



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6YES  
Title : Crystal structure of type I-D CRISPR-Cas nuclease Cas10d  
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Deposited on : 2020-03-25  
Resolution : 4.10 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](mailto: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.

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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 : 2.20  
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) : 2.20

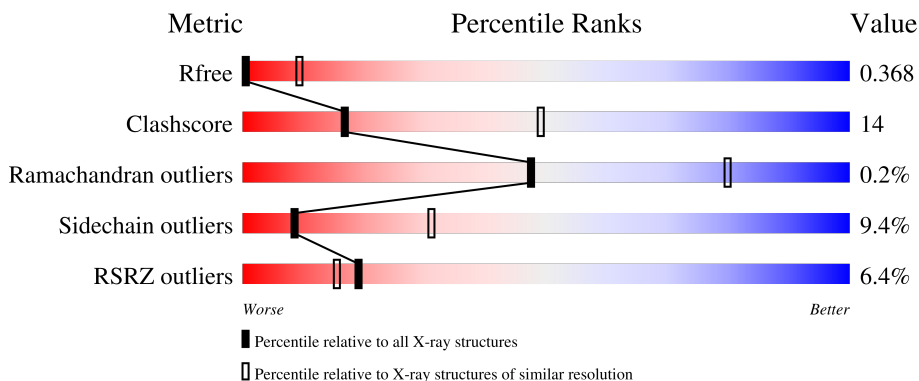
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.10 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	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	855	 2% 63% 27% 7%
1	B	855	 10% 62% 26% 9%

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 12534 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 protein called CRISPR-associated protein, CscA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	791	6325	4088	1009	1203	25	0	0	0
1	B	776	6207	4013	992	1180	22	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	848	LEU	-	expression tag	UNP M9U4Y8
A	849	GLU	-	expression tag	UNP M9U4Y8
A	850	HIS	-	expression tag	UNP M9U4Y8
A	851	HIS	-	expression tag	UNP M9U4Y8
A	852	HIS	-	expression tag	UNP M9U4Y8
A	853	HIS	-	expression tag	UNP M9U4Y8
A	854	HIS	-	expression tag	UNP M9U4Y8
A	855	HIS	-	expression tag	UNP M9U4Y8
B	848	LEU	-	expression tag	UNP M9U4Y8
B	849	GLU	-	expression tag	UNP M9U4Y8
B	850	HIS	-	expression tag	UNP M9U4Y8
B	851	HIS	-	expression tag	UNP M9U4Y8
B	852	HIS	-	expression tag	UNP M9U4Y8
B	853	HIS	-	expression tag	UNP M9U4Y8
B	854	HIS	-	expression tag	UNP M9U4Y8
B	855	HIS	-	expression tag	UNP M9U4Y8

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.43Å 141.43Å 223.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.31 – 4.10 119.57 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (91.31-4.10) 80.6 (119.57-4.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.32 (at 4.01Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.343 , 0.370 0.341 , 0.368	Depositor DCC
$R_{free}$ test set	953 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	163.5	Xtrriage
Anisotropy	0.325	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 208.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	12534	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	263.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
ZN

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	0.61	0/6446	0.75	2/8697 (0.0%)
1	B	0.62	0/6325	0.72	0/8533
All	All	0.62	0/12771	0.73	2/17230 (0.0%)

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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	339	PRO	N-CA-C	-7.30	93.12	112.10
1	A	337	ASP	CB-CG-OD2	5.26	123.04	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	356	ASP	Mainchain

### 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	6325	0	6422	183	7
1	B	6207	0	6315	172	31
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	12534	0	12737	355	38

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 355 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:359:ARG:NH1	1:A:384:LYS:HB2	1.52	1.22
1:A:735:ALA:HB1	1:A:796:HIS:CE1	1.76	1.19
1:A:334:ASN:O	1:A:337:ASP:HB2	1.42	1.16
1:A:214:GLU:HG3	1:A:219:PHE:CE1	1.83	1.13
1:B:379:GLN:N	1:B:379:GLN:OE1	1.81	1.11

The worst 5 of 38 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:GLU:CD	1:B:841:VAL:C[6_555]	0.69	1.51
1:B:292:GLU:OE2	1:B:841:VAL:CA[6_555]	0.80	1.40
1:B:292:GLU:OE2	1:B:841:VAL:C[6_555]	0.98	1.22
1:B:293:GLU:OE2	1:B:843:GLN:C[6_555]	1.11	1.09
1:B:293:GLU:CD	1:B:844:GLY:N[6_555]	1.18	1.02

## 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	
1	A	783/855 (92%)	698 (89%)	85 (11%)	0	100	100
1	B	770/855 (90%)	691 (90%)	76 (10%)	3 (0%)	34	71
All	All	1553/1710 (91%)	1389 (89%)	161 (10%)	3 (0%)	47	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	261	GLU
1	B	360	LYS
1	B	386	LEU

### 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	
1	A	718/775 (93%)	653 (91%)	65 (9%)	9	33
1	B	703/775 (91%)	635 (90%)	68 (10%)	8	29
All	All	1421/1550 (92%)	1288 (91%)	133 (9%)	8	31

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	571	SER
1	B	603	SER
1	B	815	GLU
1	A	657	ARG
1	A	652	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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 monosaccharides 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.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	791/855 (92%)	0.08	19 (2%) 59 49	138, 225, 308, 329	0
1	B	776/855 (90%)	0.53	82 (10%) 6 6	176, 264, 467, 602	0
All	All	1567/1710 (91%)	0.30	101 (6%) 19 15	138, 241, 441, 602	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	282	ASN	10.2
1	B	374	ASN	8.2
1	B	301	ALA	8.2
1	B	376	GLY	7.8
1	B	310	PRO	7.7

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	901	1/1	0.51	0.14	284,284,284,284	0
2	ZN	B	901	1/1	0.89	0.27	257,257,257,257	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.