A:661:ARG:CG	1.91	0.83
1:A:636:PHE:O	1:A:639:THR:HB	1.81	0.80
1:A:640:ARG:CG	1:A:640:ARG:HH11	1.94	0.79
1:A:661:ARG:HH21	1:A:661:ARG:HG3	1.46	0.79
1:A:480:GLY:CA	1:A:486:ARG:HB3	2.16	0.75
1:A:492:CYS:SG	1:A:526:THR:HB	2.27	0.73
1:A:575:LYS:HE3	3:Y:9:C:H5'	1.69	0.73
1:A:11:LEU:HD11	1:A:13:ARG:HG3	1.69	0.73
1:A:415:TRP:HZ3	1:A:668:ARG:HD2	1.51	0.72
1:A:483:GLU:HG2	1:A:484:SER:H	1.53	0.72
1:A:13:ARG:HB2	1:A:309:VAL:CG1	2.23	0.69
1:A:289:ARG:O	1:A:293:ILE:HG12	1.93	0.69
1:A:124:LEU:HB2	1:A:127:VAL:HG21	1.74	0.69
1:A:437:VAL:HG12	1:A:438:PRO:HD3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ARG:HD3	1:A:303:LEU:HA	1.76	0.68
1:A:480:GLY:HA2	1:A:487:PHE:H	1.58	0.68
1:A:471:ALA:HB3	1:A:634:GLN:HE22	1.58	0.68
1:A:415:TRP:CZ3	1:A:668:ARG:HD2	2.29	0.67
1:A:11:LEU:HD12	1:A:11:LEU:C	2.14	0.67
1:A:640:ARG:HG3	1:A:640:ARG:NH1	2.08	0.67
1:A:513:ARG:NH1	1:A:513:ARG:HG3	1.97	0.67
1:A:327:VAL:HG21	1:A:332:ASP:HB2	1.77	0.66
1:A:80:ALA:HB2	1:A:85:THR:HA	1.77	0.66
1:A:121:LEU:HD22	1:A:134:VAL:HG21	1.77	0.65
1:A:593:TYR:CZ	1:A:595:PRO:HG3	2.31	0.65
1:A:446:ARG:HG2	2:X:2:DG:C8	2.31	0.65
1:A:4:LEU:HG	1:A:314:TYR:HD1	1.63	0.64
2:X:6:DT:C2	2:X:7:DA:C8	2.85	0.64
1:A:480:GLY:HA2	1:A:486:ARG:HB3	1.78	0.63
1:A:480:GLY:HA3	1:A:486:ARG:HB3	1.80	0.63
1:A:18:PRO:HA	1:A:162:ALA:HA	1.80	0.63
1:A:513:ARG:NH1	1:A:513:ARG:CG	2.57	0.63
1:A:639:THR:HG22	1:A:640:ARG:HD2	1.81	0.62
1:A:437:VAL:O	1:A:439:LEU:N	2.32	0.62
1:A:316:LEU:HB2	1:A:591:GLY:O	1.99	0.62
1:A:483:GLU:CG	1:A:484:SER:H	2.10	0.62
1:A:158:SER:O	1:A:159:ASP:HB2	2.00	0.62
1:A:13:ARG:HB2	1:A:309:VAL:HG13	1.82	0.61
1:A:575:LYS:HB3	1:A:651:ARG:NH2	2.15	0.61
1:A:483:GLU:HG2	1:A:484:SER:N	2.15	0.61
1:A:135:TYR:CE2	1:A:172:ARG:HB2	2.36	0.61
2:X:3:DA:H2'	2:X:4:DG:C8	2.35	0.61
1:A:10:PHE:HB3	1:A:310:ARG:HA	1.83	0.60
2:X:15:DG:C2	3:Y:6:A:C2	2.90	0.60
1:A:327:VAL:HG23	1:A:332:ASP:CB	2.29	0.60
2:X:6:DT:C2	2:X:7:DA:N7	2.70	0.59
1:A:59:ARG:HA	1:A:64:LEU:HA	1.84	0.59
1:A:366:LEU:HD23	1:A:376:LEU:HD23	1.83	0.59
1:A:11:LEU:CD1	1:A:13:ARG:CG	2.73	0.58
3:Y:17:U:O2'	3:Y:18:C:H5'	2.04	0.58
1:A:44:PRO:O	1:A:48:GLN:HB3	2.04	0.58
3:Y:17:U:H2'	3:Y:18:C:C6	2.39	0.57
1:A:11:LEU:HD11	1:A:13:ARG:CG	2.35	0.56
1:A:12:ASN:ND2	1:A:580:ARG:HB2	2.20	0.56
