W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:57 AM GMT

PDB ID : 2EXY
Title : Crystal structure of the E148Q Mutant of EcClC, Fab complexed in absence of bound ions
Authors : Lobet, S.; Dutzler, R.
Deposited on : 2005-11-09
Resolution : 3.10 Å(reported)

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.
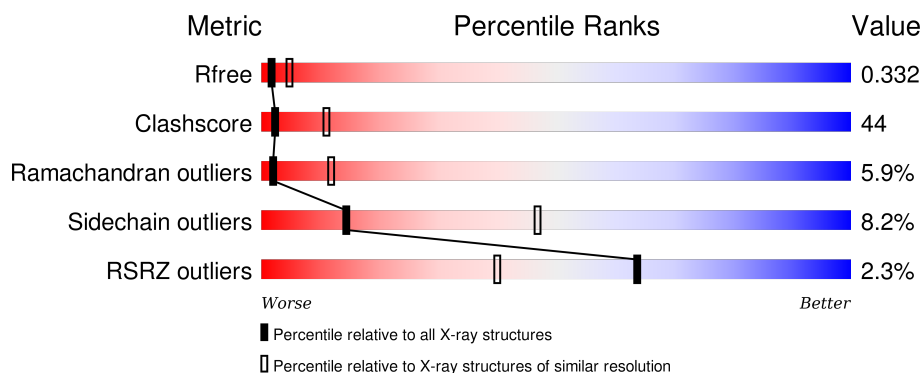
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 <=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	4% 42% 51% 7%

2 Entry composition (i)

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
1	A	444	Total	C	N	O	S	0	0	0
			3333	2190	561	562	20			
1	B	441	Total	C	N	O	S	0	0	0
			3304	2174	554	556	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	GLN	GLU	ENGINEERED	UNP P37019
B	148	GLN	GLU	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			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 (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.

- Molecule 1: H(+)/Cl(-) exchange transporter clcA

- Molecule 1: H(+)/Cl(-) exchange transporter clcA

Q207 F208 R209 Y210 T211 L212 I215 K216 A217 V218 P219 I220 G221 V222 I223 M224 I227 M228 Y229 R230 I231 E232 E235 I239 D240 V241 G242 K243 L244 A247 P248 L249 N250 T251 L252 Y255 L258 G259 I260 I261 F262 G263 I264 F265 G266 I267 I268 F269 N270 K271 W272 V273 L274

G275 M276 Q277 D278 L279 L280 H281 R282 V283 H284 G285 G286 N287 I288 T289 K290 L293 M294 G295 G296 A297 I298 G299 G303 L304 L305 F307 V308 A309 T312 S313 G314 F317 N318 L319 I320 P321 T324 G331 M332 L333 I336 F337 V338 A339 R340 V341 I342 T343 T344 L345 L346

C347 S350 G351 A352 P353 G354 G355 I356 F357 A358 P359 M360 L361 A362 L363 L367 G368 T369 A370 M373 V374 L378 F379 P380 Q381 V382 H383 L384 E385 A386 G387 M394 L397 L398 A399 A400 S401 I402 R403 A404 P405 L406 T407 I410 L411 V412 L413 E414 M415 T416 Y419 Q420

L421 I422 L423 P424 M425 I426 I427 L430 L434 L435 A436 Q437 F438 T439 G440 Q441 K442 P443 L444 Y445 S446 A447 I448 L449 A450 R451 T452 L453 A454 K455 Q456 E457 A458 GLU GLN LEU ALA ARG SER LYS ALA ALA SER ALA SER GLU ASN THR

