



wwPDB EM Validation Summary Report ⓘ

Jun 10, 2025 – 02:17 PM JST

PDB ID : 8ZP9 / pdb_00008zp9
EMDB ID : EMD-60330
Title : Cryo-EM structure of Cas5-HNH Cascade bound with sDNA, Conf2
Authors : Liu, Y.N.; Wang, L.; Zhang, H.; Zhu, H.
Deposited on : 2024-05-29
Resolution : 2.80 Å(reported)

This is a wwPDB EM Validation Summary 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 Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

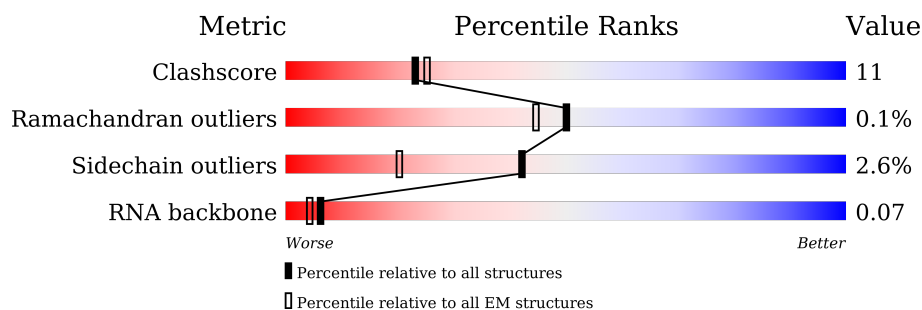
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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.



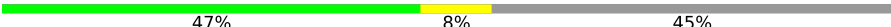
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	61	
2	F	378	
2	G	378	
2	H	378	
2	I	378	
2	J	378	
2	K	378	
3	B	388	

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Mol	Chain	Length	Quality of chain
4	M	60	 A horizontal bar chart showing the quality of chain M. The bar is divided into three segments: a green segment on the left labeled '47%', a yellow segment in the middle labeled '8%', and a grey segment on the right labeled '45%'. The total length of the bar represents 100%.

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 19297 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 RNA chain called RNA (61-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	41	Total	C	N	O	P	0	0
			879	393	162	284	40		

- Molecule 2 is a protein called CRISPR system Cascade subunit CasC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	368	Total	C	N	O	S	0	0
			2819	1782	489	536	12		
2	H	375	Total	C	N	O	S	0	0
			2878	1812	503	551	12		
2	I	373	Total	C	N	O	S	0	0
			2854	1800	498	544	12		
2	J	374	Total	C	N	O	S	0	0
			2845	1794	496	543	12		
2	K	344	Total	C	N	O	S	0	0
			2646	1670	468	497	11		
2	G	255	Total	C	N	O	S	0	0
			1927	1220	336	363	8		

- Molecule 3 is a protein called CRISPR system Cascade subunit CasD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	228	Total	C	N	O	S	0	0
			1780	1139	321	313	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	303	HIS	ALA	conflict	UNP A0A1V6F8C5

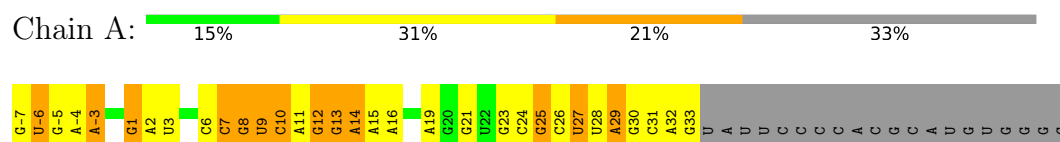
- Molecule 4 is a DNA chain called DNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	33	Total 669	C 319	N 119	O 198	P 33	0	0

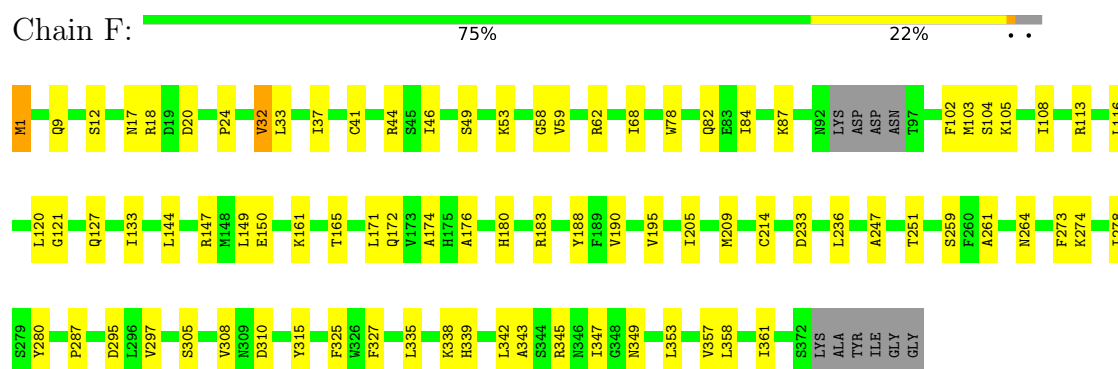
3 Residue-property plots [i](#)

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.

