



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 13, 2024 – 07:52 AM EST

PDB ID : 4KK6  
Title : Structure of CLC-ec1 deltaNC construct in 20mM Bromide  
Authors : Lim, H.-H.; Miller, C.  
Deposited on : 2013-05-05  
Resolution : 3.18 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.

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:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

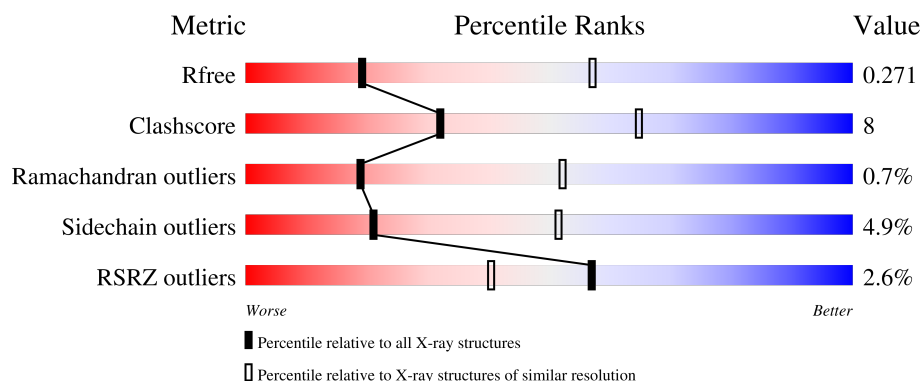
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.18 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))
$R_{free}$	164625	1851 (3.20-3.16)
Clashscore	180529	1999 (3.20-3.16)
Ramachandran outliers	177936	1961 (3.20-3.16)
Sidechain outliers	177891	1960 (3.20-3.16)
RSRZ outliers	164620	1852 (3.20-3.16)

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	446	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>..</div> </div> </div>
1	B	446	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>..</div> </div> </div>
2	C	222	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>.</div> </div> </div>
2	E	222	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>.</div> </div> </div>
3	D	211	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div> </div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	F	211	 89%8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BR	A	501	-	-	X	-
4	BR	A	502	-	-	X	-
4	BR	B	501	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13218 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 H(+)/Cl(-) exchange transporter ClcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3324	2185	558	561	20			
1	B	441	Total	C	N	O	S	0	0	0
			3304	2174	553	557	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	expression tag	UNP P37019
A	461	LYS	-	expression tag	UNP P37019
B	16	MET	-	expression tag	UNP P37019
B	461	LYS	-	expression tag	UNP P37019

- Molecule 2 is a protein called Fab, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			
2	E	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			

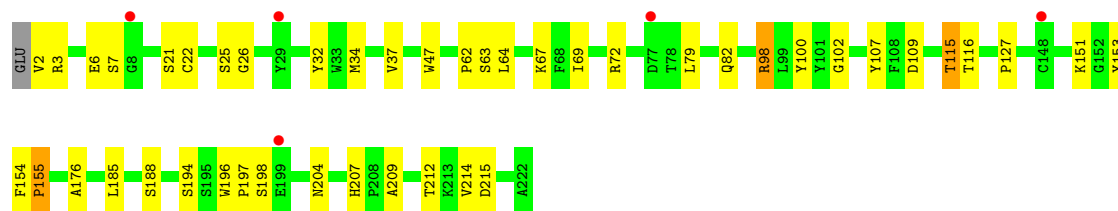
- Molecule 3 is a protein called Fab, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	F	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			

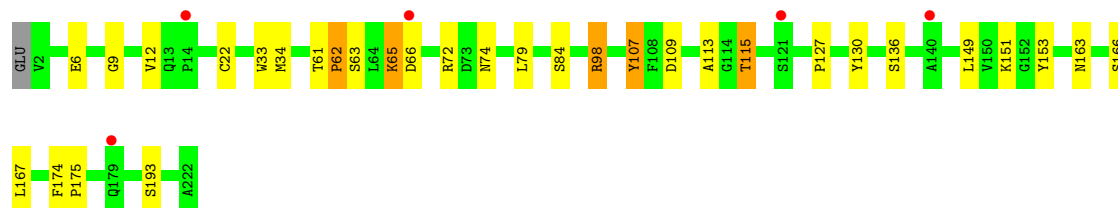
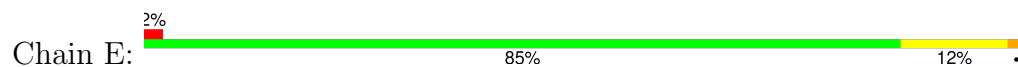
- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Br 2	0	0
4	B	2	Total 2	Br 2	0	0

