



wwPDB EM Validation Summary Report ⓘ

Apr 26, 2026 – 12:16 AM JST

PDB ID : 9WA9 / pdb_00009wa9
EMDB ID : EMD-65809
Title : SuperFi Cas9 - 22nt sgRNA - DNA ternary complex Class B
Authors : Zheng, R.; Ma, L.J.
Deposited on : 2025-08-11
Resolution : 4.12 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

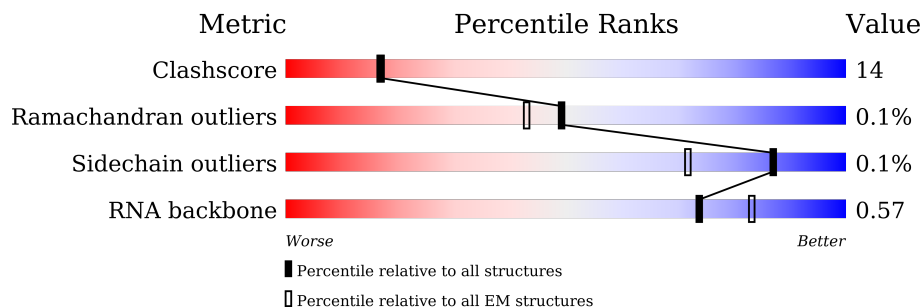
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.12 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	1368	
2	B	50	
3	C	50	
4	D	102	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12788 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	1171	Total	C	N	O	S	1	0
			9610	6108	1688	1792	22		

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).

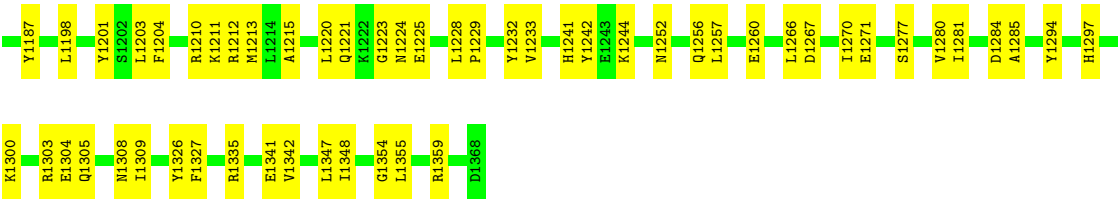
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	37	Total	C	N	O	P	0	0
			761	361	143	221	36		

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

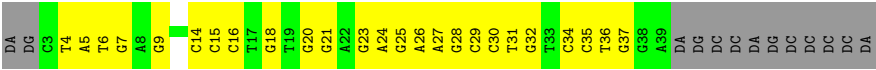
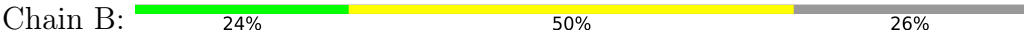
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	14	Total	C	N	O	P	0	0
			286	136	56	81	13		

- Molecule 4 is a RNA chain called RNA (102-MER).

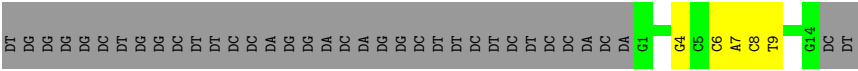
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	100	Total	C	N	O	P	0	0
			2131	955	385	692	99		



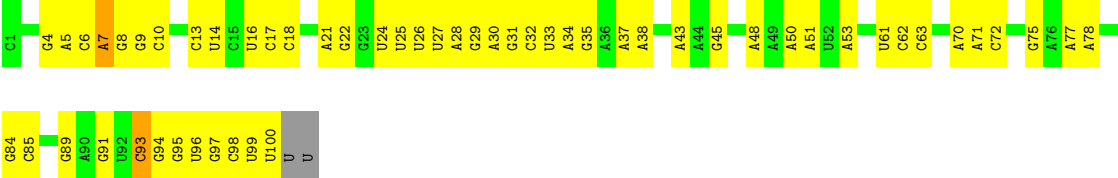
• Molecule 2: DNA (50-MER)



• Molecule 3: DNA (50-MER)



• Molecule 4: RNA (102-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58500	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 ($e^-/\text{\AA}^2$)	1.25, 1.02	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k), 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	0.12	0/9778	0.34	0/13124
2	B	0.21	0/854	0.38	0/1318
3	C	0.14	0/321	0.28	0/494
4	D	0.10	0/2385	0.23	0/3715
All	All	0.13	0/13338	0.32	0/18651

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	759	ILE	Peptide
1	A	760	VAL	Peptide

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	9610	0	9778	265	0
2	B	761	0	417	33	0
3	C	286	0	158	6	0
4	D	2131	0	1076	56	0
All	All	12788	0	11429	333	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 14.

The worst 5 of 333 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:1335:ARG:NH2	3:C:4:DG:N7	2.29	0.80
1:A:760:VAL:HG13	1:A:761:ILE:H	1.48	0.78
1:A:778:ARG:NH1	1:A:779:GLU:OE2	2.15	0.78
1:A:117:PRO:HG2	1:A:118:ILE:HD12	1.66	0.77
1:A:51:LEU:HD11	1:A:1097:LYS:HB2	1.67	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	1166/1368 (85%)	1130 (97%)	35 (3%)	1 (0%)	48 81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	760	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	1056/1227 (86%)	1054 (100%)	2 (0%)	87 86

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	783[A]	ARG
1	A	783[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	926	GLN
1	A	990	ASN
1	A	1177	ASN
1	A	413	GLN
1	A	799	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	99/102 (97%)	12 (12%)	0

5 of 12 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	7	A
4	D	21	A
4	D	22	G
4	D	30	A
4	D	31	G

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](#)

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.