



Full wwPDB EM Validation Report ⓘ

Apr 14, 2026 – 10:23 PM JST

PDB ID : 9VZX / pdb_00009vzx
EMDB ID : EMD-65487
Title : Cryo-EM structure of TasH-tigRNA-gap dsDNA complex
Authors : Zhang, H.; Liu, Z.
Deposited on : 2025-07-23
Resolution : 2.78 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

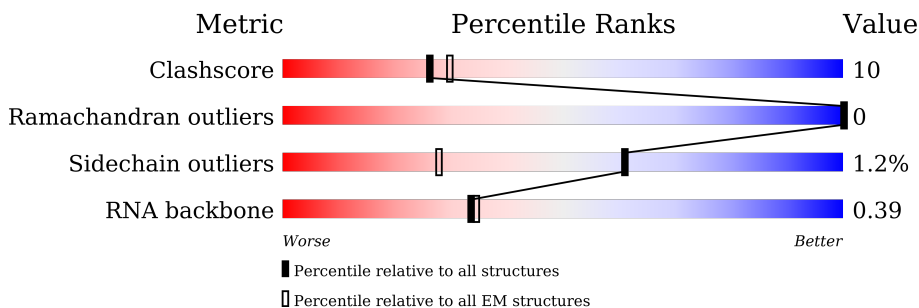
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.78 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	354	56% 13% 31%
1	B	354	53% 14% 33%
2	C	37	51% 27% 22%
3	D	38	21% 18% 61%
4	E	38	21% 16% 63%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5222 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 HNH nuclease domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	245	Total	C	N	O	S	0	0
			1952	1221	359	360	12		
1	B	238	Total	C	N	O	S	0	0
			1900	1190	349	349	12		

