Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2017 – 02:20 AM EST

PDB ID	:	4N41
Title	:	Structure of Thermus thermophilus Argonaute bound to guide DNA and 15-mer target DNA
Authors	:	Sheng, G.; Zhao, H.; Wang, J.; Rao, Y.; Wang, Y.
Deposited on	:	2013-10-08
Resolution	:	2.25 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 ⓘ symbol.

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

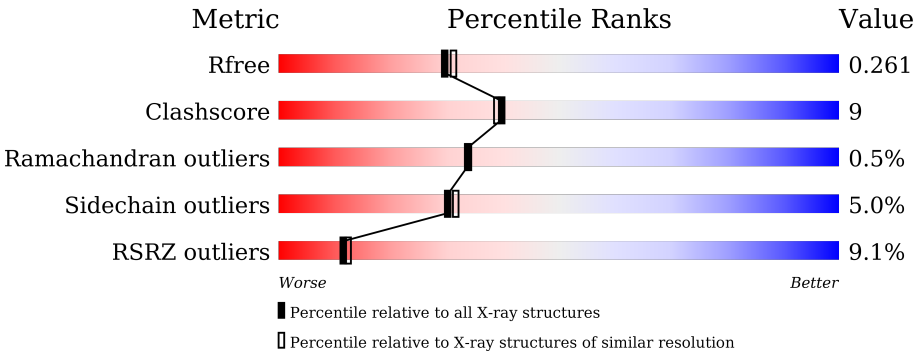
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.25 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	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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	8% 77% 17%
1	B	685	10% 76% 20%
2	C	21	24% 33% 14% 29%
2	E	21	5% 33% 33% 10% 24%
3	D	13	38% 46% 15%
4	F	14	29% 57% 14%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11432 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	658	Total	C	N	O	S	0	1	0
			4977	3177	937	857	6			
1	B	667	Total	C	N	O	S	0	0	0
			5093	3261	949	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*T*GP*TP*AP*TP*AP*GP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	P	0	0	0
			315	150	60	91	14			
2	E	16	Total	C	N	O	P	0	0	0
			338	160	62	100	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	13	Total	C	N	O	P	0	0	0
			259	124	44	78	13			

- Molecule 4 is a DNA chain called 5'-D(*AP*AP*CP*CP*TP*AP*CP*TP*GP*CP*CP*TP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	14	Total	C	N	O	P	0	0	0
			277	134	49	81	13			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	E	1	Total Mg 1 1	0	0

- Molecule 6 is water.

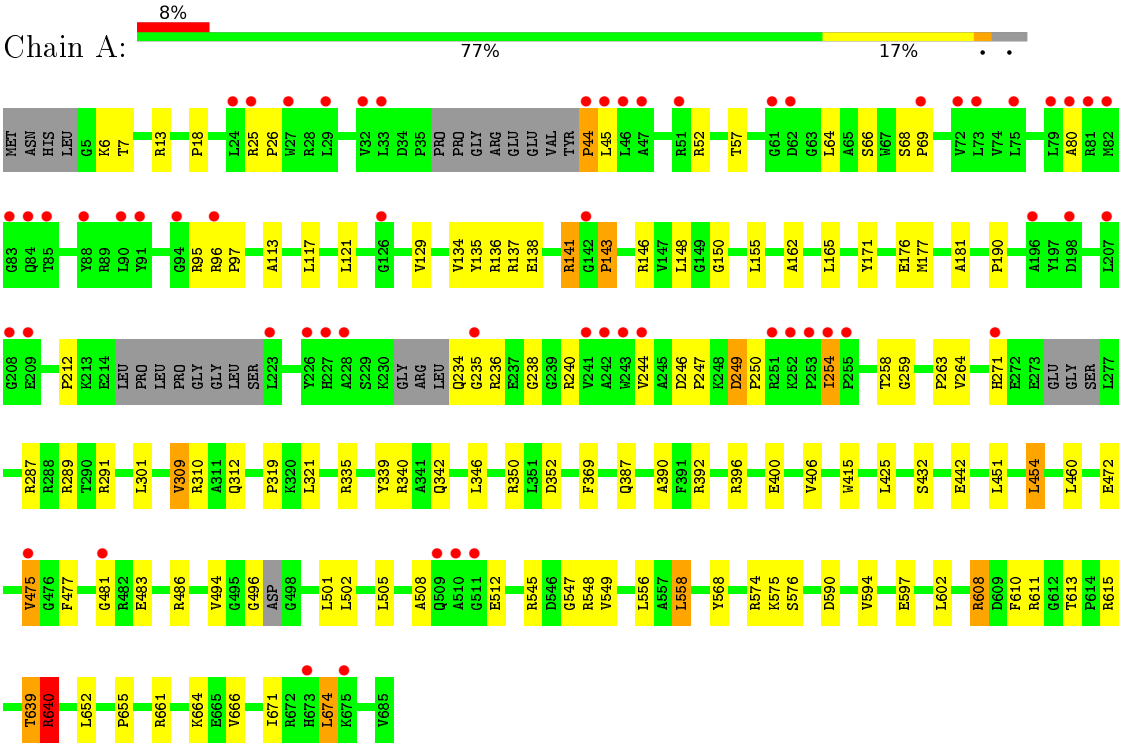
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	126	Total O 126 126	0	0
6	B	14	Total O 14 14	0	0
6	C	15	Total O 15 15	0	0
6	E	6	Total O 6 6	0	0
6	D	8	Total O 8 8	0	0
6	F	1	Total O 1 1	0	0