- **Molecule 2: Fab Fragment (Heavy Chain)**

Chain C: 5%   46%   45%   8%

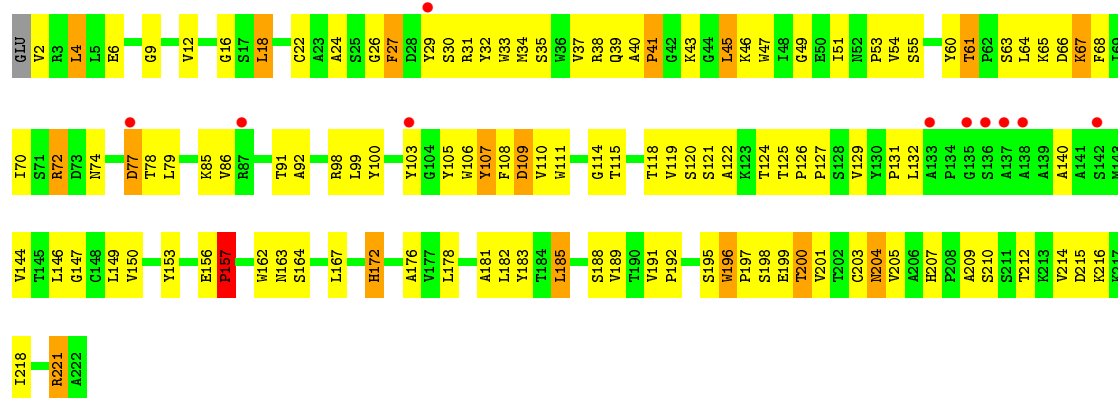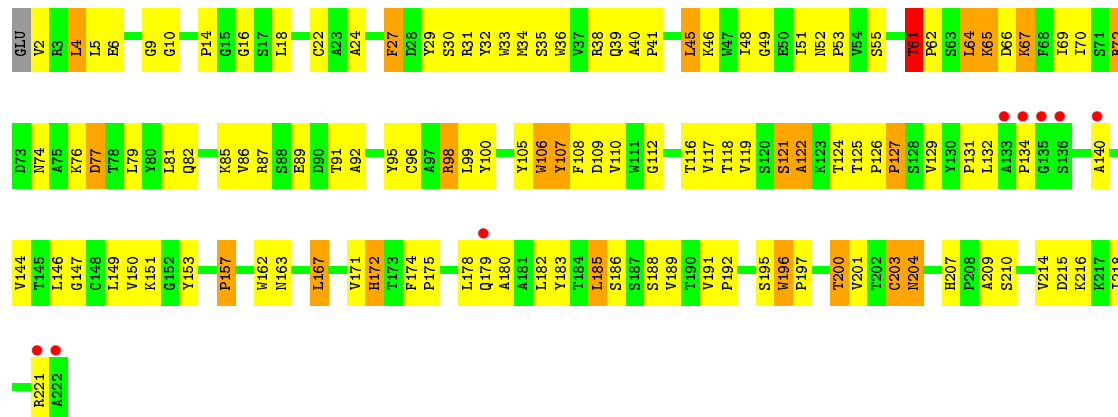GLU V2 R3 L4 L5 E6 G9 V12 G16 S17 L18 C22 A23 A24 S25 G26 F27 D28 Y29 S30 R31 Y32 W33 M34 S35 W36 V37 R38 Q39 A40 P41 G42 K43 G44 L45 K46 W47 I48 G49 E50 I51 N52 P53 S54 S55 Y60 T61 P62 S63 L64 K65 D66 K67 F68 I69

I70 S71 R72 D73 N74 D77 T78 L79 K85 V86 R87 T91 A92 R98 L99 Y100 Y103 G104 Y105 W106 Y107 F108 D109 V110 W111 G114 T115 T118 V119 S120 S121 A122 K123 T124 T125 P126 P127 S128 V129 Y130 P131 L132 A133 P134 G135 S136 A137 A138 A139 A140 A141 S142 M143

V144 T145 L146 G147 C148 L149 V150 Y153 E156 P157 W162 N163 S164 L167 H172 A176 V177 L178 A181 L182 Y183 T184 L185 S188 V189 T190 V191 P192 S195 W196 P197 S198 E199 T200 V201 T202 C203 N204 V205 A206 H207 P208 A209 S210 S211 T212 K213 V214 D215 K216 K217

I218 R221 A222

- **Molecule 2: Fab Fragment (Heavy Chain)**

Chain E: 4%   45%   44%   10%

GLU V2 R3 L4 L5 E6 G9 G10 P14 G15 G16 S17 L18 C22 A23 A24 F27 D28 Y29 S30 R31 Y32 W33 M34 S35 W36 V37 R38 Q39 A40 P41 L45 K46 W47 I48 G49 E50 I51 N52 P53 S54 S55 T61 P62 S63 L64 K65 D66 K67 F68 I69 I70 S71 R72

D73 N74 A75 K76 D77 T78 L79 Y80 L81 Q82 K85 V86 R87 S88 E89 D90 T91 A92 Y95 C96 A97 R98 L99 Y100 Y105 W106 Y107 F108 D109 V110 W111 G112 T116 V117 T118 V119 S120 S121 A122 K123 T124 T125 P126 P127 S128 V129 Y130 P131 L132 A133 P134 G135 S136 A140

V144 T145 L146 G147 C148 L149 V150 K151 G152 Y153 P157 W162 N163 L167 V171 H172 T173 F174 P175 L178 Q179 A180 A181 L182 Y183 T184 L185 S186 S187 S188 V189 T190 V191 P192 S195 W196 P197 T200 V201 T202 C203 N204 H207 P208 A209 S210 V214 D215 K216 K217 I218

R221 A222

- **Molecule 3: Fab Fragment (Light Chain)**

Chain D: %   49%   45%   5%

• Molecule 3: Fab Fragment (Light Chain)