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLY	-	expression tag	UNP M4R212
A	311	GLY	-	expression tag	UNP M4R212
A	312	SER	-	expression tag	UNP M4R212
A	313	TRP	-	expression tag	UNP M4R212
A	314	SER	-	expression tag	UNP M4R212
A	315	HIS	-	expression tag	UNP M4R212
A	316	PRO	-	expression tag	UNP M4R212
A	317	GLN	-	expression tag	UNP M4R212
A	318	PHE	-	expression tag	UNP M4R212
A	319	GLU	-	expression tag	UNP M4R212
A	320	LYS	-	expression tag	UNP M4R212
A	321	GLY	-	expression tag	UNP M4R212
A	322	GLY	-	expression tag	UNP M4R212
A	323	GLY	-	expression tag	UNP M4R212
A	324	SER	-	expression tag	UNP M4R212
A	325	GLY	-	expression tag	UNP M4R212
A	326	GLY	-	expression tag	UNP M4R212
A	327	GLY	-	expression tag	UNP M4R212
A	328	SER	-	expression tag	UNP M4R212
A	329	GLY	-	expression tag	UNP M4R212
A	330	GLY	-	expression tag	UNP M4R212
A	331	SER	-	expression tag	UNP M4R212
A	332	ALA	-	expression tag	UNP M4R212
A	333	TRP	-	expression tag	UNP M4R212
A	334	SER	-	expression tag	UNP M4R212
A	335	HIS	-	expression tag	UNP M4R212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	336	PRO	-	expression tag	UNP M4R212
A	337	GLN	-	expression tag	UNP M4R212
A	338	PHE	-	expression tag	UNP M4R212
A	339	GLU	-	expression tag	UNP M4R212
A	340	LYS	-	expression tag	UNP M4R212
A	341	ASN	-	expression tag	UNP M4R212
A	342	LEU	-	expression tag	UNP M4R212
A	343	TYR	-	expression tag	UNP M4R212
A	344	PHE	-	expression tag	UNP M4R212
A	345	GLN	-	expression tag	UNP M4R212
A	346	SER	-	expression tag	UNP M4R212
A	347	GLY	-	expression tag	UNP M4R212
A	348	SER	-	expression tag	UNP M4R212
A	349	HIS	-	expression tag	UNP M4R212
A	350	HIS	-	expression tag	UNP M4R212
A	351	HIS	-	expression tag	UNP M4R212
A	352	HIS	-	expression tag	UNP M4R212
A	353	HIS	-	expression tag	UNP M4R212
A	354	HIS	-	expression tag	UNP M4R212
B	310	GLY	-	expression tag	UNP M4R212
B	311	GLY	-	expression tag	UNP M4R212
B	312	SER	-	expression tag	UNP M4R212
B	313	TRP	-	expression tag	UNP M4R212
B	314	SER	-	expression tag	UNP M4R212
B	315	HIS	-	expression tag	UNP M4R212
B	316	PRO	-	expression tag	UNP M4R212
B	317	GLN	-	expression tag	UNP M4R212
B	318	PHE	-	expression tag	UNP M4R212
B	319	GLU	-	expression tag	UNP M4R212
B	320	LYS	-	expression tag	UNP M4R212
B	321	GLY	-	expression tag	UNP M4R212
B	322	GLY	-	expression tag	UNP M4R212
B	323	GLY	-	expression tag	UNP M4R212
B	324	SER	-	expression tag	UNP M4R212
B	325	GLY	-	expression tag	UNP M4R212
B	326	GLY	-	expression tag	UNP M4R212
B	327	GLY	-	expression tag	UNP M4R212
B	328	SER	-	expression tag	UNP M4R212
B	329	GLY	-	expression tag	UNP M4R212
B	330	GLY	-	expression tag	UNP M4R212
B	331	SER	-	expression tag	UNP M4R212
B	332	ALA	-	expression tag	UNP M4R212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	333	TRP	-	expression tag	UNP M4R212
B	334	SER	-	expression tag	UNP M4R212
B	335	HIS	-	expression tag	UNP M4R212
B	336	PRO	-	expression tag	UNP M4R212
B	337	GLN	-	expression tag	UNP M4R212
B	338	PHE	-	expression tag	UNP M4R212
B	339	GLU	-	expression tag	UNP M4R212
B	340	LYS	-	expression tag	UNP M4R212
B	341	ASN	-	expression tag	UNP M4R212
B	342	LEU	-	expression tag	UNP M4R212
B	343	TYR	-	expression tag	UNP M4R212
B	344	PHE	-	expression tag	UNP M4R212
B	345	GLN	-	expression tag	UNP M4R212
B	346	SER	-	expression tag	UNP M4R212
B	347	GLY	-	expression tag	UNP M4R212
B	348	SER	-	expression tag	UNP M4R212
B	349	HIS	-	expression tag	UNP M4R212
B	350	HIS	-	expression tag	UNP M4R212
B	351	HIS	-	expression tag	UNP M4R212
B	352	HIS	-	expression tag	UNP M4R212
B	353	HIS	-	expression tag	UNP M4R212
B	354	HIS	-	expression tag	UNP M4R212

- Molecule 2 is a RNA chain called RNA (36-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	37	Total	C	N	O	P	0	0
			774	346	147	245	36		

- Molecule 3 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	15	Total	C	N	O	P	0	0
			315	148	65	87	15		

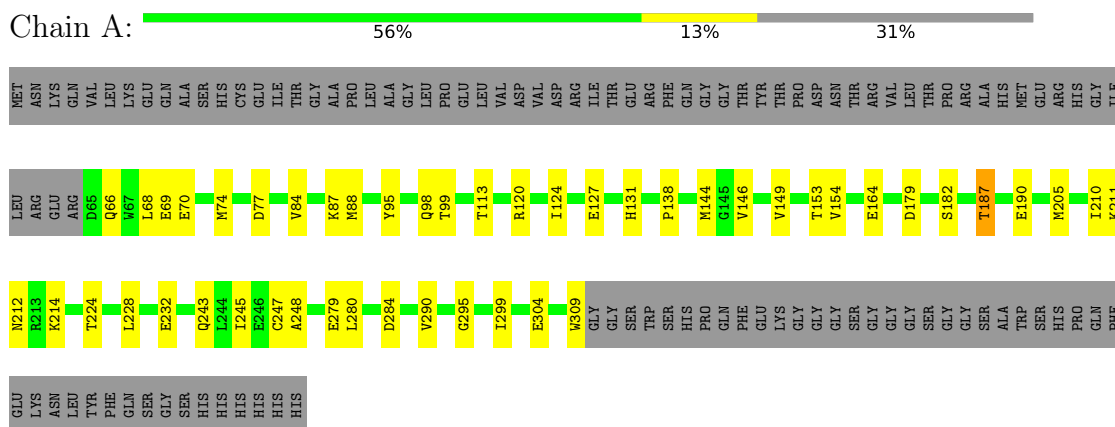
- Molecule 4 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	14	Total	C	N	O	P	0	0
			281	135	45	87	14		

