



Full wwPDB EM Validation Report ⓘ

Apr 14, 2026 – 10:29 PM JST

PDB ID : 9W04 / pdb_00009w04
EMDB ID : EMD-65491
Title : Cryo-EM structure of TasH-tigRNA-dsDNA complex
Authors : Zhang, H.; Liu, Z.
Deposited on : 2025-07-23
Resolution : 2.33 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

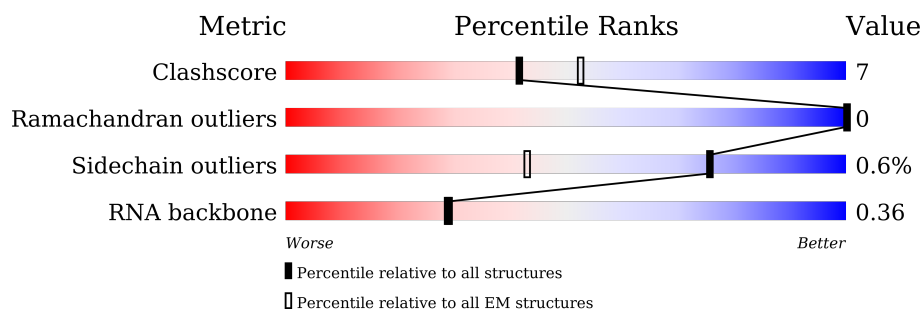
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.33 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	74% 11% 15%
1	B	354	75% 12% 13%
2	C	37	43% 46% 11%
3	D	38	37% 13% 50%
3	E	38	24% 8% 68%
4	F	38	29% 18% 53%
4	G	38	8% 26% 66%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6927 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	302	Total	C	N	O	S	0	0
			2412	1504	449	444	15		
1	B	309	Total	C	N	O	S	0	0
			2468	1538	460	455	15		

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

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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

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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	19	Total	C	N	O	P	0	0
			389	186	69	115	19		
3	E	12	Total	C	N	O	P	0	0
			242	116	40	74	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	18	Total	C	N	O	P	0	0
			374	177	75	104	18		

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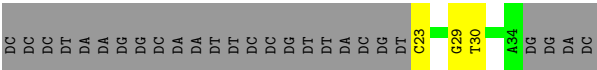
Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	13	Total	C	N	O	P	0	0
			266	127	47	79	13		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Mg	0
			1	1	
5	F	1	Total	Mg	0
			1	1	

Chain E:

24%8%68%



● Molecule 4: DNA (38-MER)

Chain F:

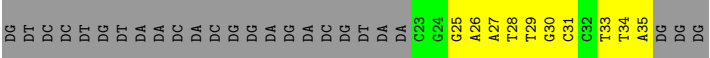
29%18%53%



● Molecule 4: DNA (38-MER)

Chain G:

8%26%66%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	242496	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](#)

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	0.42	1/2459 (0.0%)	0.55	0/3318
1	B	0.35	0/2517	0.49	0/3397
2	C	0.28	0/867	0.37	0/1351
3	D	0.30	0/435	0.58	0/669
3	E	0.28	0/269	0.49	0/412
4	F	0.26	0/421	0.49	0/648
4	G	0.52	0/297	0.84	0/456
All	All	0.37	1/7265 (0.0%)	0.52	0/10251

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	THR	C-N	-5.37	1.27	1.33

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	2412	0	2415	34	0
1	B	2468	0	2471	34	0
2	C	774	0	392	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	389	0	215	5	0
3	E	242	0	137	2	0
4	F	374	0	201	6	0
4	G	266	0	148	9	0
5	B	1	0	0	0	0
5	F	1	0	0	0	0
All	All	6927	0	5979	87	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 7.

