wwPDB EM Validation Summary Report

Apr 26, 2026 – 12:13 AM JST

PDB ID	:	9W7Q / pdb_00009w7q
EMDB ID	:	EMD-65730
Title	:	SuperFi Cas9 - 20nt sgRNA - DNA ternary complex Class A
Authors	:	Zheng, R.; Ma, L.J.
Deposited on	:	2025-08-06
Resolution	:	3.79 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:

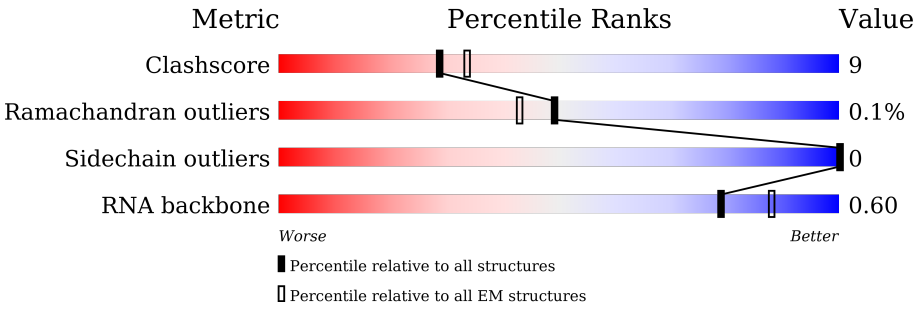
EMDB validation analysis	:	FAILED
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	NOT EXECUTED
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.79 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	1368	66% 16% 17%
2	B	50	30% 30% 40%
3	C	50	14% 16% 70%
4	D	100	24% 65% . 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12105 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 CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1129	Total	C	N	O	S	0	0
			9201	5869	1594	1719	19		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1010	ASP	TYR	engineered mutation	UNP Q99ZW2
A	1013	ASP	TYR	engineered mutation	UNP Q99ZW2
A	1016	ASP	TYR	engineered mutation	UNP Q99ZW2
A	1018	ASP	VAL	engineered mutation	UNP Q99ZW2
A	1019	ASP	ARG	engineered mutation	UNP Q99ZW2
A	1027	ASP	GLN	engineered mutation	UNP Q99ZW2
A	1031	ASP	LYS	engineered mutation	UNP Q99ZW2

- Molecule 2 is a DNA chain called DNA (50-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	30	Total	C	N	O	P	0	0
			618	293	118	178	29		

- Molecule 3 is a DNA chain called DNA (50-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	15	Total	C	N	O	P	0	0
			305	145	59	87	14		

- Molecule 4 is a RNA chain called RNA (100-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	93	Total	C	N	O	P	0	0
			1981	888	357	644	92		

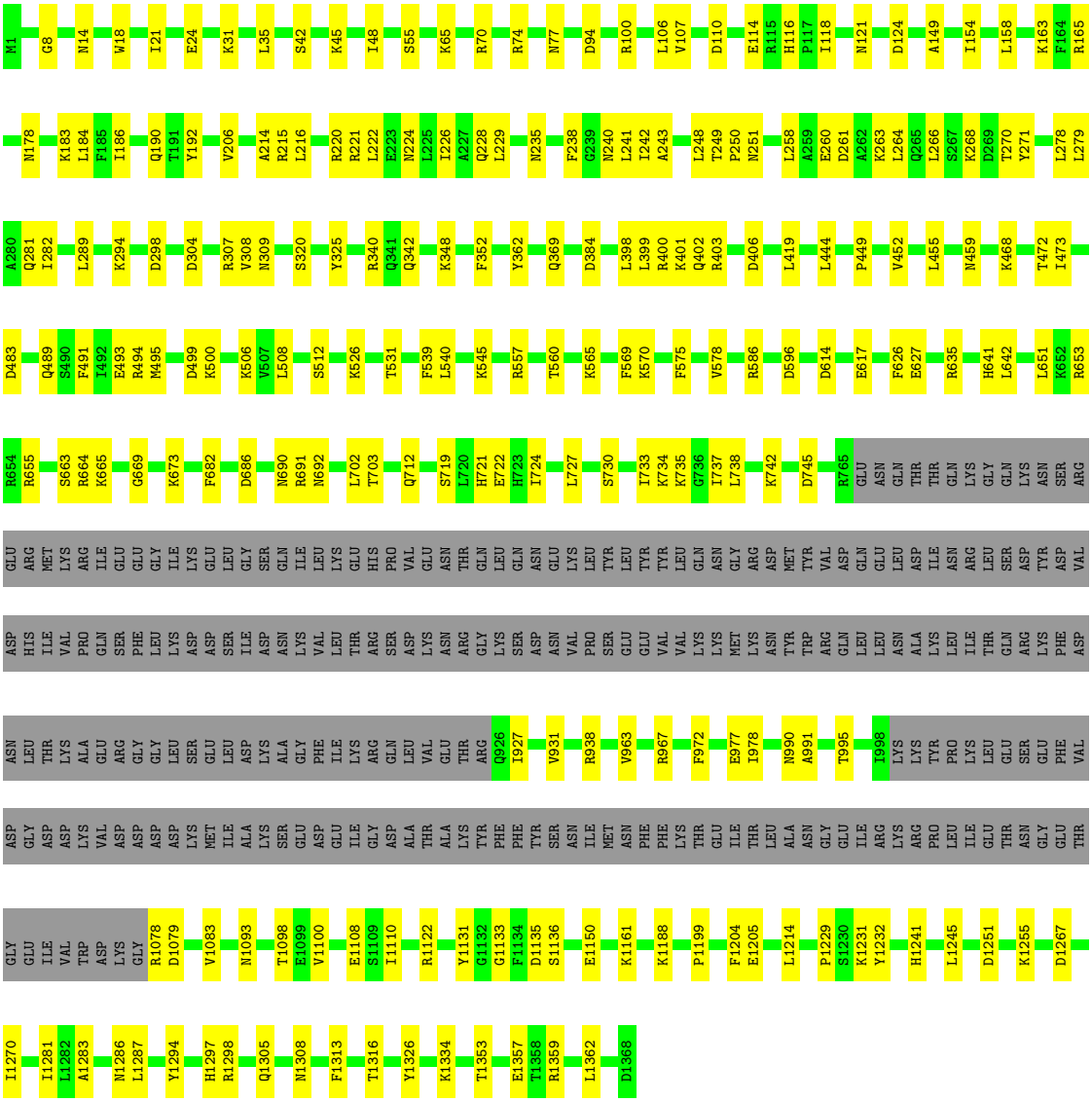
3 Residue-property plots (i)

