



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 06:01 AM EDT

PDB ID : 2EXW / pdb\_00002exw  
Title : Crystal structure of a EcCIC-Fab complex in the absence of bound ions  
Authors : Lobet, S.; Dutzler, R.  
Deposited on : 2005-11-09  
Resolution : 3.20 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

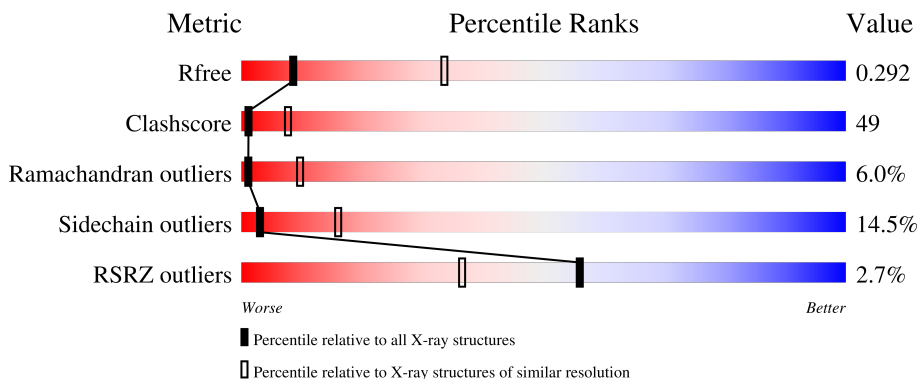
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 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	473	
1	B	473	
2	C	222	
2	E	222	
3	D	211	

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Mol	Chain	Length	Quality of chain
3	F	211	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a green segment on the left labeled '26%', a yellow segment in the middle labeled '48%', and an orange segment on the right labeled '23%'. A small red square is at the far left end, and a small black dot is at the far right end. A '%' symbol is positioned above the bar.</p>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13223 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
			Total	C	N	O	S			
1	A	444	3333	2190	560	563	20	0	0	0
1	B	441	3304	2174	553	557	20	0	0	0

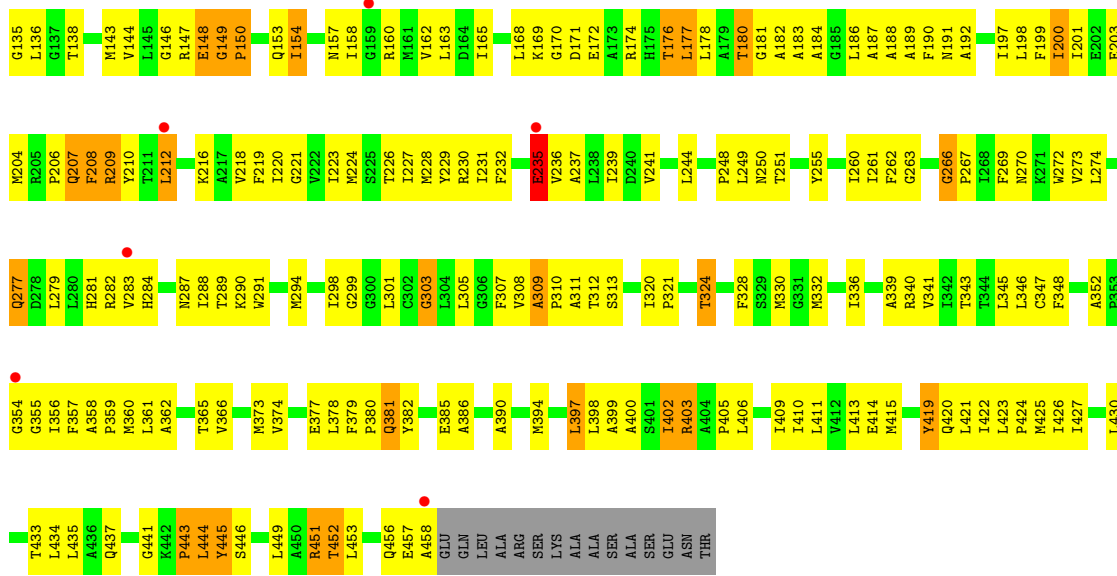
- Molecule 2 is a protein called Fab Fragment (Heavy Chain).

