



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 02:04 pm BST

PDB ID : 6K57
Title : Crystal structure of dCas9 in complex with sgRNA and DNA (CGA PAM)
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Deposited on : 2019-05-28
Resolution : 2.98 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

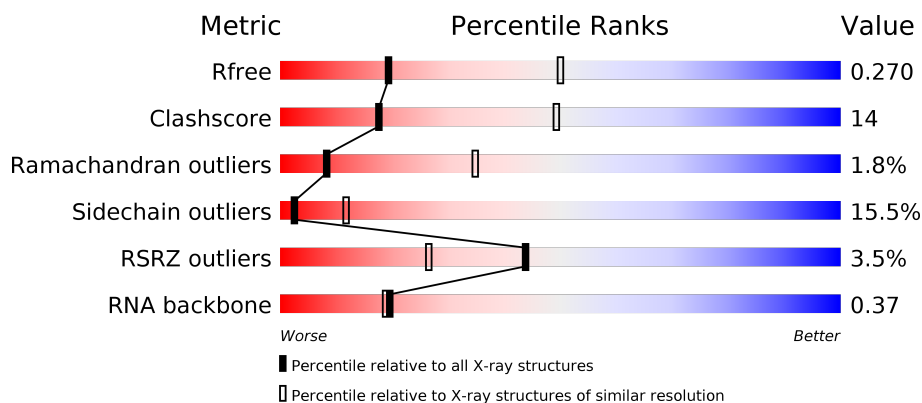
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

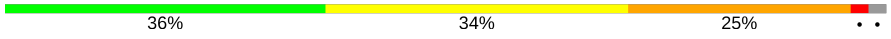



The reported resolution of this entry is 2.98 Å.

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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)
RNA backbone	3102	1088 (3.26-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	83	
2	B	1368	
3	C	28	
4	D	12	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13302 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 sgRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	81	Total	C	N	O	P	0	0	0
			1732	778	318	555	81			

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1315	Total	C	N	O	S	0	0	0
			10754	6856	1865	2011	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2

- Molecule 3 is a DNA chain called target DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	28	Total	C	N	O	P	0	0	0
			569	277	95	170	27			

- Molecule 4 is a DNA chain called non-target DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	0	0	0
			225	109	44	62	10			

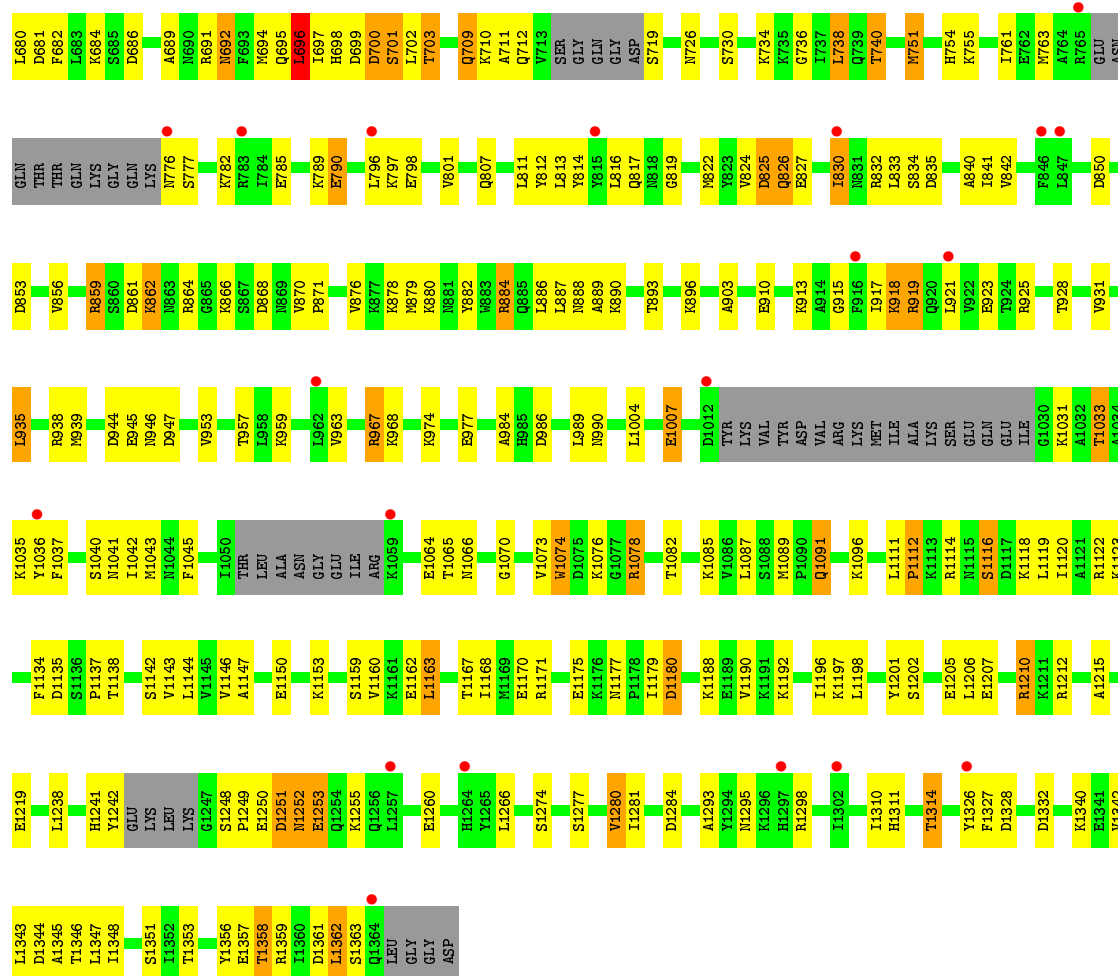
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	19	Total	O	0	0
			19	19		
5	C	1	Total	O	0	0
			1	1		



