



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 02:01 am GMT

PDB ID : 3DET
Title : Structure of the E148A, Y445A doubly ungated mutant of E.coli CLC_Ec1,
Cl⁻/H⁺ antiporter
Authors : Jayaram, H.; Accardi, A.; Wu, F.; Williams, C.; Miller, C.
Deposited on : 2008-06-10
Resolution : 2.80 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

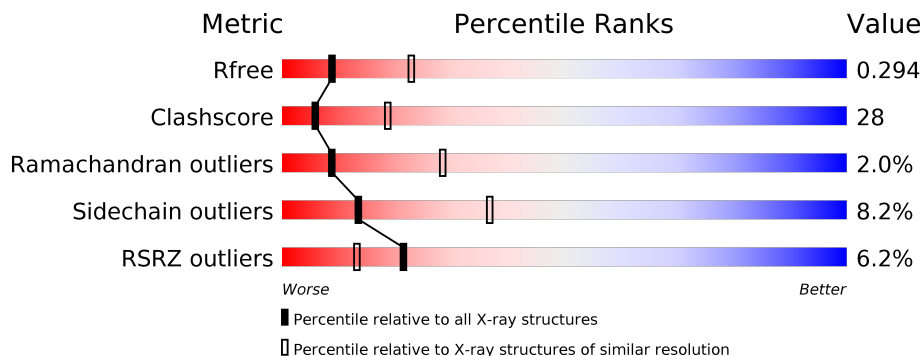
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>4%</div> <div> <div>48%</div> <div>41%</div> <div>6%</div> </div> </div>
1	B	473	<div> <div>6%</div> <div> <div>45%</div> <div>41%</div> <div>7%</div> <div>7%</div> </div> </div>
2	C	221	<div> <div>5%</div> <div> <div>63%</div> <div>32%</div> <div>5%</div> </div> </div>
2	E	221	<div> <div>3%</div> <div> <div>63%</div> <div>34%</div> </div> </div>
3	D	211	<div> <div>9%</div> <div> <div>52%</div> <div>41%</div> <div>7%</div> </div> </div>
3	F	211	<div> <div>11%</div> <div> <div>53%</div> <div>43%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13201 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	444	Total	C	N	O	S	0	0	0
			3322	2182	560	560	20			
1	B	441	Total	C	N	O	S	0	0	0
			3293	2166	553	554	20			

There are 4 discrepancies between the modelled and reference sequences:

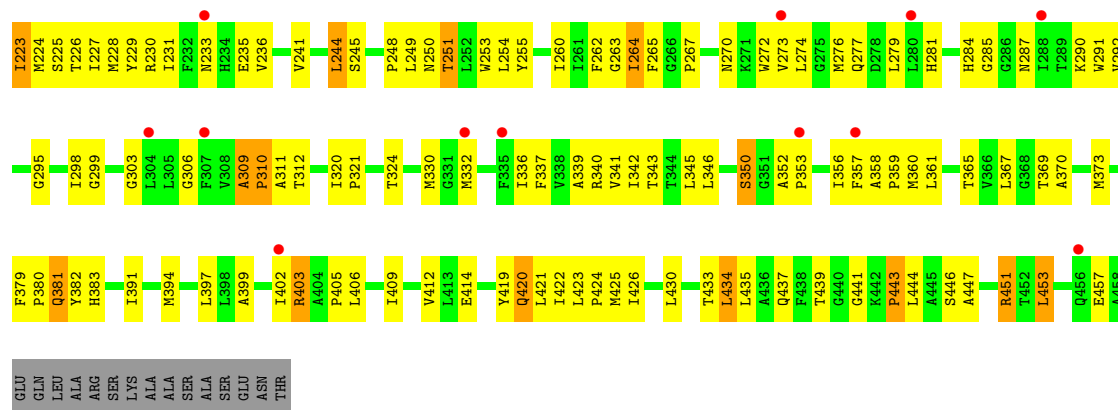
Chain	Residue	Modelled	Actual	Comment	Reference
A	148	ALA	GLU	ENGINEERED	UNP P37019
A	445	ALA	TYR	ENGINEERED	UNP P37019
B	148	ALA	GLU	ENGINEERED	UNP P37019
B	445	ALA	TYR	ENGINEERED	UNP P37019

- Molecule 2 is a protein called Fab fragment, Heavy chain.