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.

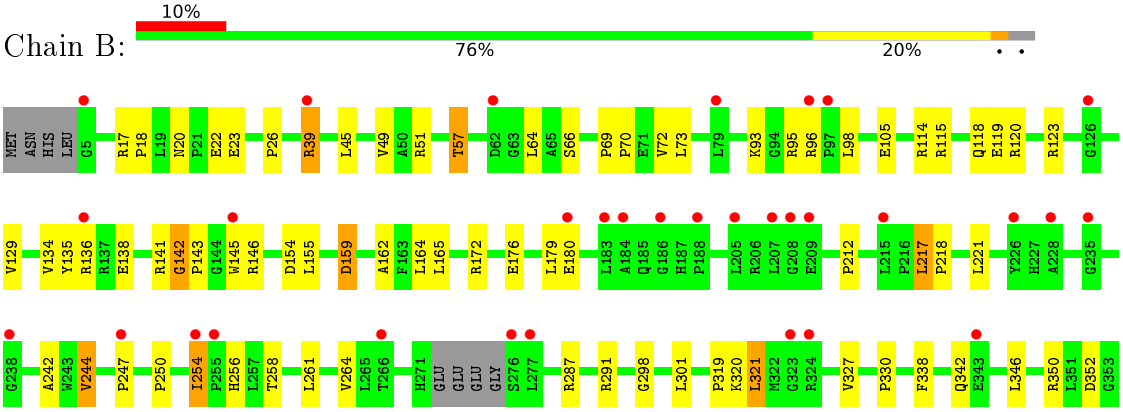
- Molecule 1: Argonaute

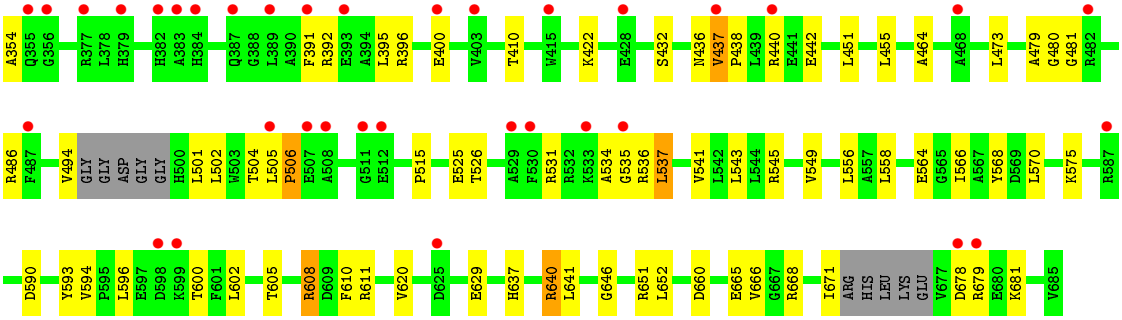
Chain A:



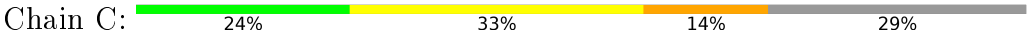
- Molecule 1: Argonaute

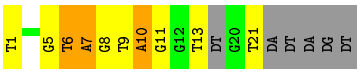
Chain B:



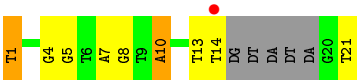


• Molecule 2: 5'-D(P*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*T*GP*TP*AP*T P*AP*GP*T)-3'

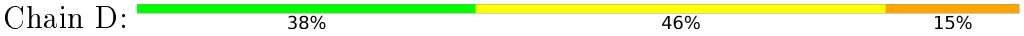


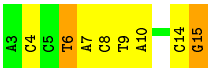


• Molecule 2: 5'-D(P*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*T*GP*TP*AP*T P*AP*GP*T)-3'