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

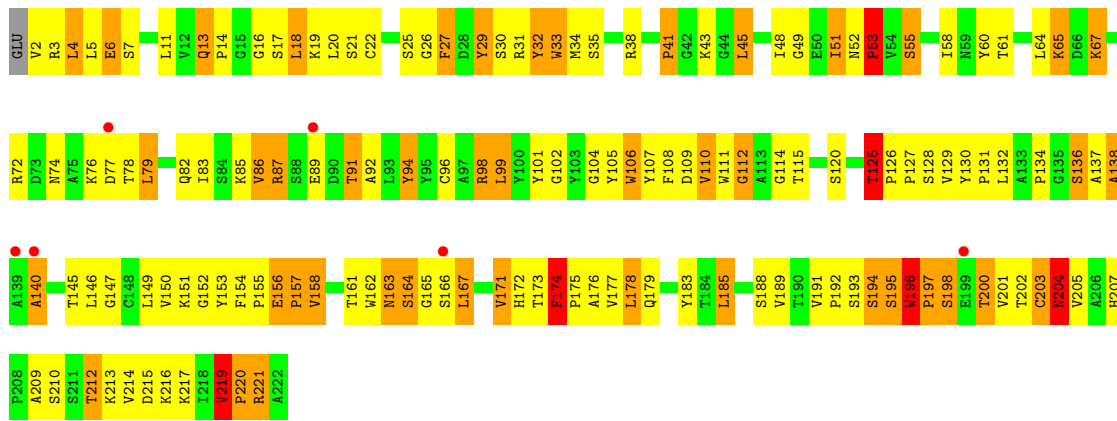
- Molecule 3 is a protein called Fab Fragment (Light Chain).

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

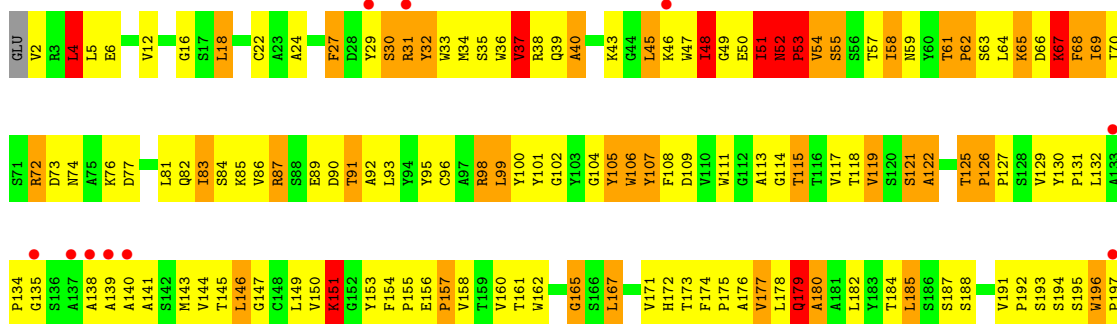




• Molecule 2: Fab Fragment (Heavy Chain)

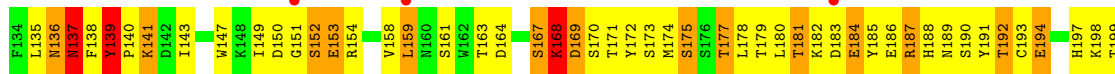
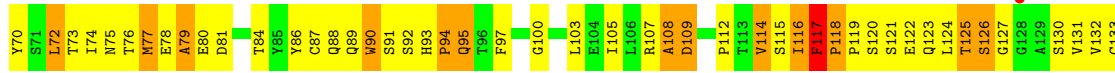


• Molecule 2: Fab Fragment (Heavy Chain)

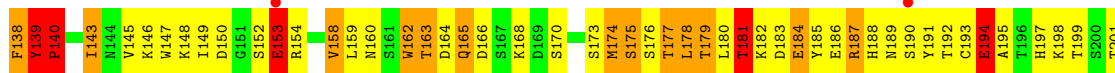
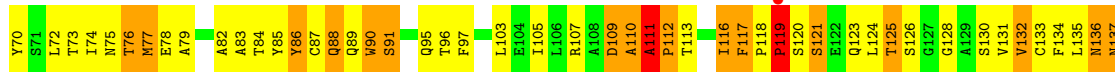
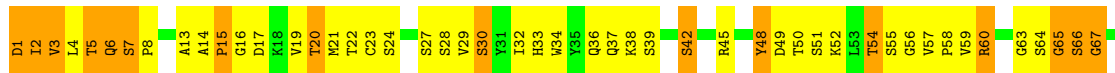




● Molecule 3: Fab Fragment (Light Chain)



● Molecule 3: Fab Fragment (Light Chain)