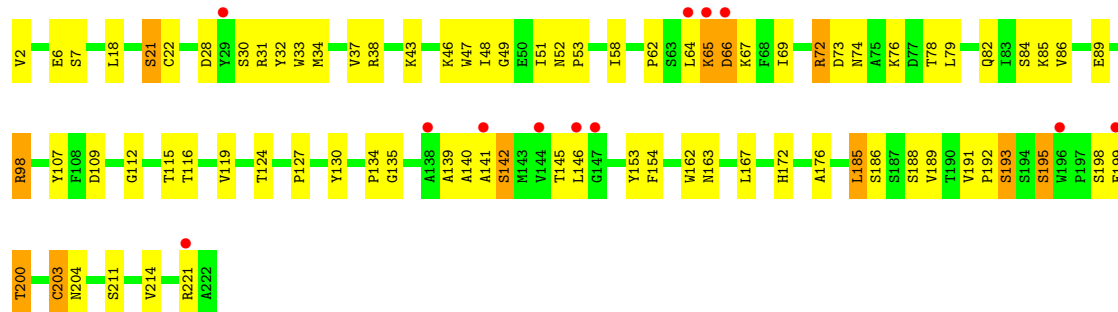
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			
2	E	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			

- Molecule 3 is a protein called Fab fragment, Light chain.

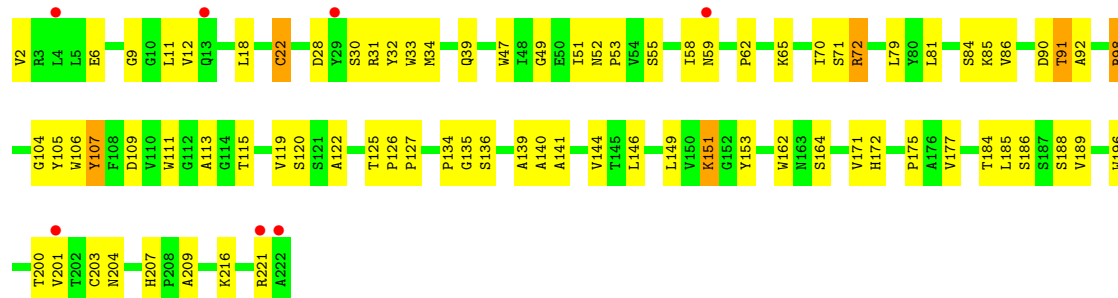
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	F	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			



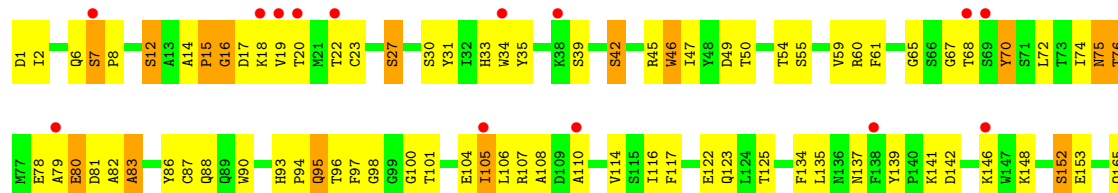
• Molecule 2: Fab fragment, Heavy chain

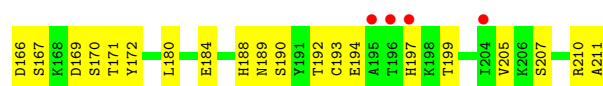


• Molecule 2: Fab fragment, Heavy chain

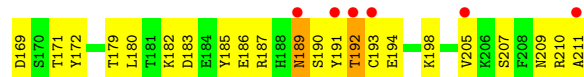
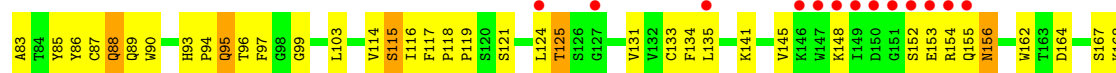