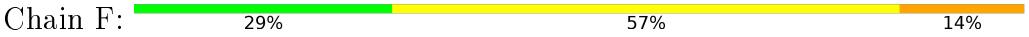


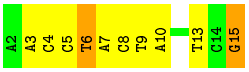
• Molecule 3: 5'-D(P*AP*CP*CP*TP*AP*CP*TP*AP*CP*CP*TP*CP*G)-3'





• Molecule 4: 5'-D(*AP*AP*CP*CP*TP*AP*CP*TP*GP*CP*CP*TP*CP*G)-3'





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.51Å 101.70Å 153.02Å 90.00° 93.52° 90.00°	Depositor
Resolution (Å)	45.52 – 2.25 45.52 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.52-2.25) 99.7 (45.52-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.223 , 0.259 0.225 , 0.261	Depositor DCC
R_{free} test set	4327 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11432	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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, 0.333 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	0.50	1/5092 (0.0%)	0.64	9/6922 (0.1%)
1	B	0.32	0/5212	0.54	5/7090 (0.1%)
2	C	1.03	1/353 (0.3%)	1.71	9/542 (1.7%)
2	E	0.82	1/378 (0.3%)	1.52	2/580 (0.3%)
3	D	0.85	0/288	1.67	4/440 (0.9%)
4	F	0.61	0/309	1.35	3/473 (0.6%)
All	All	0.49	3/11632 (0.0%)	0.79	32/16047 (0.2%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	PRO	C-N	14.55	1.67	1.34
2	E	1	DT	OP3-P	-10.77	1.48	1.61
2	C	1	DT	OP3-P	-10.02	1.49	1.61

