



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:54 am BST

PDB ID : 5XPA
Title : Crystal structure of T. thermophilus Argonaute protein complexed with a bulge 9'U10' on the target strand
Authors : Sheng, G.; Gogakos, T.; Wang, J.; Zhao, H.; Serganov, A.; Juranek, S.; Tuschl, T.; Patel, J.D.; Wang, Y.
Deposited on : 2017-06-01
Resolution : 2.90 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

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

with specific help available everywhere you see the ⓘ symbol.

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

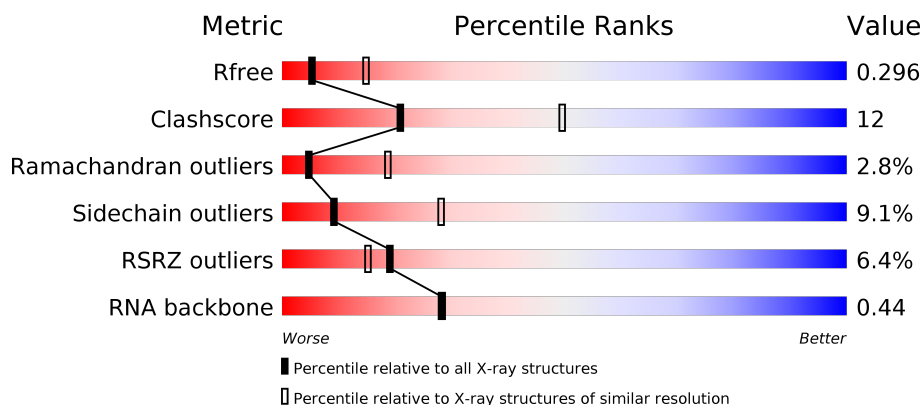
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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 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	
2	C	21	
3	D	20	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5967 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 Uncharacterized protein Ago.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	679	Total	C	N	O	S	0	0	0
			5150	3296	968	880	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	546	ASN	ASP	engineered mutation	UNP Q746M7

- Molecule 2 is a DNA chain called DNA (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	21	Total	C	N	O	P	0	0	0
			440	208	81	130	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	19	Total	C	N	O	P	0	0	0
			376	168	61	128	19			

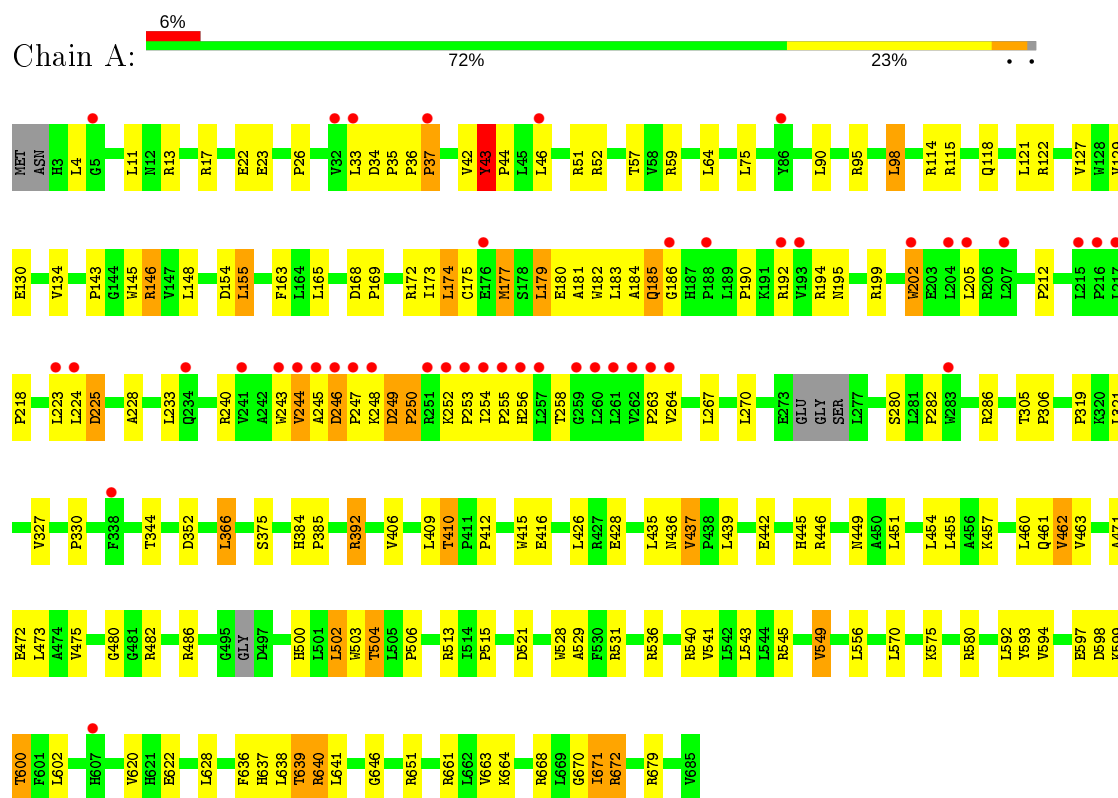
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