Chain F:

4%

42%   51%   7%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	219.64Å 119.79Å 151.30Å 90.00° 128.09° 90.00°	Depositor
Resolution (Å)	19.97 – 3.10	Depositor
	49.45 – 3.10	EDS
% Data completeness	95.6 (19.97-3.10)	Depositor
(in resolution range)	95.5 (49.45-3.10)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.328 , 0.352	Depositor
	0.309 , 0.332	DCC
R_{free} test set	2591 reflections (4.84%)	DCC
Wilson B-factor (Å^2)	82.6	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.36$	Xtriage
Outliers	0 of 53580 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	13223	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.50	0/3405	0.68	0/4621
1	B	0.51	0/3376	0.69	0/4583
2	C	0.77	1/1721 (0.1%)	0.88	1/2355 (0.0%)
2	E	0.77	4/1721 (0.2%)	0.86	0/2355
3	D	0.62	0/1660	0.77	1/2257 (0.0%)
3	F	0.74	1/1660 (0.1%)	0.83	0/2257
All	All	0.63	6/13543 (0.0%)	0.77	2/18428 (0.0%)

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
2	E	0	1
3	F	0	1
All	All	0	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	61	THR	CB-CG2	-7.07	1.29	1.52
2	E	121	SER	C-N	-6.33	1.19	1.34
2	E	121	SER	C-O	5.50	1.33	1.23
2	E	121	SER	CA-C	5.16	1.66	1.52
3	F	201	THR	CB-CG2	-5.14	1.35	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	61	THR	OG1-CB-CG2	-9.16	88.94	110.00
3	D	201	THR	OG1-CB-CG2	-5.44	97.48	110.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	419	TYR	Sidechain
2	E	95	TYR	Sidechain
3	F	31	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	3486	388	0
1	B	3304	0	3459	372	0
2	C	1672	0	1654	119	0
2	E	1672	0	1654	127	0
3	D	1621	0	1546	94	0
3	F	1621	0	1546	130	0
All	All	13223	0	13345	1156	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 44.

The worst 5 of 1156 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)
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.28	1.06
1:A:381:GLN:NE2	1:A:381:GLN:H	1.54	1.06
1:B:381:GLN:H	1:B:381:GLN:NE2	1.53	1.05
3:F:192:THR:HA	3:F:207:SER:HB3	1.37	1.05
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.39	1.04

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%)	311 (70%)	103 (23%)	28 (6%)	2	10
1	B	439/473 (93%)	296 (67%)	111 (25%)	32 (7%)	1	7
2	C	219/222 (99%)	174 (80%)	35 (16%)	10 (5%)	3	17
2	E	219/222 (99%)	180 (82%)	28 (13%)	11 (5%)	3	16
3	D	209/211 (99%)	169 (81%)	27 (13%)	13 (6%)	2	10
3	F	209/211 (99%)	165 (79%)	36 (17%)	8 (4%)	4	22
All	All	1737/1812 (96%)	1295 (75%)	340 (20%)	102 (6%)	2	12

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	PHE
1	A	171	ASP
1	A	201	ILE
1	A	283	VAL
1	A	307	PHE

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%)	305 (91%)	30 (9%)	12	41
1	B	332/358 (93%)	304 (92%)	28 (8%)	14	46
2	C	181/182 (100%)	163 (90%)	18 (10%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	181/182 (100%)	162 (90%)	19 (10%)	8	31
3	D	185/185 (100%)	177 (96%)	8 (4%)	35	72
3	F	185/185 (100%)	173 (94%)	12 (6%)	21	57
All	All	1399/1450 (96%)	1284 (92%)	115 (8%)	14	47

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	379	PHE
2	C	67	LYS
3	F	46	TRP
1	B	381	GLN
2	C	4	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	157	ASN
1	B	287	ASN
3	F	137	ASN
1	B	270	ASN
1	B	318	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%)	-0.03	6 (1%)	78	60	50, 77, 100, 111	0
1	B	441/473 (93%)	-0.02	5 (1%)	82	66	46, 76, 103, 121	0
2	C	221/222 (99%)	0.14	10 (4%)	37	17	43, 74, 94, 125	0
2	E	221/222 (99%)	0.18	8 (3%)	46	23	40, 75, 95, 116	0
3	D	211/211 (100%)	0.26	2 (0%)	85	72	57, 85, 98, 103	0
3	F	211/211 (100%)	0.18	9 (4%)	39	18	40, 71, 99, 110	0
All	All	1749/1812 (96%)	0.08	40 (2%)	64	40	40, 77, 99, 125	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	ALA	5.1
2	C	136	SER	4.9
1	B	235	GLU	3.9
1	A	235	GLU	3.8
3	F	153	GLU	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.