



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 08:18 am BST

PDB ID : 2D2Z  
Title : Crystal structure of Soluble Form Of CLIC4  
Authors : Li, Y.F.; Li, D.F.; Wang, D.C.  
Deposited on : 2005-09-21  
Resolution : 2.20 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

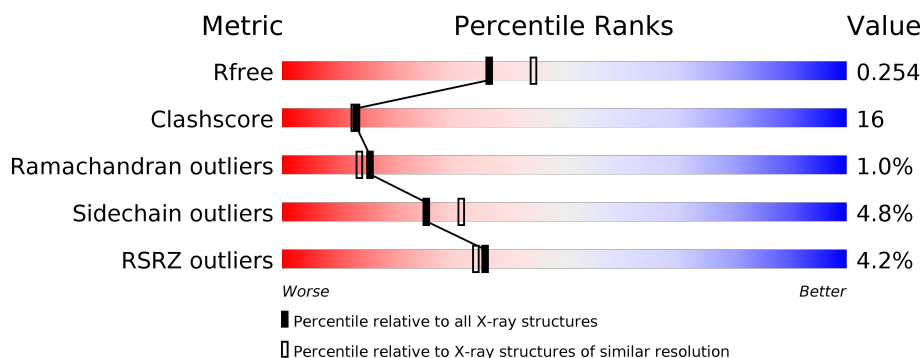
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	261	
1	B	261	
1	C	261	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6238 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 Chloride intracellular channel protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1764	1138	290	328	8			
1	B	240	Total	C	N	O	S	0	0	0
			1889	1211	311	359	8			
1	C	231	Total	C	N	O	S	0	0	0
			1821	1171	298	344	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	LEU	-	EXPRESSION TAG	UNP Q9Y696
A	255	GLU	-	EXPRESSION TAG	UNP Q9Y696
A	256	HIS	-	EXPRESSION TAG	UNP Q9Y696
A	257	HIS	-	EXPRESSION TAG	UNP Q9Y696
A	258	HIS	-	EXPRESSION TAG	UNP Q9Y696
A	259	HIS	-	EXPRESSION TAG	UNP Q9Y696
A	260	HIS	-	EXPRESSION TAG	UNP Q9Y696
A	261	HIS	-	EXPRESSION TAG	UNP Q9Y696
B	254	LEU	-	EXPRESSION TAG	UNP Q9Y696
B	255	GLU	-	EXPRESSION TAG	UNP Q9Y696
B	256	HIS	-	EXPRESSION TAG	UNP Q9Y696
B	257	HIS	-	EXPRESSION TAG	UNP Q9Y696
B	258	HIS	-	EXPRESSION TAG	UNP Q9Y696
B	259	HIS	-	EXPRESSION TAG	UNP Q9Y696
B	260	HIS	-	EXPRESSION TAG	UNP Q9Y696
B	261	HIS	-	EXPRESSION TAG	UNP Q9Y696
C	254	LEU	-	EXPRESSION TAG	UNP Q9Y696
C	255	GLU	-	EXPRESSION TAG	UNP Q9Y696
C	256	HIS	-	EXPRESSION TAG	UNP Q9Y696
C	257	HIS	-	EXPRESSION TAG	UNP Q9Y696
C	258	HIS	-	EXPRESSION TAG	UNP Q9Y696
C	259	HIS	-	EXPRESSION TAG	UNP Q9Y696
C	260	HIS	-	EXPRESSION TAG	UNP Q9Y696

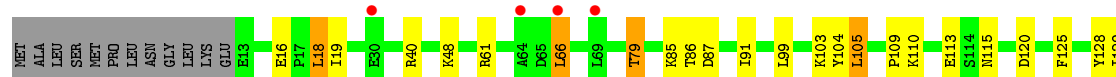
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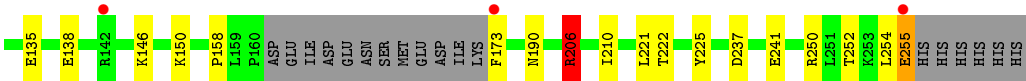
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Chain	Residue	Modelled	Actual	Comment	Reference
C	261	HIS	-	EXPRESSION TAG	UNP Q9Y696

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	229	Total 229	O 229	0	0
2	B	254	Total 254	O 254	0	0
2	C	281	Total 281	O 281	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.19Å 86.05Å 73.38Å 90.00° 112.99° 90.00°	Depositor
Resolution (Å)	23.49 – 2.20 23.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (23.49-2.20) 99.8 (23.49-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 2.19Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.216 , 0.262 0.212 , 0.254	Depositor DCC
$R_{free}$ test set	4285 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 61.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6238	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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](#)

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	0.36	0/1803	0.57	0/2436
1	B	0.36	0/1929	0.63	3/2607 (0.1%)
1	C	0.39	0/1861	0.63	1/2517 (0.0%)
All	All	0.37	0/5593	0.61	4/7560 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	THR	N-CA-C	6.08	127.42	111.00
1	C	206	ARG	N-CA-C	-5.88	95.11	111.00
1	B	6	PRO	N-CA-CB	5.77	110.22	103.30
1	B	210	ILE	N-CA-C	-5.01	97.46	111.00

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	1764	0	1776	54	0
1	B	1889	0	1880	94	0
1	C	1821	0	1813	36	0
2	A	229	0	0	10	0
2	B	254	0	0	13	0
2	C	281	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6238	0	5469	178	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 16.

The worst 5 of 178 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:B:174:SER:HB2	2:B:422:HOH:O	1.47	1.15
1:A:98:VAL:HG23	1:A:99:LEU:HD13	1.49	0.95
1:B:50:VAL:HG11	1:B:99:LEU:HD13	1.57	0.86
1:B:34:ASN:HD21	1:B:197:ILE:HD12	1.43	0.84
1:A:193:PRO:O	1:A:197:ILE:HD13	1.80	0.81

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	217/261 (83%)	209 (96%)	7 (3%)	1 (0%)	29	31
1	B	236/261 (90%)	215 (91%)	16 (7%)	5 (2%)	7	4
1	C	227/261 (87%)	219 (96%)	7 (3%)	1 (0%)	34	37
All	All	680/783 (87%)	643 (95%)	30 (4%)	7 (1%)	15	14

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	ASN
1	C	61	ARG
1	B	15	LYS

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Mol	Chain	Res	Type
1	A	68	ASN
1	B	69	LEU

### 5.3.2 Protein sidechains ⓘ

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	197/237 (83%)	190 (96%)	7 (4%)	35	45
1	B	209/237 (88%)	196 (94%)	13 (6%)	18	21
1	C	202/237 (85%)	193 (96%)	9 (4%)	27	34
All	All	608/711 (86%)	579 (95%)	29 (5%)	25	32

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	125	PHE
1	B	233	THR
1	C	138	GLU
1	B	135	GLU
1	B	234	CYS

Some 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	232	ASN
1	B	34	ASN
1	C	34	ASN
1	A	207	ASN
1	B	196	HIS

### 5.3.3 RNA ⓘ

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 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, 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	223/261 (85%)	0.21	7 (3%) 49 47	18, 37, 68, 80	0
1	B	240/261 (91%)	0.29	15 (6%) 20 19	21, 39, 67, 80	0
1	C	231/261 (88%)	-0.03	7 (3%) 50 48	17, 30, 65, 89	0
All	All	694/783 (88%)	0.15	29 (4%) 36 34	17, 35, 68, 89	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	PRO	4.8
1	B	6	PRO	4.1
1	B	64	ALA	3.9
1	C	173	PHE	3.7
1	B	161	ASP	3.6

### 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.