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: CRISPR-associated endonuclease Cas9/Csn1

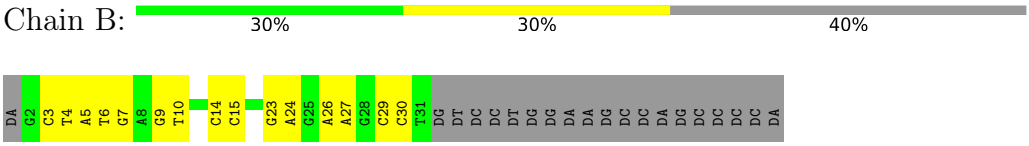
Chain A:





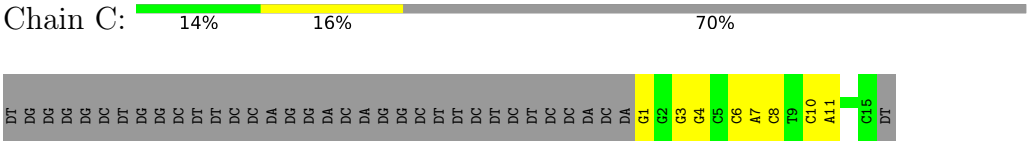
- Molecule 2: DNA (50-MER)

Chain B:



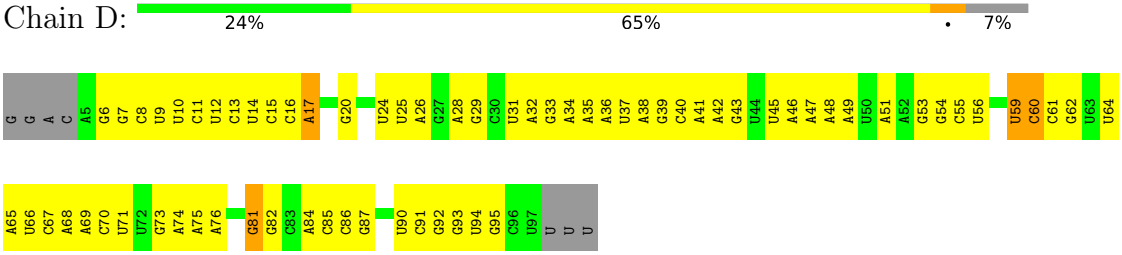
• Molecule 3: DNA (50-MER)

Chain C:



• Molecule 4: RNA (100-MER)

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39173	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.5625	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	0.18	0/9366	0.38	0/12588
2	B	0.26	0/694	0.42	0/1071
3	C	0.26	0/342	0.40	0/526
4	D	0.18	0/2217	0.27	0/3453
All	All	0.19	0/12619	0.36	0/17638

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

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	9201	0	9354	144	0
2	B	618	0	338	15	0
3	C	305	0	169	6	0
4	D	1981	0	1000	73	0
All	All	12105	0	10861	215	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.

The worst 5 of 215 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:178:ASN:HD21	1:A:298:ASP:HB2	1.44	0.81
1:A:403:ARG:NH2	4:D:46:A:OP1	2.15	0.79
1:A:724:ILE:HG23	1:A:734:LYS:HB3	1.65	0.78
1:A:468:LYS:HE3	1:A:483:ASP:HB2	1.63	0.78
1:A:65:LYS:NZ	1:A:1108:GLU:OE2	2.19	0.76

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	1123/1368 (82%)	1084 (96%)	38 (3%)	1 (0%)	48 79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	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
1	A	1009/1227 (82%)	1009 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	595	HIS
1	A	726	ASN
1	A	926	GLN
1	A	739	GLN
1	A	309	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	92/100 (92%)	12 (13%)	1 (1%)

5 of 12 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	17	A
4	D	28	A
4	D	29	G
4	D	51	A
4	D	59	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	D	59	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 (i)

There are no chain breaks in this entry.