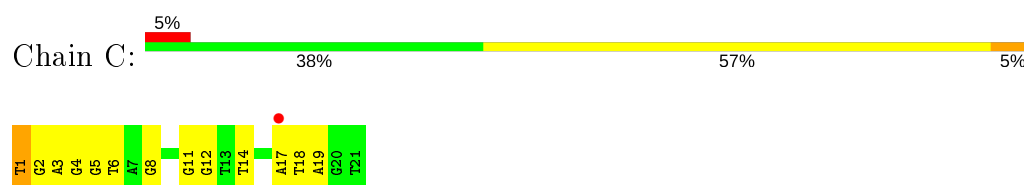
3 Residue-property plots [i](#)

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



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



• Molecule 3: RNA (5'-R(P*AP*UP*AP*CP*AP*AP*CP*CP*GP*UP*UP*CP*UP*AP*CP*U P*CP*CP*G)-3')





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	109.13Å 109.13Å 184.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.15 – 2.90 43.15 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.15-2.90) 99.9 (43.15-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.215 , 0.281 0.241 , 0.296	Depositor DCC
R_{free} test set	1292 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	87.1	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5967	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.36	0/5269	0.57	5/7170 (0.1%)
2	C	0.69	1/494 (0.2%)	1.26	1/761 (0.1%)
3	D	0.38	0/417	0.99	3/645 (0.5%)
All	All	0.40	1/6180 (0.0%)	0.70	9/8576 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	DT	OP3-P	-10.70	1.48	1.61

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ASP	C-N-CD	-18.57	79.75	120.60
3	D	12	U	C5-C6-N1	7.38	126.39	122.70
2	C	11	DG	O4'-C1'-N9	6.46	112.52	108.00
1	A	282	PRO	N-CA-CB	5.97	110.47	103.30
1	A	506	PRO	N-CA-CB	5.84	110.31	103.30
1	A	37	PRO	N-CA-CB	5.53	109.93	103.30
3	D	11	U	P-O3'-C3'	5.48	126.28	119.70
3	D	12	U	C6-N1-C2	-5.24	117.86	121.00
1	A	246	ASP	C-N-CD	-5.20	109.15	120.60

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	5150	0	5105	124	0
2	C	440	0	234	11	0
3	D	376	0	193	11	0
4	A	1	0	0	0	0
All	All	5967	0	5532	139	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 12.