1:A:11:LEU:O	1:A:11:LEU:HD12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ALA:CB	1:A:594:VAL:HG22	2.36	0.55
1:A:76:GLU:HG2	1:A:89:ARG:HD3	1.87	0.55
1:A:661:ARG:CG	1:A:661:ARG:NH2	2.59	0.55
1:A:287:ARG:O	1:A:291:ARG:HG3	2.07	0.55
1:A:165:LEU:HD13	1:A:167:VAL:HG23	1.88	0.54
1:A:640:ARG:HD2	1:A:640:ARG:N	2.23	0.53
1:A:666:VAL:HG22	1:A:674:LEU:HD11	1.89	0.53
1:A:11:LEU:CD1	1:A:11:LEU:C	2.76	0.53
1:A:433:GLN:HG2	1:A:450:ALA:O	2.09	0.53
1:A:297:ILE:O	1:A:301:LEU:HB2	2.09	0.53
1:A:472:GLU:O	1:A:495:GLY:N	2.41	0.53
2:X:3:DA:H2'	2:X:4:DG:H8	1.74	0.53
1:A:347:ALA:HB2	1:A:403:VAL:HG11	1.91	0.53
1:A:554:PHE:O	1:A:558:LEU:HG	2.09	0.52
3:Y:16:C:OP2	3:Y:16:C:H6	1.91	0.52
1:A:349:LEU:HB3	1:A:408:VAL:HG22	1.92	0.52
1:A:10:PHE:CZ	1:A:291:ARG:NH2	2.78	0.52
1:A:313:ALA:HB2	1:A:594:VAL:HG22	1.92	0.52
1:A:80:ALA:CB	1:A:85:THR:HA	2.40	0.51
1:A:506:PRO:HG2	1:A:666:VAL:HG21	1.93	0.51
1:A:411:PRO:O	1:A:412:PRO:C	2.49	0.51
1:A:621:HIS:CE1	1:A:631:LEU:HD11	2.45	0.51
1:A:575:LYS:HB3	1:A:651:ARG:HH22	1.75	0.51
1:A:569:ASP:OD2	1:A:626:THR:OG1	2.29	0.51
1:A:319:PRO:HG2	1:A:640:ARG:HD3	1.92	0.50
1:A:575:LYS:HE3	3:Y:9:C:C5'	2.40	0.50
1:A:545:ARG:HD2	1:A:553:GLU:OE1	2.12	0.50
1:A:348:LEU:HD21	1:A:350:ARG:HG3	1.94	0.50
1:A:295:SER:HA	1:A:306:PRO:HG2	1.94	0.50
1:A:54:GLY:O	1:A:57:THR:OG1	2.30	0.50
1:A:117:LEU:HB2	1:A:155:LEU:HG	1.94	0.49
1:A:652:LEU:CB	1:A:653:PRO:HD2	2.43	0.49
1:A:639:THR:HG22	1:A:640:ARG:CD	2.42	0.48
1:A:19:LEU:HD23	1:A:23:GLU:HB3	1.96	0.48
1:A:97:PRO:O	1:A:98:LEU:HD12	2.14	0.48
1:A:45:LEU:HA	1:A:48:GLN:HG2	1.96	0.47
1:A:437:VAL:CG1	1:A:438:PRO:HD3	2.44	0.47
1:A:475:VAL:HG23	1:A:477:PHE:CE1	2.50	0.47
1:A:347:ALA:HB3	1:A:406:VAL:HB	1.96	0.46
1:A:480:GLY:HA2	1:A:487:PHE:N	2.29	0.46
1:A:509:GLN:HE22	1:A:514:ILE:HG23	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:LEU:HD23	1:A:435:LEU:HB3	1.97	0.46
1:A:19:LEU:HG	1:A:163:PHE:CE1	2.51	0.46
1:A:640:ARG:HA	1:A:649:PHE:CD2	2.50	0.46
1:A:439:LEU:HA	1:A:443:GLU:OE1	2.17	0.45
1:A:314:TYR:N	1:A:314:TYR:CD2	2.84	0.45
1:A:628:LEU:HA	1:A:631:LEU:HD12	1.99	0.45
1:A:312:GLN:CD	1:A:312:GLN:H	2.20	0.45
2:X:15:DG:N2	3:Y:6:A:C2	2.85	0.45
1:A:431:PRO:HB2	1:A:457:LYS:HB3	1.99	0.44
1:A:475:VAL:HG22	1:A:543:LEU:HD12	2.00	0.43
1:A:31:VAL:HG12	1:A:32:VAL:H	1.81	0.43