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	4	DC	O4'-C1'-N1	9.72	114.81	108.00
2	E	10	DA	O4'-C4'-C3'	-9.46	100.33	106.00
2	E	1	DT	OP1-P-OP2	-8.46	106.90	119.60
3	D	15	DG	O4'-C1'-N9	-8.32	102.17	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	13	DT	O4'-C1'-N1	7.54	113.28	108.00
2	C	6	DT	O4'-C1'-N1	7.18	113.03	108.00
1	A	143	PRO	N-CA-CB	6.99	111.69	103.30
2	C	1	DT	O4'-C1'-N1	-6.93	103.15	108.00
4	F	6	DT	O4'-C1'-N1	6.80	112.76	108.00
2	C	1	DT	OP1-P-OP2	-6.77	109.45	119.60
1	A	44	PRO	O-C-N	-6.45	112.39	122.70
1	A	640	ARG	NE-CZ-NH2	-6.34	117.13	120.30
2	C	11	DG	O4'-C4'-C3'	-6.30	101.98	104.50
3	D	6	DT	O4'-C1'-N1	6.26	112.38	108.00
1	B	218	PRO	N-CA-CB	6.26	110.81	103.30
1	A	249	ASP	N-CA-C	-6.14	94.43	111.00
1	B	247	PRO	N-CA-CB	6.04	110.55	103.30
1	B	250	PRO	N-CA-CB	5.84	110.31	103.30
2	C	7	DA	O4'-C1'-N9	5.83	112.08	108.00
4	F	3	DA	O4'-C1'-N9	5.82	112.08	108.00
1	B	212	PRO	N-CA-CB	5.79	110.25	103.30
1	B	143	PRO	N-CA-CB	5.77	110.22	103.30
1	A	640	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	247	PRO	N-CA-CB	5.54	109.95	103.30
4	F	15	DG	O4'-C1'-N9	-5.54	104.12	108.00
1	A	212	PRO	N-CA-CB	5.41	109.79	103.30
2	C	10	DA	O4'-C4'-C3'	-5.35	102.36	104.50
1	A	454	LEU	CA-CB-CG	5.14	127.13	115.30
2	C	9	DT	C4'-C3'-C2'	-5.12	98.50	103.10
3	D	7	DA	O4'-C1'-N9	5.11	111.58	108.00
1	A	250	PRO	N-CA-CB	5.09	109.41	103.30
2	C	10	DA	O4'-C1'-N9	5.05	111.53	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	508	ALA	Peptide
1	A	597	GLU	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	4977	0	4894	82	0
1	B	5093	0	5046	92	0
2	C	315	0	173	10	0
2	E	338	0	184	7	0
3	D	259	0	147	6	0
4	F	277	0	159	9	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
6	A	126	0	0	9	0
6	B	14	0	0	1	0
6	C	15	0	0	1	0
6	D	8	0	0	1	0
6	E	6	0	0	0	0
6	F	1	0	0	0	0
All	All	11432	0	10603	191	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 (191) 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:44:PRO:C	1:A:45:LEU:N	1.67	1.48
1:A:545:ARG:NH2	1:A:549:VAL:O	2.11	0.84
1:B:545:ARG:NH2	1:B:549:VAL:O	2.11	0.82
1:A:113:ALA:HB1	1:A:155:LEU:HD13	1.62	0.80
1:A:350:ARG:NH2	1:A:352:ASP:OD1	2.16	0.79
1:A:246:ASP:O	1:A:249:ASP:O	2.01	0.78
1:B:575:LYS:HE2	1:B:652:LEU:HD11	1.70	0.74
1:A:472:GLU:O	1:A:496:GLY:N	2.24	0.69
1:B:440:ARG:NE	1:B:442:GLU:OE2	2.25	0.68
1:A:141:ARG:NH2	1:A:176:GLU:OE1	2.26	0.68
1:A:335:ARG:NH1	6:A:785:HOH:O	2.22	0.66
1:B:350:ARG:NH2	1:B:352:ASP:OD1	2.29	0.66
1:B:22:GLU:OE1	1:B:95:ARG:NH2	2.27	0.66
1:B:575:LYS:O	1:B:651:ARG:NH2	2.26	0.66
1:A:52:ARG:HH12	1:A:80:ALA:H	1.42	0.65
1:A:129:VAL:HG22	1:A:134:VAL:HG12	1.77	0.65
2:E:13:DT:H2"	2:E:14:DT:H5'	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4:DG:H2'	2:E:5:DG:C8	2.32	0.65
1:B:473:LEU:HB3	1:B:541:VAL:HG12	1.78	0.64
1:A:319:PRO:HG2	1:A:640:ARG:HG3	1.79	0.64
1:B:605:THR:O	1:B:640:ARG:NH2	2.28	0.63
1:B:120:ARG:NH1	1:B:301:LEU:O	2.31	0.63
1:B:504:THR:HG22	1:B:679:ARG:HH21	1.62	0.62
1:B:525:GLU:HG3	1:B:679:ARG:HH22	1.64	0.62
3:D:8:DC:H2'	3:D:9:DT:C6	2.35	0.62
1:A:590:ASP:OD2	3:D:15:DG:N1	2.18	0.61
1:B:531:ARG:HE	1:B:537:LEU:HD13	1.65	0.61
1:A:146:ARG:NH1	1:A:176:GLU:OE2	2.34	0.61
1:A:350:ARG:NH1	6:A:797:HOH:O	2.30	0.60
1:A:25:ARG:HH22	1:A:95:ARG:NH2	2.00	0.60
1:A:271:HIS:HD2	3:D:10:DA:H5"	1.66	0.59
4:F:9:DT:H2'	4:F:10:DA:C8	2.38	0.59
1:A:639:THR:HG21	1:A:640:ARG:HH21	1.68	0.59
1:B:17:ARG:NH1	1:B:18:PRO:O	2.33	0.58
1:A:639:THR:CG2	1:A:640:ARG:HH21	2.16	0.58
4:F:8:DC:H2'	4:F:9:DT:C6	2.38	0.58