All (139) 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:130:GLU:OE1	1:A:172:ARG:NH1	1.60	1.30
1:A:184:ALA:O	1:A:186:GLY:N	1.88	1.05
1:A:246:ASP:CB	1:A:247:PRO:HD2	2.00	0.91
1:A:246:ASP:CB	1:A:247:PRO:CD	2.51	0.88
1:A:254:ILE:HG23	1:A:255:PRO:HD2	1.59	0.84
1:A:130:GLU:CD	1:A:172:ARG:NH1	2.32	0.83
1:A:177:MET:HE1	1:A:182:TRP:HA	1.63	0.79
1:A:177:MET:HE1	1:A:182:TRP:CA	2.13	0.78
1:A:184:ALA:C	1:A:186:GLY:N	2.41	0.72
1:A:184:ALA:C	1:A:186:GLY:H	1.89	0.72
1:A:202:TRP:CD2	1:A:244:VAL:HG11	2.25	0.72
1:A:473:LEU:HB3	1:A:541:VAL:HG12	1.71	0.70
1:A:344:THR:HG21	1:A:460:LEU:HD11	1.72	0.70
1:A:146:ARG:HH11	1:A:146:ARG:HG3	1.57	0.69
1:A:254:ILE:CG2	1:A:255:PRO:HD2	2.22	0.69
3:D:16:C:H2'	3:D:17:C:O4'	1.93	0.68
1:A:184:ALA:O	1:A:185:GLN:C	2.33	0.68
1:A:639:THR:HG22	1:A:640:ARG:HE	1.59	0.68
1:A:482:ARG:NH1	2:C:14:DT:OP1	2.24	0.68
1:A:180:GLU:OE1	1:A:258:THR:OG1	2.06	0.67
1:A:545:ARG:NH2	1:A:549:VAL:O	2.27	0.67
1:A:148:LEU:HD12	1:A:174:LEU:CD2	2.24	0.67
1:A:146:ARG:NH1	1:A:146:ARG:HG3	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LEU:HD12	1:A:240:ARG:NH2	2.09	0.67
2:C:18:DT:H2''	2:C:19:DA:H5'	1.74	0.67
1:A:180:GLU:OE2	1:A:240:ARG:NH2	2.28	0.66
1:A:392:ARG:NH2	1:A:428:GLU:OE2	2.29	0.64
1:A:202:TRP:CG	1:A:244:VAL:HG11	2.32	0.64
3:D:11:U:O2'	3:D:12:U:H6	1.79	0.63
1:A:664:LYS:HB3	1:A:668:ARG:NH1	2.14	0.63
1:A:513:ARG:NH2	1:A:521:ASP:OD2	2.34	0.60
3:D:11:U:O2'	3:D:12:U:O5'	2.20	0.59
1:A:545:ARG:NH1	1:A:622:GLU:OE2	2.36	0.59
1:A:43:TYR:H	1:A:44:PRO:HD2	1.67	0.59
1:A:636:PHE:O	1:A:639:THR:HB	2.02	0.58
1:A:600:THR:HB	1:A:620:VAL:HG22	1.86	0.58
1:A:480:GLY:HA2	1:A:663:VAL:HG11	1.87	0.57
1:A:330:PRO:HB2	1:A:646:GLY:HA2	1.86	0.57
3:D:11:U:O2'	3:D:12:U:O4'	2.25	0.55
1:A:190:PRO:HG3	1:A:263:PRO:HB3	1.87	0.55
2:C:3:DA:H2''	2:C:4:DG:H8	1.72	0.55
1:A:168:ASP:OD1	1:A:286:ARG:NH1	2.40	0.54
1:A:410:THR:O	1:A:436:ASN:HA	2.07	0.54
1:A:180:GLU:O	1:A:183:LEU:HB2	2.07	0.54
1:A:471:ALA:HB2	1:A:540:ARG:HG2	1.90	0.54
1:A:664:LYS:HB3	1:A:668:ARG:HH12	1.73	0.53
1:A:181:ALA:O	1:A:184:ALA:N	2.42	0.53
1:A:192:ARG:HG3	1:A:202:TRP:O	2.08	0.53
1:A:446:ARG:HG3	2:C:2:DG:C8	2.44	0.53
1:A:17:ARG:NH2	1:A:23:GLU:OE1	2.37	0.53
1:A:22:GLU:OE1	1:A:95:ARG:NH1	2.43	0.52
1:A:177:MET:CE	1:A:182:TRP:HB2	2.39	0.52
1:A:246:ASP:CB	1:A:247:PRO:HD3	2.39	0.51
1:A:254:ILE:HG22	1:A:255:PRO:N	2.25	0.50
1:A:502:LEU:HG	1:A:503:TRP:N	2.27	0.50
1:A:254:ILE:CG2	1:A:255:PRO:CD	2.89	0.50
2:C:8:DG:C8	2:C:8:DG:H5'	2.47	0.50
1:A:26:PRO:HG2	1:A:98:LEU:HD22	1.94	0.50
1:A:594:VAL:HB	1:A:602:LEU:HB2	1.93	0.50
1:A:52:ARG:NH1	1:A:52:ARG:O	2.45	0.49
1:A:575:LYS:O	1:A:651:ARG:NH2	2.29	0.49
2:C:12:DG:N2	3:D:9:C:O2	2.46	0.49
3:D:8:C:H2'	3:D:9:C:C6	2.47	0.49
1:A:46:LEU:HD23	1:A:59:ARG:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:LEU:HB2	1:A:243:TRP:O	2.13	0.49
1:A:173:ILE:HG23	1:A:270:LEU:HD11	1.94	0.48
1:A:212:PRO:HB2	1:A:224:LEU:HB2	1.94	0.48
1:A:409:LEU:HD23	1:A:435:LEU:HB3	1.96	0.48
1:A:415:TRP:CZ2	1:A:668:ARG:HG2	2.48	0.48
1:A:228:ALA:HB2	1:A:233:LEU:HD12	1.95	0.48