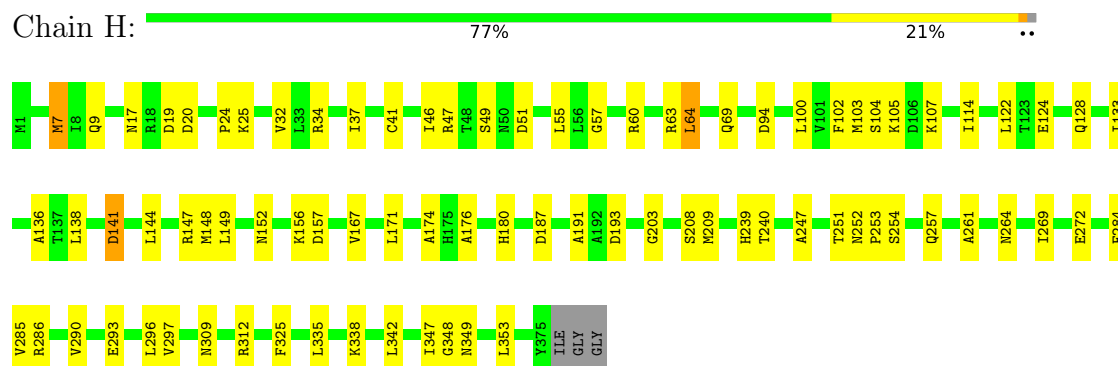
- Molecule 1: RNA (61-MER)



- Molecule 2: CRISPR system Cascade subunit CasC

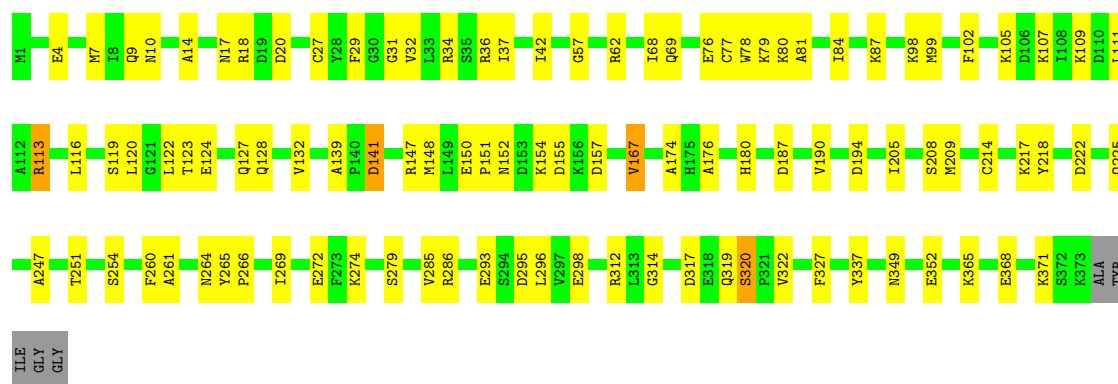


- Molecule 2: CRISPR system Cascade subunit CasC



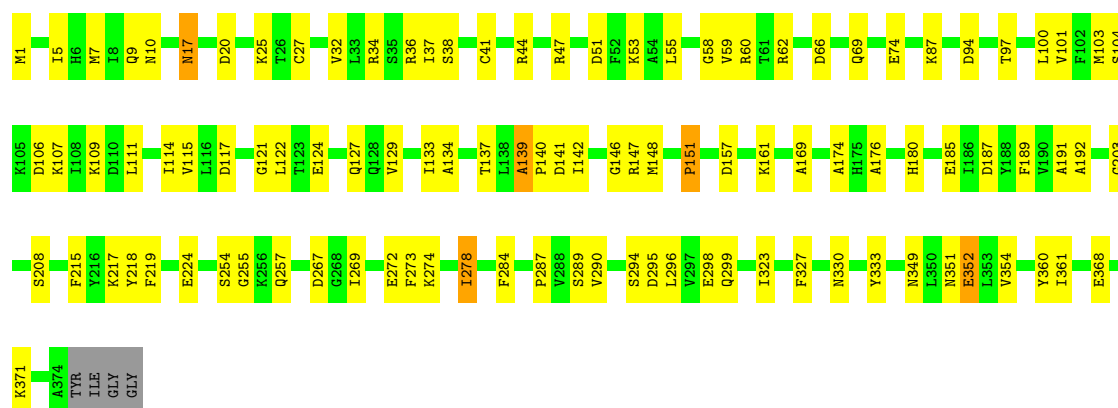
- Molecule 2: CRISPR system Cascade subunit CasC