1:A:575:LYS:HE2	1:A:652:LEU:HD11	1.84	0.58
1:A:350:ARG:HH21	1:A:350:ARG:HB3	1.68	0.58
1:A:481:GLY:HA3	3:D:6:DT:H5'	1.86	0.58
1:B:242:ALA:HB2	1:B:258:THR:HG22	1.85	0.57
1:B:330:PRO:HB2	1:B:646:GLY:HA2	1.85	0.57
1:B:593:TYR:CE2	1:B:629:GLU:HG3	2.39	0.57
1:A:171:TYR:OH	1:A:289:ARG:NH2	2.37	0.57
1:A:350:ARG:HH22	1:A:352:ASP:CG	2.07	0.57
1:B:437:VAL:HG23	1:B:438:PRO:HD3	1.87	0.56
1:B:138:GLU:OE2	1:B:141:ARG:HB3	2.06	0.55
1:A:392:ARG:HB3	1:A:396:ARG:HH21	1.71	0.55
1:B:45:LEU:O	1:B:49:VAL:HG23	2.07	0.55
1:B:534:ALA:O	1:B:536:ARG:N	2.39	0.55
1:B:537:LEU:HD23	1:B:566:ILE:HD11	1.88	0.54
1:A:138:GLU:OE2	1:A:141:ARG:HG3	2.08	0.54
1:B:464:ALA:HA	1:B:641:LEU:HD21	1.90	0.54
1:B:558:LEU:HG	1:B:568:TYR:CE1	2.43	0.54
1:B:608:ARG:HG2	1:B:610:PHE:CE2	2.43	0.54
1:A:611:ARG:HD3	2:C:5:DG:H1'	1.90	0.53
1:B:665:GLU:OE1	1:B:668:ARG:NH2	2.41	0.53
1:A:608:ARG:HG2	1:A:610:PHE:CE2	2.44	0.53
1:B:590:ASP:OD2	4:F:15:DG:N1	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:VAL:HG22	1:B:134:VAL:HG12	1.92	0.52
1:B:217:LEU:HD11	2:E:21:DT:H2'	1.91	0.52
1:B:481:GLY:HA3	4:F:6:DT:H5'	1.90	0.52
1:A:234:GLN:O	1:A:236:ARG:N	2.36	0.52
1:B:115:ARG:NH1	1:B:118:GLN:OE1	2.43	0.52
1:A:287:ARG:HD3	1:A:291:ARG:CZ	2.41	0.51
1:B:180:GLU:OE1	1:B:258:THR:OG1	2.21	0.51
6:A:737:HOH:O	2:C:7:DA:H5"	2.09	0.51
1:A:18:PRO:HA	1:A:162:ALA:HA	1.91	0.51
3:D:9:DT:H2'	3:D:10:DA:C8	2.46	0.51
2:C:7:DA:OP1	6:C:202:HOH:O	2.19	0.51
4:F:4:DC:H2'	4:F:5:DC:C6	2.46	0.51
1:B:57:THR:HG22	1:B:66:SER:OG	2.11	0.51
1:B:594:VAL:HB	1:B:602:LEU:HB2	1.93	0.51
1:B:319:PRO:HG2	1:B:640:ARG:HG3	1.93	0.50
4:F:4:DC:H2'	4:F:5:DC:H6	1.77	0.50
1:A:594:VAL:HB	1:A:602:LEU:HB2	1.94	0.50
1:B:531:ARG:NE	1:B:537:LEU:HD13	2.26	0.50
2:C:6:DT:H2'	2:C:7:DA:H8	1.77	0.50
1:B:422:LYS:NZ	2:E:1:DT:OP1	2.36	0.50
1:A:44:PRO:C	1:A:45:LEU:CA	2.71	0.49
1:A:240:ARG:O	1:A:258:THR:HG23	2.12	0.49
1:B:159:ASP:OD2	1:B:159:ASP:N	2.45	0.49
1:B:70:PRO:HA	1:B:73:LEU:HD12	1.94	0.49
1:A:291:ARG:NH1	6:A:711:HOH:O	2.46	0.49
1:B:525:GLU:HG3	1:B:679:ARG:NH2	2.27	0.49
1:A:350:ARG:NE	6:A:797:HOH:O	2.42	0.49
1:A:13:ARG:HG3	1:A:309:VAL:HG13	1.95	0.49
1:A:608:ARG:NH2	6:A:723:HOH:O	2.45	0.48
1:A:135:TYR:HA	1:A:150:GLY:HA3	1.96	0.48
1:B:410:THR:O	1:B:436:ASN:HA	2.14	0.48
2:E:7:DA:H2'	2:E:8:DG:C8	2.48	0.48
1:A:494:VAL:HG22	1:A:501:LEU:CD2	2.44	0.48
1:A:264:VAL:HG11	2:C:10:DA:H5'	1.96	0.48
1:B:264:VAL:HG11	2:E:10:DA:H5'	1.96	0.48
1:B:114:ARG:NH2	1:B:154:ASP:OD2	2.43	0.48
1:B:319:PRO:HG3	1:B:637:HIS:CD2	2.49	0.48
1:A:611:ARG:HD3	2:C:5:DG:C1'	2.44	0.47
1:B:350:ARG:HH21	1:B:350:ARG:HB3	1.79	0.47
1:B:392:ARG:NH1	1:B:396:ARG:HH22	2.12	0.47
1:A:547:GLY:HA3	1:A:574:ARG:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:PRO:HG3	1:A:263:PRO:HB3	1.96	0.47
1:B:217:LEU:HB2	1:B:221:LEU:O	2.15	0.47
1:B:506:PRO:O	1:B:671:ILE:HD11	2.14	0.47
1:A:483:GLU:HA	1:A:548:ARG:HG3	1.95	0.47
1:B:600:THR:HG22	1:B:620:VAL:HG22	1.96	0.47
1:A:319:PRO:HG2	1:A:640:ARG:CG	2.45	0.47
1:A:666:VAL:HA	1:A:671:ILE:HG22	1.97	0.47
4:F:9:DT:H2'	4:F:10:DA:H8	1.79	0.47
1:B:142:GLY:N	1:B:145:TRP:O	2.48	0.47
1:B:494:VAL:HG22	1:B:501:LEU:HD22	1.96	0.46
1:A:26:PRO:HD2	1:A:96:ARG:O	2.15	0.46
1:A:310:ARG:HD3	6:A:776:HOH:O	2.15	0.46
1:A:238:GLY:HA2	1:A:259:GLY:HA3	1.96	0.46
1:B:396:ARG:O	1:B:400:GLU:HG3	2.16	0.46
1:B:146:ARG:HD3	1:B:176:GLU:OE2	2.16	0.46
1:A:396:ARG:O	1:A:400:GLU:HG3	2.16	0.46
3:D:14:DC:OP1	6:D:102:HOH:O	2.21	0.46
1:A:671:ILE:HD11	1:A:674:LEU:HB2	1.97	0.46
1:B:666:VAL:HG13	1:B:671:ILE:HB	1.98	0.46