1:A:319:PRO:HB3	1:A:637:HIS:CG	2.49	0.47
1:A:437:VAL:O	1:A:439:LEU:N	2.47	0.47
1:A:661:ARG:HD3	1:A:661:ARG:HA	1.76	0.47
1:A:599:LYS:HD3	1:A:628:LEU:HD11	1.96	0.47
1:A:181:ALA:O	1:A:182:TRP:C	2.51	0.47
1:A:183:LEU:CD1	1:A:240:ARG:NH2	2.78	0.46
1:A:179:LEU:HD13	1:A:258:THR:HG22	1.97	0.46
1:A:445:HIS:NE2	3:D:19:C:O2'	2.47	0.46
3:D:6:A:H2'	3:D:7:A:C8	2.50	0.46
1:A:129:VAL:HG22	1:A:134:VAL:HG23	1.96	0.46
1:A:148:LEU:CD1	1:A:174:LEU:CD2	2.93	0.46
1:A:671:ILE:O	1:A:672:ARG:C	2.54	0.46
1:A:145:TRP:CE3	1:A:145:TRP:C	2.89	0.46
1:A:179:LEU:O	1:A:180:GLU:C	2.53	0.46
1:A:639:THR:CG2	1:A:640:ARG:HE	2.27	0.46
1:A:75:LEU:HD22	1:A:90:LEU:HB2	1.97	0.45
1:A:121:LEU:HB3	1:A:129:VAL:HG21	1.98	0.45
1:A:148:LEU:CD1	1:A:174:LEU:HD23	2.46	0.45
1:A:145:TRP:O	1:A:145:TRP:CE3	2.70	0.45
1:A:205:LEU:HD21	1:A:245:ALA:HB2	1.98	0.45
1:A:486:ARG:HB2	1:A:515:PRO:HG3	1.98	0.45
1:A:205:LEU:CG	1:A:245:ALA:HB2	2.47	0.44
1:A:449:ASN:ND2	2:C:2:DG:H21	2.15	0.44
1:A:183:LEU:HA	1:A:183:LEU:HD23	1.66	0.44
1:A:177:MET:CE	1:A:182:TRP:N	2.81	0.44
1:A:202:TRP:CG	1:A:244:VAL:CG1	3.00	0.44
1:A:503:TRP:CZ2	1:A:679:ARG:HG2	2.52	0.43
1:A:249:ASP:HA	1:A:250:PRO:HD2	1.77	0.43
1:A:641:LEU:HA	1:A:641:LEU:HD23	1.83	0.43
1:A:118:GLN:O	1:A:122:ARG:HG3	2.18	0.43
2:C:17:DA:H2	3:D:3:U:H3	1.65	0.43
1:A:513:ARG:HD2	1:A:513:ARG:HA	1.70	0.43
1:A:352:ASP:OD2	1:A:437:VAL:HG21	2.18	0.43
1:A:384:HIS:CG	1:A:385:PRO:HD2	2.54	0.43
1:A:246:ASP:CB	1:A:250:PRO:HG3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ASP:HA	1:A:35:PRO:HA	1.89	0.43
1:A:502:LEU:HD13	1:A:529:ALA:HB1	2.01	0.43
1:A:366:LEU:HD13	1:A:366:LEU:HA	1.76	0.43
1:A:461:GLN:O	1:A:463:VAL:N	2.45	0.42
1:A:51:ARG:HG2	1:A:115:ARG:HH12	1.84	0.42
1:A:155:LEU:HD21	1:A:163:PHE:HB3	2.01	0.42
1:A:168:ASP:OD1	1:A:169:PRO:HD2	2.19	0.42
1:A:225:ASP:HA	1:A:228:ALA:HB3	2.01	0.42
2:C:3:DA:H2''	2:C:4:DG:C8	2.51	0.42
1:A:43:TYR:HA	1:A:43:TYR:HD1	1.68	0.42
1:A:457:LYS:NZ	2:C:1:DT:OP1	2.52	0.42
1:A:148:LEU:HD12	1:A:174:LEU:HD22	2.00	0.42
1:A:252:LYS:HA	1:A:253:PRO:HD3	1.93	0.41
1:A:305:THR:HA	1:A:306:PRO:HD3	1.82	0.41
1:A:593:TYR:OH	1:A:628:LEU:HB3	2.20	0.41
1:A:638:LEU:HA	1:A:638:LEU:HD23	1.89	0.41
1:A:177:MET:HE1	1:A:182:TRP:CB	2.50	0.41
1:A:472:GLU:OE1	1:A:536:ARG:NH1	2.41	0.41
1:A:114:ARG:NH2	1:A:154:ASP:OD2	2.53	0.41
1:A:267:LEU:HD12	1:A:267:LEU:HA	1.90	0.41
1:A:455:LEU:HD22	1:A:460:LEU:HD22	2.02	0.41
1:A:175:CYS:SG	1:A:175:CYS:O	2.79	0.41
1:A:194:ARG:HG2	1:A:195:ASN:O	2.21	0.41
1:A:416:GLU:CD	1:A:416:GLU:H	2.24	0.41
2:C:5:DG:H2'	2:C:6:DT:C6	2.56	0.41
1:A:11:LEU:C	1:A:13:ARG:H	2.24	0.41
1:A:504:THR:HG22	1:A:679:ARG:NH1	2.36	0.41
3:D:3:U:H2'	3:D:4:A:C8	2.56	0.41
1:A:254:ILE:CG2	1:A:255:PRO:N	2.84	0.40
1:A:22:GLU:OE1	1:A:95:ARG:NH2	2.54	0.40
3:D:17:C:H2'	3:D:18:U:C6	2.57	0.40
1:A:177:MET:HE3	1:A:177:MET:HB3	1.94	0.40
1:A:177:MET:CE	1:A:182:TRP:CA	2.93	0.40
1:A:321:LEU:HB3	1:A:327:VAL:HG23	2.04	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	673/685 (98%)	609 (90%)	45 (7%)	19 (3%)	5	19

