



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 04:05 am BST

PDB ID : 3KRN  
Title : Crystal Structure of C. elegans cell-death-related nuclease 5(CRN-5)  
Authors : Yang, C.-C.; Wang, Y.-T.; Hsiao, Y.-Y.; Doudeva, L.G.; Chow, S.Y.; Yuan, H.S.  
Deposited on : 2009-11-19  
Resolution : 3.92 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	:	2.11
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

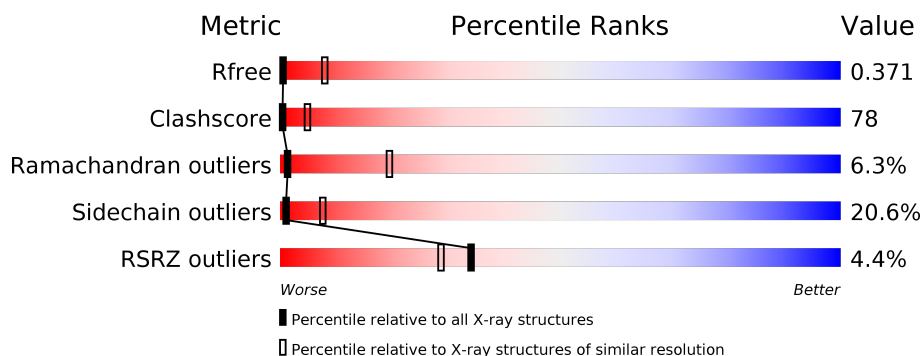
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.92 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	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)

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  $\geq 3$ , 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	222	<div> <div>5%</div> <div>20% 47% 14% 18%</div> </div>
1	B	222	<div> <div>2%</div> <div>19% 38% 14% 28%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2575 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 Protein C14A4.5, confirmed by transcript evidence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1374	864	235	261	14			
1	B	160	Total	C	N	O	S	0	0	0
			1201	758	205	225	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	215	LEU	-	EXPRESSION TAG	UNP Q17952
A	216	GLU	-	EXPRESSION TAG	UNP Q17952
A	217	HIS	-	EXPRESSION TAG	UNP Q17952
A	218	HIS	-	EXPRESSION TAG	UNP Q17952
A	219	HIS	-	EXPRESSION TAG	UNP Q17952
A	220	HIS	-	EXPRESSION TAG	UNP Q17952
A	221	HIS	-	EXPRESSION TAG	UNP Q17952
A	222	HIS	-	EXPRESSION TAG	UNP Q17952
B	215	LEU	-	EXPRESSION TAG	UNP Q17952
B	216	GLU	-	EXPRESSION TAG	UNP Q17952
B	217	HIS	-	EXPRESSION TAG	UNP Q17952
B	218	HIS	-	EXPRESSION TAG	UNP Q17952
B	219	HIS	-	EXPRESSION TAG	UNP Q17952
B	220	HIS	-	EXPRESSION TAG	UNP Q17952
B	221	HIS	-	EXPRESSION TAG	UNP Q17952
B	222	HIS	-	EXPRESSION TAG	UNP Q17952

These plots are drawn for all protein, RNA and DNA 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

- Chain A:
- 
- 5% 20% 47% 14% 18%
- MET ALA ASP G3 R4 L5 R6 E7 M8 G10 E11 L12 S13 F14 L15 LYS ASN LEU ALA ASP G20 S21 A22 C23 F24 S25 Q26 G27 A28 T29 C30 I31 W32 A33 S34 C35 S36 G37 P38 G39 D40 VAL HIS ALA SER LYS ALA SER ASP ASP GLU MET THR LEU D64 I55 S56 Y57 R58 A59 W60 C61 G62 ASP ASN K65 F66 M67 V68 L69 N70 W71 I72 T73 H74 S75 T76 LEU SER N79 A80 I81 N82 L83 GLU LEU PHE PRQ HIS T89 T90 I91 S92 V93 T94 V95 H96 G97 I98 Q99 D100 S103 A106 V107 A108 I109 N110 G111 A112 C113 F114 A115 L116 D117 D118 N119 G120 A121 H122 C123 F123 T124 T125 V126 I127 C128 G129 V130 L131 I132 I133 V134 A134 V135 K136 D137 E138 L139 I140 I141 D142 P143 T144 A145 E148 S151 T152 GLY A154 V155 L156 F157 S158 V159 C160 K161 H166 P167 E168 V169 M172 D173 A174 I175 W178 D179 F180 I181 Q182 L183 A185 W187 S188 I189 A190 Q191 P192 S193 A194 S195 A196 I197 F198 D199 F200 Y201 R202 T203 V204 R207 K208 V211 D212 GLU GLN LEU GLU LEU HIS HIS HIS HIS HIS HIS