1:B:17:ARG:NH2	1:B:23:GLU:OE1	2.44	0.46
1:B:422:LYS:HD2	1:B:432:SER:OG	2.16	0.46
1:B:531:ARG:NH1	1:B:536:ARG:HA	2.31	0.45
1:B:298:GLY:O	6:B:801:HOH:O	2.21	0.45
1:A:177:MET:HB2	1:A:181:ALA:HB3	1.98	0.45
1:A:136:ARG:HG3	1:A:137:ARG:N	2.31	0.45
1:A:339:TYR:CD2	1:A:340:ARG:HG3	2.52	0.45
1:B:486:ARG:HG2	1:B:515:PRO:HD3	1.99	0.45
1:A:576:SER:HA	1:A:615:ARG:HH21	1.82	0.44
1:B:352:ASP:HB3	1:B:437:VAL:HG21	1.99	0.44
1:B:479:ALA:C	1:B:481:GLY:H	2.19	0.44
1:A:57:THR:HG22	1:A:66:SER:OG	2.18	0.44
1:B:504:THR:HG21	1:B:526:THR:OG1	2.16	0.44
1:B:479:ALA:O	1:B:481:GLY:N	2.45	0.44
1:A:254:ILE:HG13	2:C:21:DT:H1'	1.99	0.44
1:B:287:ARG:HD3	1:B:291:ARG:CZ	2.47	0.44
1:B:610:PHE:CG	4:F:13:DT:H4'	2.53	0.44
1:B:244:VAL:HG12	1:B:254:ILE:HG23	2.00	0.44
1:B:564:GLU:HB3	1:B:566:ILE:HG13	1.99	0.44
1:A:494:VAL:HG23	1:A:655:PRO:HG3	1.99	0.44
1:A:6:LYS:HD3	1:A:312:GLN:HE21	1.83	0.44
1:B:338:PHE:CZ	1:B:455:LEU:HD13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ARG:NE	1:B:39:ARG:H	2.15	0.44
1:A:319:PRO:CG	1:A:640:ARG:HG3	2.47	0.43
1:B:155:LEU:HD12	1:B:164:LEU:O	2.18	0.43
1:A:442:GLU:CD	1:A:442:GLU:H	2.20	0.43
1:A:574:ARG:NH2	6:A:751:HOH:O	2.52	0.43
1:B:494:VAL:HG11	1:B:641:LEU:HD13	1.99	0.43
1:B:69:PRO:O	1:B:72:VAL:HG22	2.17	0.43
1:A:68:SER:HA	1:A:69:PRO:HD3	1.90	0.43
1:B:18:PRO:HA	1:B:162:ALA:HA	2.00	0.43
2:C:6:DT:H2'	2:C:7:DA:C8	2.54	0.43
1:A:425:LEU:HD12	1:A:432:SER:HB3	2.01	0.43
1:B:678:ASP:HB2	1:B:681:LYS:HG3	2.00	0.43
1:A:350:ARG:CZ	6:A:797:HOH:O	2.67	0.43
1:A:96:ARG:HA	1:A:97:PRO:HD3	1.82	0.43
1:A:369:PHE:CZ	1:A:460:LEU:HD21	2.53	0.43
1:A:613:THR:O	2:C:6:DT:H5"	2.18	0.43
1:B:611:ARG:HD3	2:E:5:DG:H1'	2.00	0.43
1:A:121:LEU:HD22	1:A:134:VAL:HG11	2.01	0.42
1:B:98:LEU:HD22	1:B:105:GLU:HG2	2.00	0.42
1:B:321:LEU:HB3	1:B:327:VAL:HG23	2.00	0.42
1:B:115:ARG:O	1:B:119:GLU:HG2	2.19	0.42
1:A:13:ARG:HG3	1:A:309:VAL:CG1	2.49	0.42
1:A:475:VAL:HG22	1:A:477:PHE:CE1	2.55	0.42
1:A:486:ARG:HD3	1:A:512:GLU:OE2	2.19	0.42
1:B:20:ASN:OD1	1:B:23:GLU:N	2.48	0.42
1:A:558:LEU:HG	1:A:568:TYR:CE1	2.55	0.42
1:B:505:LEU:HD21	1:B:666:VAL:HG21	2.01	0.42
1:A:146:ARG:HE	1:A:148:LEU:HD21	1.85	0.42
1:A:505:LEU:HA	1:A:505:LEU:HD23	1.79	0.42
1:A:505:LEU:HD21	1:A:666:VAL:HG21	2.02	0.42
1:A:674:LEU:HD23	1:A:674:LEU:HA	1.73	0.42
1:A:664:LYS:HB2	1:A:664:LYS:HE3	1.85	0.41
1:A:117:LEU:O	1:A:121:LEU:HG	2.20	0.41
1:B:135:TYR:CE2	1:B:172:ARG:HB2	2.55	0.41
1:B:51:ARG:NH2	1:B:115:ARG:HH12	2.18	0.41
1:B:26:PRO:HD2	1:B:96:ARG:O	2.19	0.41
1:A:387:GLN:HB3	1:A:390:ALA:HB3	2.03	0.41
1:B:17:ARG:HH22	1:B:23:GLU:CD	2.22	0.41
1:B:179:LEU:N	1:B:261:LEU:O	2.48	0.41
1:A:287:ARG:HD3	1:A:291:ARG:NH1	2.35	0.41
1:B:256:HIS:HB3	1:B:261:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:6:DT:H2'	4:F:7:DA:C8	2.55	0.41
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.85	0.41
1:B:93:LYS:HD3	1:B:93:LYS:HA	1.92	0.41
1:B:596:LEU:HD11	1:B:602:LEU:HG	2.03	0.40
1:A:117:LEU:HD22	1:A:155:LEU:HB2	2.02	0.40
1:B:51:ARG:NH2	1:B:115:ARG:HH22	2.20	0.40
1:B:536:ARG:NH1	1:B:537:LEU:O	2.55	0.40
2:C:7:DA:H2'	2:C:8:DG:C8	2.56	0.40
1:B:350:ARG:NH2	1:B:354:ALA:HB3	2.37	0.40
1:B:391:PHE:CE2	1:B:395:LEU:HD11	2.57	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	647/685 (94%)	623 (96%)	22 (3%)	2 (0%)	46	51
1	B	659/685 (96%)	638 (97%)	16 (2%)	5 (1%)	24	20
All	All	1306/1370 (95%)	1261 (97%)	38 (3%)	7 (0%)	34	34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	PRO
1	B	142	GLY
1	A	235	GLY
1	B	535	GLY
1	B	506	PRO
1	B	480	GLY
1	B	437	VAL