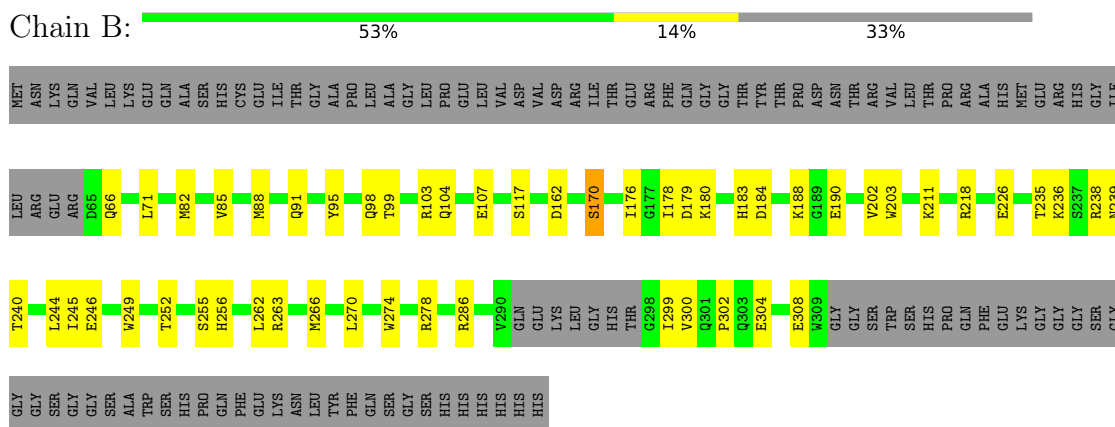
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

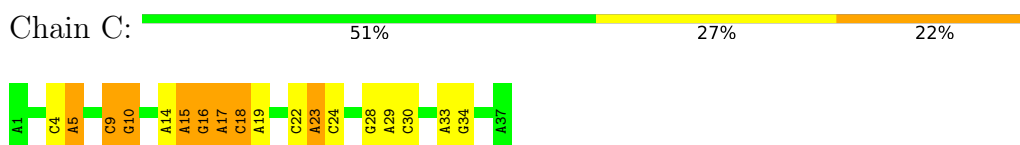
- Molecule 1: HNH nuclease domain-containing protein



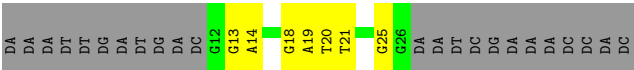
- Molecule 1: HNH nuclease domain-containing protein



- Molecule 2: RNA (36-MER)



- Molecule 3: DNA (38-MER)



● Molecule 4: DNA (38-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65896	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.10	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.16	0/1991	0.32	0/2687
1	B	0.17	0/1937	0.36	0/2612
2	C	0.21	0/867	0.34	0/1351
3	D	0.18	0/355	0.43	0/547
4	E	0.21	0/312	0.46	0/478
All	All	0.18	0/5462	0.36	0/7675

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1952	0	1944	39	0
1	B	1900	0	1899	46	0
2	C	774	0	392	15	0
3	D	315	0	168	6	0
4	E	281	0	160	5	0
All	All	5222	0	4563	98	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 10.