• Molecule 3: Fab fragment, Light chain





● 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, α , β , γ	231.17Å 97.51Å 173.28Å 90.00° 132.88° 90.00°	Depositor
Resolution (Å)	59.03 – 2.80 59.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.4 (59.03-2.80) 91.5 (59.00-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.53 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.4.0073	Depositor
R, R_{free}	0.255 , 0.299 0.249 , 0.294	Depositor DCC
R_{free} test set	3203 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	82.1	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13201	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.75	2/3393 (0.1%)	0.84	5/4605 (0.1%)
1	B	0.76	0/3364	0.87	5/4567 (0.1%)
2	C	0.80	0/1721	0.85	0/2355
2	E	0.80	0/1721	0.82	0/2355
3	D	0.69	0/1660	0.84	1/2257 (0.0%)
3	F	0.81	0/1660	0.88	0/2257
All	All	0.77	2/13519 (0.0%)	0.85	11/18396 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	LEU	N-CA	-6.23	1.33	1.46
1	A	202	GLU	CG-CD	5.24	1.59	1.51

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	76	THR	N-CA-C	-9.00	86.70	111.00
1	B	403	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	B	75	TYR	N-CA-C	-6.45	93.59	111.00
1	A	340	ARG	NE-CZ-NH1	-6.35	117.13	120.30
1	B	194	LEU	CB-CG-CD1	-6.14	100.57	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	74	ASN	Peptide

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	3322	0	3478	222	0
1	B	3293	0	3452	248	0
2	C	1672	0	1654	71	0
2	E	1672	0	1654	65	0
3	D	1621	0	1546	98	0
3	F	1621	0	1546	89	0
All	All	13201	0	13330	738	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 28.

The worst 5 of 738 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:232:PHE:C	1:A:233:ASN:ND2	1.74	1.41
1:B:75:TYR:CB	1:B:76:PRO:HD3	1.53	1.37
1:A:232:PHE:O	1:A:233:ASN:ND2	1.58	1.35
1:A:235:GLU:O	1:A:236:VAL:HG23	1.19	1.28
1:B:73:ASP:O	1:B:77:LEU:HB3	1.39	1.22

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	387 (88%)	49 (11%)	6 (1%)	13	39
1	B	439/473 (93%)	361 (82%)	60 (14%)	18 (4%)	3	11
2	C	219/221 (99%)	191 (87%)	27 (12%)	1 (0%)	32	67
2	E	219/221 (99%)	199 (91%)	18 (8%)	2 (1%)	20	52
3	D	209/211 (99%)	179 (86%)	23 (11%)	7 (3%)	4	15
3	F	209/211 (99%)	188 (90%)	20 (10%)	1 (0%)	32	67
All	All	1737/1810 (96%)	1505 (87%)	197 (11%)	35 (2%)	9	28

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	VAL
1	B	75	TYR
1	B	144	VAL
3	D	15	PRO
1	B	72	ALA

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	333/356 (94%)	304 (91%)	29 (9%)	12	33
1	B	330/356 (93%)	304 (92%)	26 (8%)	14	38
2	C	181/181 (100%)	163 (90%)	18 (10%)	9	26
2	E	181/181 (100%)	168 (93%)	13 (7%)	17	43
3	D	185/185 (100%)	171 (92%)	14 (8%)	15	40
3	F	185/185 (100%)	171 (92%)	14 (8%)	15	40
All	All	1395/1444 (97%)	1281 (92%)	114 (8%)	13	37

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	434	LEU
2	C	185	LEU
3	F	95	GLN
1	B	451	ARG
2	C	65	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	270	ASN
1	B	381	GLN
3	F	136	ASN
1	B	277	GLN
1	B	287	ASN

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 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, 95th 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 ²)	Q<0.9
1	A	444/473 (93%)	0.45	19 (4%)	36	26	80, 99, 129, 147	0
1	B	441/473 (93%)	0.52	29 (6%)	19	11	72, 105, 140, 156	0
2	C	221/221 (100%)	0.29	12 (5%)	26	17	69, 95, 121, 145	0
2	E	221/221 (100%)	0.13	7 (3%)	48	37	70, 94, 116, 132	0
3	D	211/211 (100%)	0.43	18 (8%)	11	6	82, 107, 125, 129	0
3	F	211/211 (100%)	0.46	23 (10%)	6	3	64, 87, 126, 131	0
All	All	1749/1810 (96%)	0.40	108 (6%)	21	13	64, 99, 129, 156	0

The worst 5 of 108 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	72	ALA	10.2
1	A	168	LEU	7.2
1	B	104	ALA	6.9
3	F	147	TRP	6.5
1	B	73	ASP	6.3

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.