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	466/549 (85%)	442 (95%)	24 (5%)	29 29
1	B	484/549 (88%)	461 (95%)	23 (5%)	31 33
All	All	950/1098 (86%)	903 (95%)	47 (5%)	30 33

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	64	LEU
1	A	141	ARG
1	A	165	LEU
1	A	244	VAL
1	A	254	ILE
1	A	301	LEU
1	A	309	VAL
1	A	321	LEU
1	A	342	GLN
1	A	346	LEU
1	A	406	VAL
1	A	415	TRP
1	A	451	LEU
1	A	454	LEU
1	A	475	VAL
1	A	502	LEU
1	A	556	LEU
1	A	558	LEU
1	A	608	ARG
1	A	639	THR
1	A	640	ARG
1	A	661	ARG
1	A	674	LEU
1	B	39	ARG
1	B	57	THR
1	B	64	LEU

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Mol	Chain	Res	Type
1	B	123	ARG
1	B	136	ARG
1	B	159	ASP
1	B	165	LEU
1	B	217	LEU
1	B	244	VAL
1	B	254	ILE
1	B	320	LYS
1	B	321	LEU
1	B	342	GLN
1	B	346	LEU
1	B	451	LEU
1	B	502	LEU
1	B	537	LEU
1	B	543	LEU
1	B	556	LEU
1	B	570	LEU
1	B	608	ARG
1	B	640	ARG
1	B	660	ASP

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	271	HIS
1	A	312	GLN
1	A	342	GLN
1	B	382	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 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

