



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:20 AM GMT

PDB ID : 3ORG
Title : Crystal Structure of a eukaryotic CLC transporter
Authors : Feng, L.; MacKinnon, R.
Deposited on : 2010-09-07
Resolution : 3.50 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
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

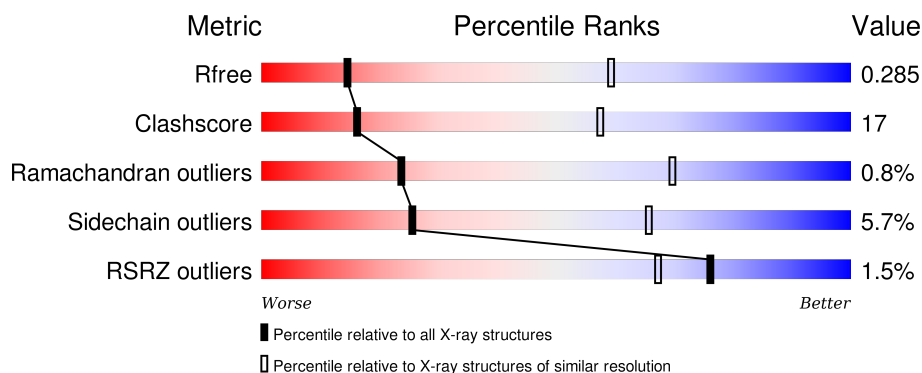
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	632	<div> <div> <div></div> <div>54%</div> <div>28%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	632	<div> <div> <div></div> <div>56%</div> <div>27%</div> <div>•</div> <div>16%</div> </div> </div>
1	C	632	<div> <div> <div></div> <div>51%</div> <div>31%</div> <div>•</div> <div>16%</div> </div> </div>
1	D	632	<div> <div> <div></div> <div>53%</div> <div>30%</div> <div>•</div> <div>16%</div> </div> </div>

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
2	CL	A	802	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16236 atoms, of which 0 are hydrogens and 0 are deuteriums.

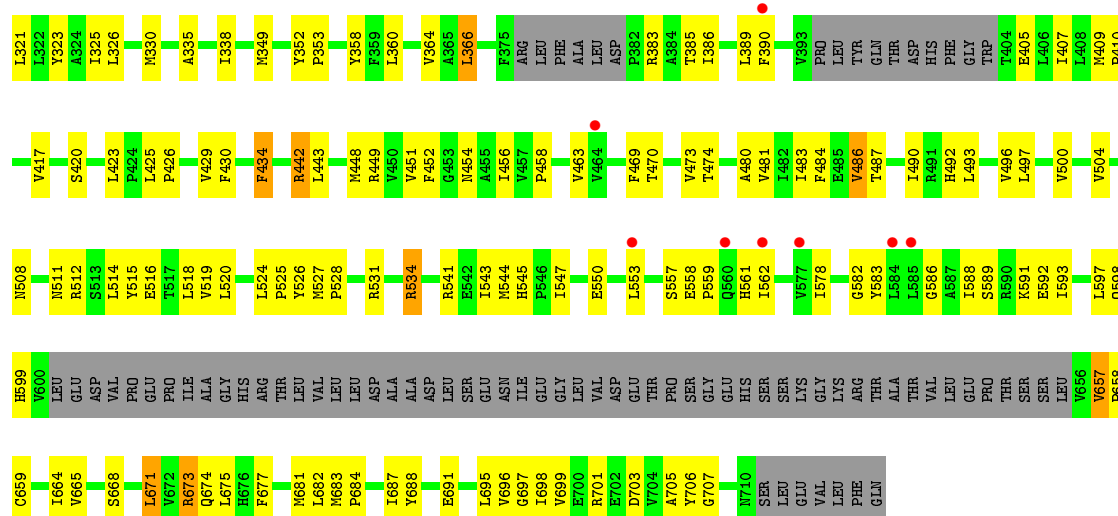
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CmCLC.