2:X:8:DG:C6	2:X:9:DT:C4	3.07	0.43
1:A:469:TYR:HB3	1:A:470:PRO:HD2	1.99	0.43
3:Y:14:A:H2'	3:Y:15:C:C6	2.53	0.43
1:A:17:ARG:O	1:A:17:ARG:HG2	2.17	0.43
1:A:314:TYR:HD2	1:A:314:TYR:N	2.17	0.43
1:A:656:LEU:HA	1:A:656:LEU:HD23	1.79	0.43
1:A:652:LEU:HB2	1:A:653:PRO:HD2	2.01	0.43
1:A:105:GLU:O	1:A:106:ARG:C	2.57	0.42
3:Y:15:C:H2'	3:Y:16:C:O4'	2.20	0.42
1:A:26:PRO:HD2	1:A:98:LEU:HD13	2.02	0.42
1:A:6:LYS:HE2	1:A:314:TYR:CZ	2.55	0.42
1:A:358:PRO:O	1:A:359:GLU:C	2.57	0.42
1:A:27:TRP:CE3	1:A:70:PRO:HD3	2.55	0.41
1:A:662:LEU:HB2	1:A:684:PHE:CZ	2.56	0.41
1:A:629:GLU:CD	1:A:629:GLU:H	2.23	0.41
1:A:168:ASP:HA	1:A:169:PRO:HD3	1.79	0.41
1:A:505:LEU:HA	1:A:505:LEU:HD23	1.95	0.41
1:A:99:ASP:HA	1:A:100:PRO:HD3	1.82	0.41
1:A:27:TRP:CE3	1:A:95:ARG:HD2	2.55	0.41
1:A:286:ARG:HG2	1:A:582:TYR:OH	2.19	0.41
3:Y:17:U:H2'	3:Y:18:C:H6	1.82	0.41
1:A:652:LEU:H	1:A:652:LEU:HD12	1.85	0.41
1:A:598:ASP:O	1:A:600:THR:HG22	2.21	0.40
1:A:155:LEU:HD13	1:A:163:PHE:HD2	1.85	0.40
1:A:11:LEU:HD13	1:A:13:ARG:CG	2.28	0.40
1:A:180:GLU:C	1:A:182:TRP:H	2.24	0.40
1:A:158:SER:O	1:A:159:ASP:CB	2.65	0.40
1:A:153:LEU:HD22	1:A:167:VAL:HG22	2.02	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	642/685 (94%)	571 (89%)	62 (10%)	9 (1%)	14	50

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	462	VAL
1	A	262	VAL
1	A	37	PRO
1	A	93	LYS
1	A	205	LEU
1	A	21	PRO
1	A	244	VAL
1	A	143	PRO
1	A	44	PRO

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	384/549 (70%)	329 (86%)	55 (14%)	4	19

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	10	PHE

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Mol	Chain	Res	Type
1	A	11	LEU
1	A	17	ARG
1	A	25	ARG
1	A	27	TRP
1	A	31	VAL
1	A	45	LEU
1	A	57	THR
1	A	108	VAL
1	A	155	LEU
1	A	165	LEU
1	A	175	CYS
1	A	178	SER
1	A	230	LYS
1	A	283	TRP
1	A	301	LEU
1	A	309	VAL
1	A	314	TYR
1	A	317	SER
1	A	318	ILE
1	A	329	LYS
1	A	348	LEU
1	A	362	ARG
1	A	375	SER
1	A	378	LEU
1	A	392	ARG
1	A	406	VAL
1	A	426	LEU
1	A	432	SER
1	A	437	VAL
1	A	446	ARG
1	A	451	LEU
1	A	454	LEU
1	A	478	ASP
1	A	505	LEU
1	A	513	ARG
1	A	531	ARG
1	A	543	LEU
1	A	545	ARG
1	A	556	LEU
1	A	559	GLU
1	A	563	ARG
1	A	566	ILE

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Mol	Chain	Res	Type
1	A	570	LEU
1	A	572	SER
1	A	580	ARG
1	A	598	ASP
1	A	600	THR
1	A	622	GLU