All (98) 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)
2:C:17:A:O2'	2:C:18:C:OP1	1.72	1.05
1:A:88:MET:HE3	1:A:113:THR:HG21	1.50	0.91
1:B:239:ASN:OD1	1:B:240:THR:N	2.05	0.90
1:B:66:GLN:N	1:B:66:GLN:OE1	2.09	0.85
1:B:308:GLU:N	1:B:308:GLU:OE2	2.09	0.85
1:B:104:GLN:N	1:B:104:GLN:OE1	2.12	0.81
1:A:304:GLU:OE1	1:A:304:GLU:N	2.15	0.79
1:A:66:GLN:N	1:A:66:GLN:OE1	2.17	0.77
1:B:179:ASP:OD1	1:B:180:LYS:N	2.17	0.76
2:C:9:C:O2'	2:C:10:G:OP1	2.05	0.74
1:B:246:GLU:OE1	1:B:246:GLU:N	2.22	0.73
1:B:236:LYS:NZ	1:B:246:GLU:OE2	2.17	0.72
1:A:138:PRO:HB2	1:A:280:LEU:HD13	1.74	0.69
1:B:304:GLU:N	1:B:304:GLU:OE2	2.28	0.67
1:B:88:MET:HE3	1:B:88:MET:HA	1.79	0.65
1:A:69:GLU:N	1:A:69:GLU:OE2	2.29	0.65
1:A:224:THR:O	1:A:228:LEU:HD12	1.98	0.64
1:A:290:VAL:O	1:A:295:GLY:N	2.31	0.63
1:A:299:ILE:O	1:A:299:ILE:HD12	2.01	0.61
1:B:170:SER:OG	2:C:17:A:O3'	2.14	0.60
1:A:87:LYS:NZ	1:B:91:GLN:OE1	2.34	0.59
1:A:247:CYS:SG	1:A:248:ALA:N	2.75	0.59
1:B:235:THR:OG1	2:C:22:C:OP1	2.15	0.58
1:A:68:LEU:HD12	1:A:68:LEU:O	2.04	0.58
1:B:238:ARG:HH11	1:B:244:LEU:HD13	1.68	0.57
1:A:187:THR:OG1	1:A:190:GLU:OE1	2.15	0.57
1:A:88:MET:HE3	1:A:113:THR:CG2	2.30	0.56
1:A:74:MET:HE1	1:A:131:HIS:CG	2.41	0.55
1:B:85:VAL:HG22	1:B:117:SER:OG	2.06	0.55
1:A:120:ARG:O	1:A:124:ILE:HD13	2.07	0.55
1:B:262:LEU:O	1:B:266:MET:HG3	2.06	0.55
1:A:210:ILE:HD12	1:A:211:LYS:N	2.22	0.54
1:A:245:ILE:C	1:A:245:ILE:HD12	2.32	0.54
1:A:84:VAL:HG22	1:B:88:MET:HE1	1.89	0.53
1:A:212:ASN:OD1	1:A:214:LYS:NZ	2.26	0.53
1:A:280:LEU:HD21	1:A:309:TRP:HB2	1.92	0.52
1:B:176:ILE:HD11	1:B:178:ILE:HD13	1.92	0.52
1:B:103:ARG:NH1	1:B:103:ARG:HB3	2.25	0.51
2:C:9:C:C5	4:E:19:DA:C4	2.99	0.51
1:A:70:GLU:HA	1:A:70:GLU:OE1	2.10	0.51
1:A:279:GLU:HA	1:A:279:GLU:OE1	2.10	0.50
1:A:164:GLU:HA	1:A:164:GLU:OE2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASP:OD2	1:A:77:ASP:C	2.55	0.49
1:B:256:HIS:NE2	2:C:23:A:OP2	2.39	0.49
1:B:71:LEU:HD13	1:B:71:LEU:C	2.37	0.49
1:B:107:GLU:C	1:B:107:GLU:OE2	2.55	0.49
1:A:232:GLU:OE1	1:A:232:GLU:N	2.43	0.49
1:B:176:ILE:HD11	1:B:178:ILE:CD1	2.43	0.48
1:B:179:ASP:OD1	1:B:180:LYS:HG3	2.14	0.48
1:A:210:ILE:HD12	1:A:210:ILE:C	2.39	0.48
2:C:9:C:C2	2:C:10:G:C8	3.02	0.48
1:A:95:TYR:CE2	1:A:99:THR:HG21	2.48	0.47
1:A:299:ILE:HD12	1:A:299:ILE:C	2.39	0.47
1:A:245:ILE:HD12	1:A:245:ILE:O	2.15	0.47
1:B:183:HIS:CD2	1:B:184:ASP:OD1	2.68	0.47
1:B:274:TRP:CE2	1:B:278:ARG:HD3	2.50	0.47
1:A:98:GLN:OE1	1:A:98:GLN:C	2.58	0.46
1:B:99:THR:HG22	1:B:99:THR:O	2.14	0.46
1:B:249:TRP:O	1:B:252:THR:HG22	2.16	0.46
2:C:17:A:O2'	2:C:18:C:P	2.69	0.46