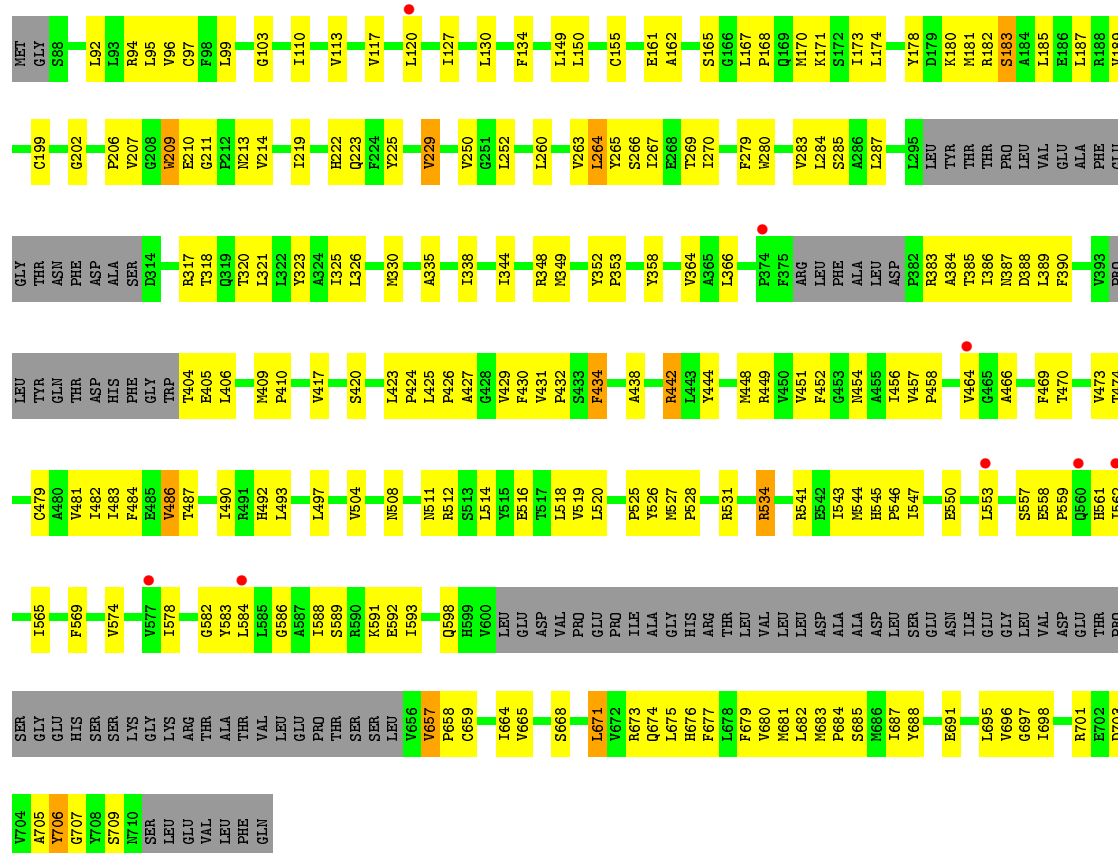
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4057	2669	675	688	25			
1	B	534	Total	C	N	O	S	0	0	0
			4057	2669	675	688	25			
1	C	534	Total	C	N	O	S	0	0	0
			4057	2669	675	688	25			
1	D	534	Total	C	N	O	S	0	0	0
			4057	2669	675	688	25			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Cl	0	0
			2	2		
2	A	2	Total	Cl	0	0
			2	2		
2	D	2	Total	Cl	0	0
			2	2		
2	C	2	Total	Cl	0	0
			2	2		



• Molecule 1: CmCLC



• Molecule 1: CmCLC



V704	ASP	ASP	LEU	S478	P559	PRO	V704
A705	ALA	ALA	TYR	S481	Q560	SER	A705
Y706	SER	SER	GLN	V481	H561	GLY	Y706
G707	THR	THR	THR	I482	I562	GLU	G707
				I483	K563	HIS	
N710	HIS	ASP	ASP	F484	V574	SER	N710
SER	THR	R317	HIS	E485		SER	SER
LEU	T318	T318	PHE	V486	V577	LYS	LEU
GLU	Q319	Q319	GLY	T487	I578	GLY	GLU
VAL	T320	T320	TRP			LYS	VAL
PHE	F230	F230				ARG	PHE
GLN	L233	L233	L406	I490	G582	THR	GLN
	A106	A106		R491	Y583	ALA	
	I110	I110	M409	H492	L584	THR	
	V113	V113	P410	L493	L585	VAL	
	A246	A246			G586	LEU	
	C248	C248	V417	V496	A587	GLU	
	A249	A249	L497	L497	I588	PRO	
	V250	V250	S420	V500	S589	THR	
	A253	A253	L423	V504	R590	SER	
	P259	P259	P424		K591	SER	
	L260	L260	L425	I593	E592	LEU	
	G261	G261	P426	N508		V656	
	V263	V263	A427		Q598	V657	
	L264	L264	G428	N511	H599	P658	
	Y265	Y265	V429	S512	V600	C659	
	S266	S266	F430	L514	LEU		
	L267	L267	V431	Y515	ASP	T664	
	E268	E268	P432	E516	VAL	V665	
	T269	T269	S433	T517	PRO	S668	
	I270	I270	F434	L518	GLU	L671	
	F279	F279	A438	V519	PRO	V672	
	W280	W280	R442	L520	ILE	Q674	
	V283	V283	L443	M521	ALA	L675	
	L284	L284	Y444	L524	GLY	H676	
	L287	L287		P525	HIS	F677	
	L295	L295		Y526	ARG	L678	
	LEU	LEU	A365	M527	THR	F679	
	TYR	TYR	L366	P528	LEU	V680	
	THR	THR	F375	R531	VAL	M681	
	THR	THR	ARG		LEU	L682	
	PRO	PRO	LEU	R534	LEU	M683	
	LEU	LEU	PHE	R541	ASP	P684	
	VAL	VAL	ALA	E542	ALA		
	GLU	GLU	LEU	I543	ASP	I687	
	ALA	ALA	ASP	M544	LEU	V688	
	PHE	PHE	I456	H545	GLU	E691	
	GLY	GLY	P458		ASN	V696	
	THR	THR	V464	E550	ILE	G697	
	ASN	ASN	A466	P551	GLY	I698	
	PHE	PHE		H552	LEU	V699	
	GLY	GLY	F469	L553	VAL	E700	
	THR	THR	T470		ASP	E701	
	PHE	PHE	V473	S557	GLU	E702	
			T474	E558	THR	D703	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.63Å 178.27Å 145.13Å 90.00° 129.21° 90.00°	Depositor
Resolution (Å)	29.66 – 3.50 28.88 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.66-3.50) 97.1 (28.88-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.259 , 0.284 0.259 , 0.285	Depositor DCC
R_{free} test set	2774 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	111.1	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.429 for -k+l,-h-l,-l 0.418 for k+l,h+l,-l 0.428 for -h-2*l,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 55484 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16236	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.43	0/4142	0.60	2/5626 (0.0%)
1	B	0.43	0/4142	0.61	2/5626 (0.0%)
1	C	0.43	0/4142	0.60	1/5626 (0.0%)
1	D	0.43	0/4142	0.60	1/5626 (0.0%)
All	All	0.43	0/16568	0.60	6/22504 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	LEU	CA-CB-CG	5.99	129.07	115.30
1	C	95	LEU	CA-CB-CG	5.44	127.81	115.30
1	D	95	LEU	CA-CB-CG	5.18	127.21	115.30
1	B	366	LEU	CA-CB-CG	5.09	127.02	115.30
1	B	95	LEU	CA-CB-CG	5.05	126.91	115.30