All (87) 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:B:218:ARG:NH2	3:D:13:DT:OP1	2.21	0.74
1:B:296:HIS:HB3	2:C:1:A:H5'	1.75	0.67
1:B:1:MET:O	4:F:15:DA:N6	2.30	0.65
1:A:205:MET:SD	1:A:209:MET:HE3	2.39	0.63
1:B:166:ALA:O	1:B:278:ARG:NH1	2.35	0.59
1:A:49:LEU:N	1:A:49:LEU:HD23	2.18	0.58
1:A:1:MET:O	3:D:15:DC:N4	2.37	0.58
1:B:290:VAL:HA	1:B:294:LEU:HB2	1.85	0.58
1:B:148:GLY:O	4:G:29:DT:H5''	2.05	0.56
1:A:256:HIS:NE2	2:C:23:A:OP2	2.35	0.55
1:A:31:ARG:HD2	1:A:41:TYR:CZ	2.42	0.55
1:A:6:LEU:HD23	1:A:6:LEU:O	2.06	0.54
1:A:303:GLN:NE2	1:A:304:GLU:OE1	2.40	0.54
1:B:139:LEU:HD21	1:B:273:TYR:CZ	2.44	0.53
1:B:60:ILE:HG23	2:C:31:G:H1'	1.91	0.53
1:B:47:ARG:HD3	1:B:49:LEU:HD21	1.91	0.53
1:A:300:VAL:O	1:A:300:VAL:HG13	2.10	0.52
1:A:286:ARG:HG2	1:A:287:PRO:HD2	1.92	0.51
3:D:6:DA:H4'	3:D:7:DG:OP1	2.11	0.51
1:A:77:ASP:OD2	1:B:106:THR:HG22	2.12	0.50
1:B:22:GLY:C	1:B:23:LEU:HD22	2.36	0.50
1:A:32:ILE:HG12	1:A:45:ASN:O	2.11	0.50
1:B:225:LYS:NZ	3:D:14:DC:OP1	2.45	0.49
2:C:8:C:O2'	2:C:9:C:H5''	2.12	0.49
1:A:246:GLU:N	1:A:246:GLU:OE2	2.46	0.49
1:A:60:ILE:HG23	2:C:13:A:H1'	1.94	0.49
4:G:30:DG:H4'	4:G:31:DC:OP1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:7:U:O2'	2:C:8:C:H5'	2.14	0.48
4:G:34:DT:H2''	4:G:35:DA:C8	2.49	0.48
1:A:218:ARG:NH1	4:F:13:DG:OP1	2.43	0.48
4:F:12:DC:H2''	4:F:13:DG:O5'	2.12	0.48
1:B:168:SER:O	1:B:171:ALA:N	2.46	0.48
1:A:4:GLN:NE2	1:A:8:GLU:OE1	2.48	0.47
1:A:184:ASP:O	1:A:184:ASP:CG	2.57	0.47
4:F:21:DA:H2'	4:F:22:DA:C8	2.49	0.47
1:A:36:PHE:O	1:A:37:GLN:HB2	2.14	0.47
1:B:205:MET:O	1:B:209:MET:HG3	2.15	0.47
4:G:28:DT:H2''	4:G:29:DT:O5'	2.15	0.46
1:B:276:VAL:HG22	1:B:309:TRP:CZ2	2.50	0.46
1:B:205:MET:HE1	1:B:269:PHE:CD2	2.51	0.46
1:B:157:LEU:HD12	1:B:198:LEU:HD11	1.96	0.46
1:B:290:VAL:HG22	2:C:2:G:N7	2.30	0.45
4:F:12:DC:H4'	4:F:13:DG:OP1	2.15	0.45
1:A:1:MET:C	1:A:1:MET:SD	2.99	0.45
1:A:66:GLN:OE1	1:A:66:GLN:N	2.45	0.45
1:B:290:VAL:HG12	1:B:296:HIS:HB2	1.99	0.45
1:B:161:VAL:HG23	1:B:198:LEU:HD21	2.00	0.44
1:A:60:ILE:HG23	2:C:13:A:C1'	2.48	0.44
1:A:60:ILE:O	2:C:12:U:O2'	2.36	0.44
1:A:221:TYR:HH	1:A:258:HIS:CE1	2.32	0.44
4:F:8:DA:H4'	4:F:9:DA:OP1	2.17	0.44
1:B:168:SER:O	1:B:171:ALA:HB3	2.18	0.43
1:A:205:MET:O	1:A:209:MET:HG3	2.18	0.43
1:B:6:LEU:O	1:B:6:LEU:HD23	2.18	0.43