1	A	639	THR
1	A	640	ARG
1	A	641	LEU
1	A	652	LEU
1	A	661	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	509	GLN
1	A	634	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	Y	12/19 (63%)	5 (41%)	1 (8%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	Y	8	C
3	Y	9	C
3	Y	12	C
3	Y	15	C
3	Y	16	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	Y	9	C

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 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, 95th 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(Å²)	Q<0.9
1	A	654/685 (95%)	0.36	66 (10%)	9	8	46, 58, 66, 71	0
2	X	16/21 (76%)	-0.31	0	100	100	47, 55, 60, 61	0
3	Y	13/19 (68%)	-0.48	0	100	100	45, 54, 61, 62	0
All	All	683/725 (94%)	0.32	66 (9%)	10	9	45, 58, 66, 71	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	261	LEU	15.4
1	A	189	LEU	10.8
1	A	190	PRO	7.4
1	A	260	LEU	6.6
1	A	225	ASP	6.6
1	A	34	ASP	6.6
1	A	64	LEU	6.5
1	A	29	LEU	6.4
1	A	210	GLU	6.4
1	A	195	ASN	6.1
1	A	244	VAL	6.0
1	A	258	THR	5.8
1	A	211	ASP	5.5
1	A	243	TRP	5.2
1	A	255	PRO	5.2
1	A	83	GLY	5.2
1	A	82	MET	5.2
1	A	37	PRO	4.9
1	A	63	GLY	4.9
1	A	205	LEU	4.9
1	A	188	PRO	4.9
1	A	59	ARG	4.7
1	A	39	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	40	GLU	3.9
1	A	147	VAL	3.6
1	A	239	GLY	3.6
1	A	242	ALA	3.6
1	A	191	LYS	3.6
1	A	174	LEU	3.4
1	A	204	LEU	3.4
1	A	241	VAL	3.4
1	A	35	PRO	3.4
1	A	209	GLU	3.3
1	A	91	TYR	3.2
1	A	85	THR	3.1
1	A	240	ARG	3.0
1	A	222	SER	3.0
1	A	254	ILE	2.8
1	A	229	SER	2.8
1	A	173	ILE	2.8
1	A	36	PRO	2.8
1	A	77	GLY	2.8
1	A	212	PRO	2.7
1	A	203	GLU	2.7
1	A	128	TRP	2.7
1	A	42	VAL	2.6
1	A	86	TYR	2.6
1	A	148	LEU	2.5
1	A	92	PRO	2.5
1	A	149	GLY	2.5
1	A	175	CYS	2.4
1	A	214	GLU	2.4
1	A	88	TYR	2.4
1	A	30	GLU	2.3
1	A	206	ARG	2.2
1	A	179	LEU	2.2
1	A	78	THR	2.2
1	A	192	ARG	2.2
1	A	65	ALA	2.2
1	A	264	VAL	2.1
1	A	10	PHE	2.1
1	A	235	GLY	2.1
1	A	335	ARG	2.1
1	A	33	LEU	2.0
1	A	259	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	38	GLY	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. 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, 95th 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
4	MG	A	687	1/1	0.94	0.36	6.50	68,68,68,68	0
4	MG	A	686	1/1	0.97	0.27	1.45	60,60,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.