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	PRO
1	A	143	PRO
1	A	185	GLN
1	A	250	PRO
1	A	672	ARG
1	A	500	HIS
1	A	597	GLU
1	A	670	GLY
1	A	43	TYR
1	A	248	LYS
1	A	598	ASP
1	A	671	ILE
1	A	4	LEU
1	A	462	VAL
1	A	36	PRO
1	A	375	SER
1	A	218	PRO
1	A	42	VAL
1	A	412	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	485/549 (88%)	441 (91%)	44 (9%)	9 28

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	43	TYR
1	A	57	THR
1	A	64	LEU
1	A	98	LEU
1	A	127	VAL
1	A	146	ARG
1	A	155	LEU
1	A	165	LEU
1	A	174	LEU
1	A	177	MET
1	A	179	LEU
1	A	199	ARG
1	A	202	TRP
1	A	223	LEU
1	A	225	ASP
1	A	244	VAL
1	A	256	HIS
1	A	264	VAL
1	A	280	SER
1	A	366	LEU
1	A	392	ARG
1	A	406	VAL
1	A	410	THR
1	A	426	LEU
1	A	437	VAL
1	A	442	GLU
1	A	451	LEU
1	A	454	LEU
1	A	462	VAL
1	A	475	VAL
1	A	502	LEU
1	A	504	THR
1	A	528	TRP
1	A	531	ARG
1	A	543	LEU
1	A	549	VAL
1	A	556	LEU