- Chain B:
- 
- | Amino Acid | Segment |
|------------|---------|
| S188       | 19%     |
| L189       | 19%     |
| A190       | 19%     |
| Q191       | 19%     |
| P192       | 19%     |
| S193       | 19%     |
| A194       | 19%     |
| I197       | 19%     |
| F198       | 19%     |
| D199       | 19%     |
| F200       | 19%     |
| Y201       | 19%     |
| K202       | 19%     |
| T203       | 19%     |
| V204       | 19%     |
| M205       | 19%     |
| K206       | 19%     |
| R207       | 19%     |
| K208       | 19%     |
| L209       | 19%     |
| S210       | 19%     |
| V211       | 19%     |
| ASP        | 19%     |
| GLU        | 19%     |
| GLN        | 19%     |
| LEU        | 19%     |
| GLY        | 19%     |
| HIS        | 19%     |
| HIS        | 19%     |
| HIS        | 19%     |
| HIS        | 19%     |
| HIS        | 19%     |
| HIS        | 19%     |
| HIS        | 19%     |
| C61        | 19%     |
| GLY        | 19%     |
| ASP        | 19%     |
| ASN        | 19%     |
| ASN        | 19%     |
| LYS        | 19%     |
| PHE        | 19%     |
| ASN        | 19%     |
| VAL        | 19%     |
| LEU        | 19%     |
| LEU        | 19%     |
| ASN        | 19%     |
| ASN        | 19%     |
| ILE        | 19%     |
| I73        | 19%     |
| H74        | 19%     |
| S75        | 19%     |
| L139       | 19%     |
| I140       | 19%     |
| I141       | 19%     |
| D142       | 19%     |
| P143       | 19%     |
| T144       | 19%     |
| A145       | 19%     |
| K146       | 19%     |
| Q147       | 19%     |
| E148       | 19%     |
| A149       | 19%     |
| A150       | 19%     |
| S151       | 19%     |
| T152       | 19%     |
| G153       | 19%     |
| A154       | 19%     |
| V155       | 19%     |
| L156       | 19%     |
| S157       | 19%     |
| S158       | 19%     |
| V159       | 19%     |
| CYS        | 19%     |
| LYS        | 19%     |
| GLY        | 19%     |
| SER        | 19%     |
| D164       | 19%     |
| G165       | 19%     |
| R166       | 19%     |
| P167       | 19%     |
| E168       | 19%     |
| V169       | 19%     |
| C170       | 19%     |
| A171       | 19%     |
| M172       | 19%     |
| D173       | 19%     |
| A174       | 19%     |
| H177       | 19%     |
| H178       | 19%     |
| D179       | 19%     |
| F180       | 19%     |
| I181       | 19%     |
| Q182       | 19%     |
| A186       | 19%     |
| V187       | 19%     |
| G102       | 38%     |
| S103       | 38%     |
| M104       | 38%     |
| G105       | 38%     |
| A106       | 38%     |
| V107       | 38%     |
| A108       | 38%     |
| I109       | 38%     |
| M110       | 38%     |
| C113       | 38%     |
| F114       | 38%     |
| A115       | 38%     |
| L116       | 38%     |
| L117       | 38%     |
| D118       | 38%     |
| S119       | 38%     |
| G120       | 38%     |
| A121       | 38%     |
| D122       | 38%     |
| F24        | 38%     |
| S25        | 38%     |
| Q26        | 38%     |
| G27        | 38%     |
| A28        | 38%     |
| T29        | 38%     |
| C30        | 38%     |
| I31        | 38%     |
| W32        | 38%     |
| A33        | 38%     |
| S34        | 38%     |
| C35        | 38%     |
| SER        | 38%     |
| GLY        | 38%     |
| PRO        | 38%     |
| GLY        | 38%     |
| ASP        | 38%     |
| VAL        | 38%     |
| HIS        | 38%     |
| ALA        | 38%     |
| SER        | 38%     |
| LYS        | 38%     |
| ALA        | 38%     |
| SER        | 38%     |
| ASP        | 38%     |
| GLU        | 38%     |
| ALA        | 38%     |
| MET        | 38%     |
| THR        | 38%     |
| LEU        | 38%     |
| ASP        | 38%     |
| ILE        | 38%     |
| SER        | 38%     |
| TYR        | 38%     |
| ARG        | 38%     |
| ALA        | 38%     |
| ASP        | 38%     |
| ASP        | 14%     |
| GLY        | 14%     |
| GLY        | 14%     |
| ASP        | 14%     |
| VAL        | 14%     |
| HIS        | 14%     |
| ALA        | 14%     |
| SER        | 14%     |
| LYS        | 14%     |
| ALA        | 14%     |
| SER        | 14%     |
| ASP        | 14%     |
| GLU        | 14%     |
| ALA        | 14%     |
| MET        | 14%     |
| THR        | 14%     |
| LEU        | 14%     |
| ASP        | 14%     |
| ILE        | 14%     |
| SER        | 14%     |
| TYR        | 14%     |
| ARG        | 14%     |
| ALA        | 14%     |
| ASP        | 14%     |
| ASP        | 28%     |
| GLY        | 28%     |
| ALA        | 28%     |
| MET        | 28%     |
| THR        | 28%     |
| LEU        | 28%     |
| ASP        | 28%     |
| ILE        | 28%     |
| SER        | 28%     |
| TYR        | 28%     |
| ARG        | 28%     |
| ALA        | 28%     |
| ASP        | 28%     |