1:B:143:ALA:O	1:B:146:VAL:HG12	2.18	0.43
2:C:7:U:C2'	2:C:8:C:H5'	2.48	0.43
2:C:34:G:O2'	2:C:35:C:P	2.77	0.43
4:G:25:DG:H2'	4:G:26:DA:H5'	2.01	0.43
1:A:1:MET:HE1	1:A:3:LYS:HG2	2.00	0.43
3:E:29:DG:C2'	3:E:30:DT:H72	2.49	0.43
2:C:23:A:H2'	2:C:23:A:N3	2.32	0.43
1:B:23:LEU:HD22	1:B:23:LEU:N	2.34	0.43
2:C:17:A:C4	2:C:19:A:N7	2.87	0.43
1:A:80:GLN:OE1	1:B:87:LYS:NZ	2.39	0.42
1:A:4:GLN:OE1	1:A:5:VAL:N	2.52	0.42
2:C:17:A:N7	2:C:19:A:N6	2.68	0.42
1:B:78:ARG:HH22	4:G:28:DT:P	2.42	0.42
3:D:6:DA:H1'	3:D:7:DG:H5''	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:THR:HG22	1:A:253:LYS:N	2.35	0.42
1:A:4:GLN:OE1	1:A:4:GLN:C	2.62	0.41
1:A:36:PHE:O	1:A:37:GLN:CB	2.68	0.41
1:B:136:LYS:HD2	1:B:136:LYS:N	2.34	0.41
4:G:33:DT:H4'	4:G:34:DT:OP1	2.20	0.41
1:A:30:ASP:HB2	1:A:49:LEU:HD21	2.01	0.41
1:A:205:MET:HE2	1:A:205:MET:HB3	1.95	0.41
1:B:72:LYS:HB2	1:B:159:THR:HG23	2.02	0.41
2:C:20:A:H2'	2:C:21:C:O4'	2.21	0.41
1:B:204:ASN:OD1	4:G:27:DA:H2''	2.21	0.41
1:B:28:ASP:OD1	3:E:23:DC:H2''	2.21	0.41
1:B:289:TYR:CE2	1:B:293:LYS:HG3	2.56	0.41
1:B:272:ASP:O	1:B:276:VAL:HG23	2.21	0.40
1:B:289:TYR:HB2	2:C:36:G:C5	2.56	0.40
4:G:30:DG:H2''	4:G:31:DC:O5'	2.21	0.40
1:A:299:ILE:O	1:A:305:ARG:NH2	2.52	0.40
1:A:29:VAL:O	1:A:29:VAL:HG23	2.22	0.40
1:A:136:LYS:HB3	1:A:136:LYS:NZ	2.36	0.40
1:B:82:MET:O	1:B:86:MET:HG2	2.21	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	298/354 (84%)	291 (98%)	7 (2%)	0	100	100
1	B	307/354 (87%)	302 (98%)	5 (2%)	0	100	100
All	All	605/708 (86%)	593 (98%)	12 (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	254/293 (87%)	252 (99%)	2 (1%)	73	82
1	B	260/293 (89%)	259 (100%)	1 (0%)	84	89
All	All	514/586 (88%)	511 (99%)	3 (1%)	76	86

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	132	ILE
1	B	290	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	118	ASN
1	B	91	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	35/37 (94%)	9 (25%)	0

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	3	U
2	C	8	C
2	C	16	G
2	C	23	A
2	C	24	C
2	C	27	A

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Mol	Chain	Res	Type
2	C	33	A
2	C	34	G
2	C	35	C

There are no RNA pucker outliers to report.

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](#)

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.