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	4057	0	4215	146	0
1	B	4057	0	4215	136	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4057	0	4215	151	0
1	D	4057	0	4215	146	0
2	A	2	0	0	1	0
2	B	2	0	0	1	0
2	C	2	0	0	1	0
2	D	2	0	0	0	0
All	All	16236	0	16860	556	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 17.

The worst 5 of 556 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:664:ILE:HD11	1:B:684:PRO:HG3	1.29	1.08
1:A:664:ILE:HD11	1:A:684:PRO:HG3	1.35	1.08
1:A:317:ARG:HD3	1:A:318:THR:H	1.17	1.07
1:D:664:ILE:HD11	1:D:684:PRO:HG3	1.37	1.07
1:D:317:ARG:HD3	1:D:318:THR:H	1.22	1.02

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	524/632 (83%)	484 (92%)	36 (7%)	4 (1%)	24	70
1	B	524/632 (83%)	483 (92%)	38 (7%)	3 (1%)	30	75
1	C	524/632 (83%)	481 (92%)	37 (7%)	6 (1%)	17	63
1	D	524/632 (83%)	484 (92%)	36 (7%)	4 (1%)	24	70
All	All	2096/2528 (83%)	1932 (92%)	147 (7%)	17 (1%)	24	70

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	VAL
1	B	405	GLU
1	D	405	GLU
1	B	598	GLN
1	D	319	GLN

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	426/522 (82%)	402 (94%)	24 (6%)	26	66
1	B	426/522 (82%)	404 (95%)	22 (5%)	29	68
1	C	426/522 (82%)	401 (94%)	25 (6%)	24	65
1	D	426/522 (82%)	400 (94%)	26 (6%)	23	64
All	All	1704/2088 (82%)	1607 (94%)	97 (6%)	25	66

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	657	VAL
1	C	264	LEU
1	D	492	HIS
1	B	673	ARG
1	C	134	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	511	ASN
1	C	222	HIS
1	D	215	HIS
1	B	319	GLN
1	D	222	HIS

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](#)

Of 8 ligands modelled in this entry, 8 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, 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	534/632 (84%)	0.12	7 (1%) 79 70	79, 118, 182, 225	1 (0%)
1	B	534/632 (84%)	0.12	9 (1%) 73 64	81, 117, 178, 221	1 (0%)
1	C	534/632 (84%)	0.10	8 (1%) 76 67	81, 117, 178, 221	1 (0%)
1	D	534/632 (84%)	0.12	7 (1%) 79 70	80, 117, 178, 220	1 (0%)
All	All	2136/2528 (84%)	0.12	31 (1%) 76 67	79, 117, 179, 225	4 (0%)

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	577	VAL	4.0
1	A	553	LEU	3.4
1	D	577	VAL	3.4
1	A	350	ARG	3.2
1	A	562	ILE	3.1

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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
2	CL	A	802	1/1	0.98	0.43	1.41	101,101,101,101	0
2	CL	C	802	1/1	0.94	0.38	0.35	95,95,95,95	0
2	CL	A	801	1/1	0.92	0.20	-0.07	99,99,99,99	0
2	CL	D	802	1/1	0.98	0.29	-0.25	97,97,97,97	0
2	CL	B	801	1/1	0.79	0.13	-1.34	102,102,102,102	0
2	CL	C	801	1/1	0.67	0.12	-1.48	102,102,102,102	0
2	CL	D	801	1/1	0.74	0.15	-1.50	97,97,97,97	0
2	CL	B	802	1/1	0.89	0.17	-1.78	99,99,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.