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.95Å 44.84Å 65.51Å 90.00° 100.65° 90.00°	Depositor
Resolution (Å)	26.50 – 3.92 36.79 – 3.92	Depositor EDS
% Data completeness (in resolution range)	97.2 (26.50-3.92) 85.1 (36.79-3.92)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	11.39 (at 3.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.306 , 0.356 0.302 , 0.371	Depositor DCC
$R_{free}$ test set	228 reflections (7.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.2	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 99.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	2575	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.78% 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

### 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	0.29	0/1394	0.50	0/1878
1	B	0.28	0/1219	0.55	0/1642
All	All	0.28	0/2613	0.52	0/3520

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	1374	0	1341	209	0
1	B	1201	0	1176	195	0
All	All	2575	0	2517	397	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 78.

The worst 5 of 397 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:83:LEU:HD11	1:A:121:MET:CG	1.34	1.52
1:A:83:LEU:CD1	1:A:121:MET:HG3	1.73	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:CD1	1:A:121:MET:CG	2.22	1.16
1:A:83:LEU:HD12	1:A:121:MET:HE2	1.29	1.14
1:A:128:CYS:HB2	1:A:129:GLY:CA	1.78	1.13

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	
1	A	169/222 (76%)	120 (71%)	38 (22%)	11 (6%)	1	19
1	B	148/222 (67%)	110 (74%)	29 (20%)	9 (6%)	1	20
All	All	317/444 (71%)	230 (73%)	67 (21%)	20 (6%)	1	19

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	PRO
1	B	167	PRO
1	A	27	GLY
1	A	67	ASN
1	A	93	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 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	149/182 (82%)	120 (80%)	29 (20%)	1	9
1	B	128/182 (70%)	100 (78%)	28 (22%)	1	6
All	All	277/364 (76%)	220 (79%)	57 (21%)	1	7

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	ILE
1	B	6	ARG
1	B	157	PHE
1	A	178	TRP
1	A	197	ILE

Some 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	191	GLN
1	B	26	GLN
1	B	119	ASN
1	A	119	ASN
1	B	79	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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, 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	183/222 (82%)	0.38	11 (6%) 21 17	19, 82, 164, 223	0
1	B	160/222 (72%)	0.38	4 (2%) 57 48	12, 83, 162, 265	0
All	All	343/444 (77%)	0.38	15 (4%) 34 29	12, 82, 162, 265	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	ASN	4.0
1	B	133	VAL	3.7
1	A	125	THR	3.2
1	A	134	ARG	3.0
1	B	25	SER	2.9

### 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.