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	219.83Å 122.44Å 151.34Å 90.00° 128.16° 90.00°	Depositor
Resolution (Å)	19.98 – 3.20 19.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.98-3.20) 97.7 (19.98-3.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.93 (at 3.22Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.268 , 0.314 0.261 , 0.292	Depositor DCC
$R_{free}$ test set	2524 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.6	Xtrriage
Anisotropy	0.519	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 60.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13223	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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	0.53	0/3405	1.02	17/4621 (0.4%)
1	B	0.58	1/3376 (0.0%)	1.03	14/4583 (0.3%)
2	C	0.65	0/1721	1.44	32/2355 (1.4%)
2	E	0.67	0/1721	1.37	26/2355 (1.1%)
3	D	0.54	0/1660	1.30	25/2257 (1.1%)
3	F	0.87	5/1660 (0.3%)	1.67	33/2257 (1.5%)
All	All	0.63	6/13543 (0.0%)	1.26	147/18428 (0.8%)

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	A	0	1
1	B	0	1
2	C	0	1
2	E	0	1
3	D	0	1
3	F	0	1
All	All	0	6

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	139	TYR	C-O	-13.94	1.06	1.24
3	F	140	PRO	CA-C	10.29	1.67	1.52
3	F	140	PRO	C-O	7.68	1.33	1.24
3	F	140	PRO	N-CA	6.80	1.56	1.47
1	B	235	GLU	C-O	-5.89	1.16	1.24

The worst 5 of 147 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	139	TYR	CA-C-N	-25.41	88.07	119.84
3	F	139	TYR	C-N-CA	-25.41	88.07	119.84
3	F	110	ALA	N-CA-C	16.77	130.20	110.41
2	C	174	PHE	CA-C-N	-13.02	106.79	120.85
2	C	174	PHE	C-N-CA	-13.02	106.79	120.85

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	419	TYR	Sidechain
1	B	419	TYR	Sidechain
2	C	29	TYR	Sidechain
3	D	139	TYR	Sidechain
2	E	101	TYR	Sidechain

## 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	3333	0	3484	310	0
1	B	3304	0	3457	295	0
2	C	1672	0	1654	187	0
2	E	1672	0	1654	172	0
3	D	1621	0	1546	204	0
3	F	1621	0	1546	239	0
All	All	13223	0	13341	1293	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 49.

The worst 5 of 1293 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:E:207:HIS:ND1	2:E:210:SER:HB2	1.52	1.23
1:A:235:GLU:O	1:A:236:VAL:HG23	1.47	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.33	1.10
3:F:7:SER:HB2	3:F:22:THR:HB	1.34	1.08
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.35	1.07

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	442/473 (93%)	361 (82%)	62 (14%)	19 (4%)	2	16
1	B	439/473 (93%)	342 (78%)	81 (18%)	16 (4%)	2	19
2	C	219/222 (99%)	166 (76%)	39 (18%)	14 (6%)	1	8
2	E	219/222 (99%)	173 (79%)	30 (14%)	16 (7%)	1	6
3	D	209/211 (99%)	159 (76%)	28 (13%)	22 (10%)	0	2
3	F	209/211 (99%)	158 (76%)	33 (16%)	18 (9%)	0	3
All	All	1737/1812 (96%)	1359 (78%)	273 (16%)	105 (6%)	1	10

5 of 105 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	ASP
1	A	209	ARG
1	A	236	VAL
1	A	309	ALA
1	B	73	ASP

### 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	335/358 (94%)	308 (92%)	27 (8%)	11	39
1	B	332/358 (93%)	303 (91%)	29 (9%)	9	36
2	C	181/182 (100%)	145 (80%)	36 (20%)	1	7
2	E	181/182 (100%)	138 (76%)	43 (24%)	1	4
3	D	185/185 (100%)	150 (81%)	35 (19%)	1	9
3	F	185/185 (100%)	152 (82%)	33 (18%)	2	10
All	All	1399/1450 (96%)	1196 (86%)	203 (14%)	3	16

5 of 203 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	137	ASN
2	E	59	ASN
3	F	194	GLU
3	D	175	SER
2	E	12	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	59	ASN
3	D	189	ASN
2	C	82	GLN
3	D	93	HIS
3	F	37	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](#)

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	444/473 (93%)	0.35	13 (2%) 53 35	48, 77, 111, 138	0
1	B	441/473 (93%)	0.27	10 (2%) 61 41	41, 71, 115, 151	0
2	C	221/222 (99%)	0.33	6 (2%) 56 36	43, 71, 106, 160	0
2	E	221/222 (99%)	0.45	10 (4%) 38 24	37, 78, 121, 145	0
3	D	211/211 (100%)	0.58	6 (2%) 55 35	52, 91, 118, 128	0
3	F	211/211 (100%)	0.48	3 (1%) 73 54	26, 70, 123, 140	0
All	All	1749/1812 (96%)	0.38	48 (2%) 56 36	26, 76, 117, 160	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	ALA	6.7
1	A	235	GLU	4.2
1	B	235	GLU	4.0
2	C	140	ALA	3.8
1	B	212	LEU	3.4

### 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 oligosaccharides 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.