• Molecule 3: target DNA



• Molecule 4: non-target DNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.96Å 69.14Å 189.24Å 90.00° 110.34° 90.00°	Depositor
Resolution (Å)	48.89 – 2.98 48.85 – 2.98	Depositor EDS
% Data completeness (in resolution range)	92.0 (48.89-2.98) 92.0 (48.85-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.197 , 0.274 0.204 , 0.270	Depositor DCC
R_{free} test set	2073 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13302	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	1.15	19/1942 (1.0%)	0.91	0/3023
2	B	0.74	0/10943	0.95	0/14703
3	C	1.03	4/636 (0.6%)	0.96	0/980
4	D	1.27	3/253 (1.2%)	0.96	0/389
All	All	0.84	26/13774 (0.2%)	0.94	0/19095

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	8	DT	O3'-P	-9.21	1.50	1.61
4	D	7	DA	O3'-P	-8.71	1.50	1.61
1	A	15	A	O3'-P	-7.98	1.51	1.61
1	A	5	C	O3'-P	-7.85	1.51	1.61
1	A	68	A	O3'-P	-7.76	1.51	1.61

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	1732	0	869	50	0
2	B	10754	0	10917	281	0
3	C	569	0	323	26	0
4	D	225	0	126	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	2	0	0	0	0
5	B	19	0	0	0	0
5	C	1	0	0	0	0
All	All	13302	0	12235	347	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 347 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:B:317:LEU:HD22	2:B:414:ILE:CD1	1.45	1.42
2:B:317:LEU:CD2	2:B:414:ILE:HD11	1.56	1.34
3:C:19:DA:H5''	3:C:19:DA:H8	1.14	1.13
3:C:19:DA:H5''	3:C:19:DA:C8	1.92	1.03
2:B:882:TYR:CZ	2:B:886:LEU:HD11	2.00	0.96

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 X-ray entries followed by that with respect to entries of similar resolution.

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	B	1301/1368 (95%)	1125 (86%)	153 (12%)	23 (2%)	8	35

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	197	GLU
2	B	826	GLN
2	B	696	LEU
2	B	825	ASP

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Mol	Chain	Res	Type
2	B	1036	TYR

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 X-ray entries followed by that with respect to entries of similar resolution.

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	B	1180/1225 (96%)	997 (84%)	183 (16%)	2 12

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	634	GLU
2	B	719	SER
2	B	1251	ASP
2	B	643	PHE
2	B	692	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	692	ASN
2	B	709	GLN
2	B	826	GLN
2	B	563	GLN
2	B	926	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	80/83 (96%)	24 (30%)	1 (1%)

5 of 24 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	U
1	A	17	A
1	A	24	U
1	A	28	A
1	A	29	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	38	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 carbohydrates 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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	81/83 (97%)	-0.43	0 100 100	25, 45, 101, 110	0
2	B	1315/1368 (96%)	0.11	49 (3%) 41 25	28, 60, 101, 134	0
3	C	28/28 (100%)	-0.44	1 (3%) 42 26	31, 49, 80, 113	0
4	D	11/12 (91%)	-0.22	0 100 100	38, 63, 106, 127	0
All	All	1435/1491 (96%)	0.07	50 (3%) 44 26	25, 59, 101, 134	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1	DC	5.3
2	B	350	ILE	4.1
2	B	200	PRO	3.8
2	B	346	LYS	3.5
2	B	198	GLU	3.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.