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Mol	Chain	Res	Type
1	A	570	LEU
1	A	580	ARG
1	A	592	LEU
1	A	600	THR
1	A	639	THR
1	A	640	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	D	16/20 (80%)	4 (25%)	1 (6%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	D	11	U
3	D	12	U
3	D	14	U
3	D	17	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	D	11	U

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 1 ligands modelled in this entry, 1 is 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, 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(Å ²)	Q<0.9
1	A	679/685 (99%)	0.34	44 (6%) 18 14	30, 85, 150, 192	0
2	C	21/21 (100%)	0.48	1 (4%) 30 27	74, 128, 190, 215	0
3	D	19/20 (95%)	0.63	1 (5%) 26 22	77, 161, 218, 223	0
All	All	719/726 (99%)	0.35	46 (6%) 19 15	30, 86, 164, 223	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	PRO	6.1
1	A	192	ARG	5.7
1	A	205	LEU	5.2
1	A	245	ALA	5.2
1	A	244	VAL	4.5
1	A	243	TRP	4.4
1	A	253	PRO	4.2
1	A	204	LEU	4.1
1	A	223	LEU	4.1
1	A	217	LEU	3.9
1	A	207	LEU	3.8
1	A	254	ILE	3.8
1	A	246	ASP	3.7
1	A	37	PRO	3.6
1	A	257	LEU	3.6
1	A	5	GLY	3.5
1	A	262	VAL	3.5
1	A	202	TRP	3.4
1	A	256	HIS	3.3
1	A	193	VAL	3.3
1	A	234	GLN	3.3
1	A	260	LEU	3.3
1	A	215	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	259	GLY	3.0
1	A	46	LEU	2.9
1	A	248	LYS	2.9
1	A	263	PRO	2.9
1	A	86	TYR	2.8
1	A	216	PRO	2.8
1	A	607	HIS	2.8
2	C	17	DA	2.7
1	A	188	PRO	2.7
1	A	32	VAL	2.7
1	A	255	PRO	2.6
1	A	176	GLU	2.6
1	A	251	ARG	2.6
1	A	338	PHE	2.5
1	A	252	LYS	2.5
1	A	224	LEU	2.4
1	A	186	GLY	2.3
1	A	241	VAL	2.3
1	A	261	LEU	2.2
1	A	283	TRP	2.1
1	A	33	LEU	2.1
1	A	264	VAL	2.1
3	D	2	A	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, 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	A	701	1/1	0.94	0.23	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.