3:D:19:DA:H2''	3:D:20:DT:H71	1.97	0.46
1:B:300:VAL:HG12	1:B:302:PRO:HD3	1.97	0.46
2:C:5:A:H2'	2:C:5:A:N3	2.30	0.46
1:B:190:GLU:C	1:B:190:GLU:OE2	2.59	0.45
1:B:211:LYS:HE2	3:D:13:DG:N2	2.32	0.45
1:B:176:ILE:HD13	1:B:270:LEU:HD11	1.98	0.45
1:A:144:MET:SD	1:A:154:VAL:HG21	2.57	0.45
1:B:203:TRP:N	1:B:266:MET:HE3	2.32	0.45
2:C:28:G:H2'	2:C:29:A:C8	2.52	0.45
1:A:182:SER:N	2:C:5:A:OP1	2.36	0.44
1:A:153:THR:HG21	1:A:205:MET:HB2	1.98	0.44
1:B:170:SER:OG	2:C:18:C:P	2.76	0.44
1:B:202:VAL:C	1:B:266:MET:HE3	2.43	0.44
1:B:179:ASP:OD1	1:B:179:ASP:C	2.61	0.44
1:B:82:MET:HE2	4:E:28:DG:O3'	2.18	0.43
1:B:245:ILE:HD12	1:B:245:ILE:C	2.43	0.43
1:A:179:ASP:N	1:A:179:ASP:OD1	2.52	0.43
1:A:243:GLN:N	1:A:243:GLN:CD	2.76	0.43
4:E:24:DC:H2''	4:E:25:DT:H5'	1.99	0.43
1:A:284:ASP:OD2	1:A:284:ASP:C	2.61	0.43
1:B:263:ARG:HA	1:B:266:MET:HG3	2.01	0.42
3:D:18:DG:H4'	3:D:19:DA:OP1	2.19	0.42
1:A:88:MET:CE	1:A:113:THR:HG21	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ASP:C	1:B:162:ASP:OD1	2.62	0.42
1:A:74:MET:SD	1:A:127:GLU:HG3	2.60	0.42
1:B:218:ARG:NH2	3:D:14:DA:OP1	2.44	0.42
1:B:170:SER:HB3	2:C:16:G:N7	2.34	0.41
3:D:25:DG:N3	3:D:25:DG:H2'	2.34	0.41
4:E:29:DT:H5''	4:E:29:DT:H6	1.84	0.41
1:A:146:VAL:HB	1:A:149:VAL:HG21	2.02	0.41
1:B:103:ARG:HB3	1:B:103:ARG:HH11	1.84	0.41
1:B:183:HIS:NE2	1:B:236:LYS:HG2	2.36	0.41
1:B:188:LYS:HA	3:D:21:DT:H4'	2.03	0.41
1:B:286:ARG:NH1	1:B:286:ARG:HB3	2.36	0.40
2:C:14:A:H3'	2:C:15:A:H5'	2.02	0.40
4:E:25:DT:H2''	4:E:26:DC:H5'	2.02	0.40
2:C:29:A:H2'	2:C:30:C:C6	2.56	0.40
1:B:95:TYR:O	1:B:98:GLN:HG3	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 PDB entries followed by that with respect to all EM entries.

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	243/354 (69%)	238 (98%)	5 (2%)	0	100	100
1	B	234/354 (66%)	231 (99%)	3 (1%)	0	100	100
All	All	477/708 (67%)	469 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM

entries.

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	203/293 (69%)	202 (100%)	1 (0%)	81	92
1	B	198/293 (68%)	194 (98%)	4 (2%)	48	77
All	All	401/586 (68%)	396 (99%)	5 (1%)	61	84

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	THR
1	B	170	SER
1	B	226	GLU
1	B	255	SER
1	B	299	ILE

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	35/37 (94%)	12 (34%)	2 (5%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	4	C
2	C	5	A
2	C	9	C
2	C	10	G
2	C	15	A
2	C	16	G
2	C	18	C
2	C	19	A
2	C	23	A
2	C	24	C
2	C	33	A
2	C	34	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	9	C
2	C	17	A

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.