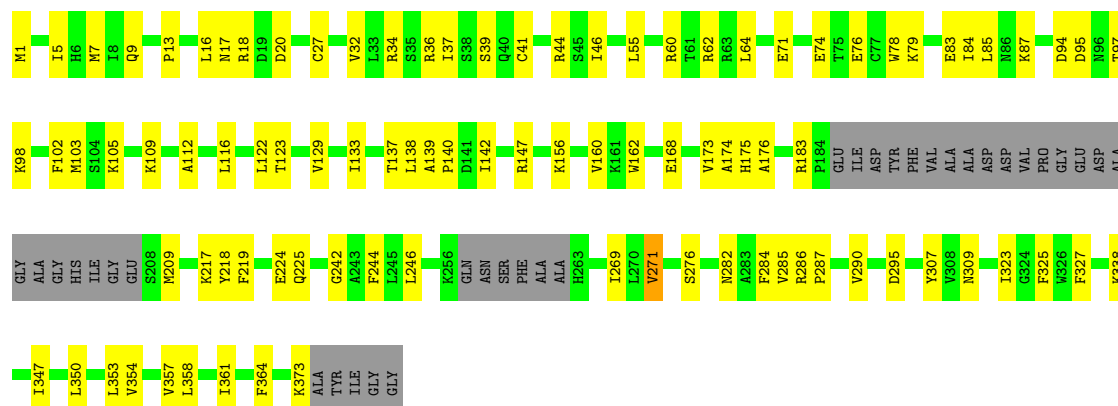
• Molecule 2: CRISPR system Cascade subunit CasC

Chain J: 71% 26% ..



• Molecule 2: CRISPR system Cascade subunit CasC

Chain K: 66% 25% 9%



• Molecule 2: CRISPR system Cascade subunit CasC

Chain G: 48% 19% 33%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53050	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	12000	Depositor
Maximum defocus (nm)	25000	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	0.14	0/984	0.35	0/1534
2	F	0.13	0/2875	0.32	0/3900
2	G	0.13	0/1967	0.34	0/2670
2	H	0.13	0/2934	0.28	0/3977
2	I	0.14	0/2911	0.33	0/3949
2	J	0.15	0/2901	0.35	0/3937
2	K	0.15	0/2695	0.37	0/3648
3	B	0.15	0/1829	0.37	0/2491
4	M	0.19	0/748	0.37	0/1150
All	All	0.14	0/19844	0.34	0/27256

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	879	0	444	29	0
2	F	2819	0	2745	61	0
2	G	1927	0	1854	52	0
2	H	2878	0	2805	61	0
2	I	2854	0	2766	69	0
2	J	2845	0	2746	79	0
2	K	2646	0	2603	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1780	0	1762	40	0
4	M	669	0	372	4	0
All	All	19297	0	18097	407	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 11.

The worst 5 of 407 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:J:272:GLU:OE2	2:J:274:LYS:NZ	2.10	0.84
1:A:6:C:N4	1:A:8:G:N7	2.29	0.81
2:F:44:ARG:HH22	2:G:194:ASP:HB3	1.44	0.81
2:F:295:ASP:HB3	2:H:286:ARG:HG2	1.62	0.81
2:J:55:LEU:HB3	2:J:140:PRO:HG2	1.64	0.80

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	
2	F	364/378 (96%)	350 (96%)	14 (4%)	0	100	100
2	G	247/378 (65%)	235 (95%)	12 (5%)	0	100	100
2	H	373/378 (99%)	349 (94%)	24 (6%)	0	100	100
2	I	371/378 (98%)	339 (91%)	31 (8%)	1 (0%)	37	67
2	J	372/378 (98%)	343 (92%)	27 (7%)	2 (0%)	25	56
2	K	338/378 (89%)	317 (94%)	21 (6%)	0	100	100
3	B	223/388 (58%)	214 (96%)	9 (4%)	0	100	100
All	All	2288/2656 (86%)	2147 (94%)	138 (6%)	3 (0%)	50	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	151	PRO
2	J	139	ALA
2	I	322	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 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	
2	F	295/313 (94%)	290 (98%)	5 (2%)	56	84
2	G	199/313 (64%)	191 (96%)	8 (4%)	27	60
2	H	302/313 (96%)	295 (98%)	7 (2%)	45	78
2	I	297/313 (95%)	289 (97%)	8 (3%)	40	74
2	J	293/313 (94%)	284 (97%)	9 (3%)	35	69
2	K	279/313 (89%)	272 (98%)	7 (2%)	42	75
3	B	183/323 (57%)	179 (98%)	4 (2%)	47	79
All	All	1848/2201 (84%)	1800 (97%)	48 (3%)	42	75

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	352	GLU
2	K	361	ILE
2	K	271	VAL
2	K	323	ILE
2	G	172	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	204	HIS
2	G	346	ASN
2	J	6	HIS

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Mol	Chain	Res	Type
3	B	22	ASN
2	K	96	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	40/61 (65%)	23 (57%)	2 (5%)

5 of 23 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	-6	U
1	A	-5	G
1	A	-3	A
1	A	1	G
1	A	2	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	C
1	A	9	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 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 ⓘ

There are no chain breaks in this entry.