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	658/685 (96%)	0.60	58 (8%) 12 13	28, 50, 120, 138	0
1	B	667/685 (97%)	0.66	67 (10%) 9 10	49, 78, 106, 126	0
2	C	15/21 (71%)	0.23	0 100 100	38, 45, 110, 114	0
2	E	16/21 (76%)	0.21	1 (6%) 23 24	58, 66, 95, 105	0
3	D	13/13 (100%)	-0.20	0 100 100	38, 53, 73, 86	0
4	F	14/14 (100%)	-0.07	0 100 100	51, 74, 92, 95	0
All	All	1383/1439 (96%)	0.61	126 (9%) 11 12	28, 69, 114, 138	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	HIS	8.2
1	A	223	LEU	8.2
1	A	243	TRP	8.1
1	A	241	VAL	8.0
1	A	47	ALA	7.5
1	A	46	LEU	7.3
1	A	208	GLY	6.8
1	B	254	ILE	6.2
1	B	487	PHE	5.9
1	B	355	GLN	5.8
1	A	72	VAL	5.5
1	A	82	MET	4.9
1	B	235	GLY	4.9
1	A	62	ASP	4.8
1	A	196	ALA	4.7
1	A	73	LEU	4.6
1	B	468	ALA	4.5
1	B	508	ALA	4.5
1	A	33	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	5	GLY	4.4
1	B	184	ALA	4.4
1	B	415	TRP	4.2
1	A	253	PRO	4.2
1	B	226	TYR	4.1
1	A	251	ARG	4.0
1	B	207	LEU	3.9
1	A	44	PRO	3.8
1	B	389	LEU	3.6
1	A	29	LEU	3.6
1	A	226	TYR	3.5
1	B	186	GLY	3.5
1	A	673	HIS	3.5
1	A	207	LEU	3.5
1	B	356	GLY	3.4
1	B	228	ALA	3.4
1	B	96	ARG	3.4
2	E	14	DT	3.4
1	B	205	LEU	3.4
1	B	79	LEU	3.4
1	A	126	GLY	3.3
1	B	188	PRO	3.3
1	A	79	LEU	3.3
1	A	94	GLY	3.3
1	B	599	LYS	3.3
1	B	511	GLY	3.2
1	A	32	VAL	3.2
1	B	266	THR	3.2
1	B	598	ASP	3.1
1	A	511	GLY	3.1
1	B	391	PHE	3.1
1	B	136	ARG	3.0
1	A	27	TRP	3.0
1	B	403	VAL	3.0
1	B	393	GLU	3.0
1	B	507	GLU	3.0
1	B	437	VAL	2.9
1	A	254	ILE	2.9
1	B	247	PRO	2.9
1	A	88	TYR	2.9
1	B	382	HIS	2.9
1	A	228	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	39	ARG	2.8
1	A	90	LEU	2.8
1	B	183	LEU	2.8
1	A	91	TYR	2.8
1	A	85	THR	2.8
1	B	440	ARG	2.8
1	B	387	GLN	2.8
1	A	25	ARG	2.8
1	A	242	ALA	2.7
1	B	535	GLY	2.7
1	B	679	ARG	2.7
1	A	255	PRO	2.7
1	B	400	GLU	2.6
1	B	625	ASP	2.6
1	A	271	HIS	2.6
1	A	45	LEU	2.6
1	B	343	GLU	2.6
1	B	323	GLY	2.6
1	A	81	ARG	2.6
1	B	533	LYS	2.6
1	B	276	SER	2.6
1	B	126	GLY	2.6
1	A	61	GLY	2.5
1	A	83	GLY	2.5
1	A	142	GLY	2.5
1	A	244	VAL	2.5
1	A	80	ALA	2.5
1	A	24	LEU	2.5
1	A	69	PRO	2.5
1	B	277	LEU	2.5
1	A	51	ARG	2.5
1	B	505	LEU	2.5
1	A	510	ALA	2.4
1	A	84	GLN	2.4
1	A	235	GLY	2.4
1	B	678	ASP	2.4
1	B	383	ALA	2.3
1	B	208	GLY	2.3
1	B	482	ARG	2.3
1	B	62	ASP	2.3
1	A	509	GLN	2.3
1	A	75	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	209	GLU	2.2
1	B	384	HIS	2.2
1	B	377	ARG	2.2
1	B	145	TRP	2.2
1	B	530	PHE	2.1
1	B	215	LEU	2.1
1	B	428	GLU	2.1
1	B	529	ALA	2.1
1	A	198	ASP	2.1
1	A	96	ARG	2.1
1	B	97	PRO	2.1
1	A	675	LYS	2.1
1	A	252	LYS	2.1
1	A	475	VAL	2.1
1	B	180	GLU	2.0
1	B	587	ARG	2.0
1	A	481	GLY	2.0
1	B	238	GLY	2.0
1	B	209	GLU	2.0
1	B	512	GLU	2.0
1	B	255	PRO	2.0
1	B	379	HIS	2.0
1	B	324	ARG	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, 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	MG	E	101	1/1	0.95	0.20	0.63	71,71,71,71	0
5	MG	C	101	1/1	0.97	0.15	-0.12	32,32,32,32	0
5	MG	B	701	1/1	0.80	0.09	-2.74	68,68,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.