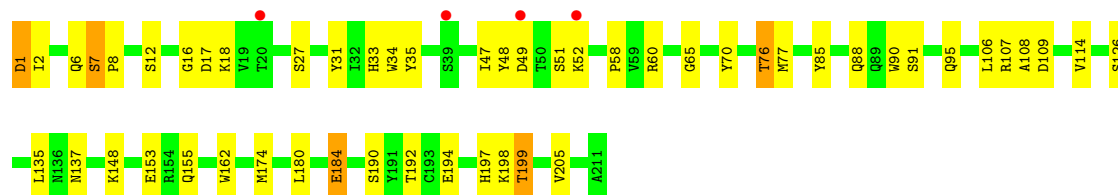
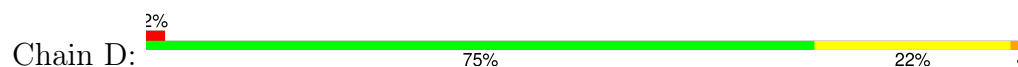




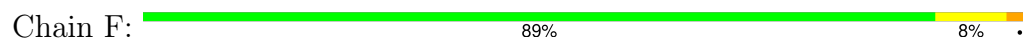
- Molecule 2: Fab, heavy chain



- Molecule 3: Fab, light chain



- Molecule 3: Fab, light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.36Å 100.92Å 171.72Å 90.00° 132.12° 90.00°	Depositor
Resolution (Å)	24.88 – 3.18 24.88 – 3.18	Depositor EDS
% Data completeness (in resolution range)	99.0 (24.88-3.18) 98.9 (24.88-3.18)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 3.17Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.235 , 0.269 0.237 , 0.271	Depositor DCC
$R_{free}$ test set	2462 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	101.9	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 8.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13218	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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

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

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	0.32	0/3396	0.42	0/4609
1	B	0.30	0/3376	0.43	0/4583
2	C	0.34	0/1721	0.44	0/2355
2	E	0.34	0/1721	0.44	0/2355
3	D	0.30	0/1660	0.47	0/2257
3	F	0.33	0/1660	0.47	1/2257 (0.0%)
All	All	0.32	0/13534	0.44	1/18416 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	7	SER	C-N-CD	6.14	141.29	128.40

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	3324	0	3476	58	0
1	B	3304	0	3457	88	0
2	C	1672	0	1654	22	0
2	E	1672	0	1654	16	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1621	0	1546	28	0
3	F	1621	0	1546	13	0
4	A	2	0	0	6	0
4	B	2	0	0	9	0
All	All	13218	0	13333	209	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 8.

The worst 5 of 209 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:356:ILE:N	4:B:501:BR:BR	2.16	1.32
1:A:107:SER:N	4:A:502:BR:BR	2.66	0.83
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.62	0.81
1:B:355:GLY:CA	4:B:501:BR:BR	2.89	0.75
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.20	0.74

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	441/446 (99%)	423 (96%)	18 (4%)	0	100	100
1	B	439/446 (98%)	407 (93%)	29 (7%)	3 (1%)	19	52
2	C	219/222 (99%)	203 (93%)	13 (6%)	3 (1%)	9	38
2	E	219/222 (99%)	195 (89%)	21 (10%)	3 (1%)	9	38
3	D	209/211 (99%)	187 (90%)	18 (9%)	4 (2%)	6	31
3	F	209/211 (99%)	187 (90%)	22 (10%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1736/1758 (99%)	1602 (92%)	121 (7%)	13 (1%)	19	52

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	62	PRO
2	E	65	LYS
1	B	107	SER
2	C	62	PRO
3	D	126	SER

### 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	334/337 (99%)	309 (92%)	25 (8%)	11	37
1	B	332/337 (98%)	319 (96%)	13 (4%)	27	57
2	C	181/182 (100%)	172 (95%)	9 (5%)	20	50
2	E	181/182 (100%)	173 (96%)	8 (4%)	24	54
3	D	185/185 (100%)	180 (97%)	5 (3%)	40	67
3	F	185/185 (100%)	176 (95%)	9 (5%)	21	51
All	All	1398/1408 (99%)	1329 (95%)	69 (5%)	21	51

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	151	LYS
2	E	193	SER
3	F	74	ILE
1	A	452	THR
1	A	451	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	284	HIS
1	B	420	GLN

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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	443/446 (99%)	-0.14	9 (2%) 64 48	45, 67, 94, 130	0
1	B	441/446 (98%)	0.10	22 (4%) 35 23	49, 77, 111, 138	0
2	C	221/222 (99%)	-0.19	5 (2%) 61 44	35, 65, 99, 133	0
2	E	221/222 (99%)	-0.23	5 (2%) 61 44	45, 65, 93, 132	0
3	D	211/211 (100%)	0.02	4 (1%) 66 50	49, 77, 98, 106	0
3	F	211/211 (100%)	-0.33	0 100 100	40, 58, 106, 120	0
All	All	1748/1758 (99%)	-0.10	45 (2%) 57 40	35, 69, 102, 138	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	ALA	7.3
1	B	73	ASP	5.9
1	B	72	ALA	4.9
1	A	168	LEU	4.7
1	B	95	PHE	4.6

### 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 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(Å <sup>2</sup> )	Q<0.9
4	BR	B	502	1/1	0.77	0.18	126,126,126,126	0
4	BR	A	502	1/1	0.84	0.21	121,121,121,121	0
4	BR	A	501	1/1	0.91	0.16	98,98,98,98	0
4	BR	B	501	1/1	0.92	0.23	115,115,115,115	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.