



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:28 AM UTC

PDB ID : 3CO2 / pdb_00003co2
Title : Mlotik1 ion channel cyclic-nucleotide binding domain mutant
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Deposited on : 2008-03-27
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at 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	:	4-5-2 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

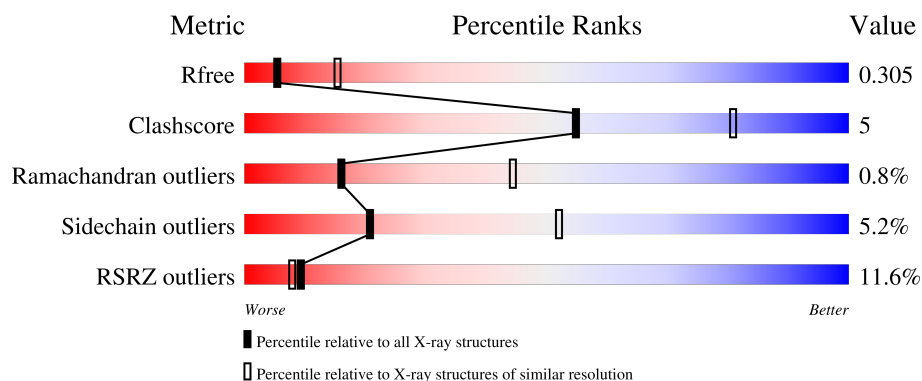
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 ≥ 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	140	12% 75% 12% • 10%
1	B	140	6% 83% 9% 9%
1	C	140	12% 75% 9% • 15%
1	D	140	11% 77% 14% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3519 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 Mlotik1 ion channel protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	126	Total	C	N	O	S	0	0	0
			886	571	147	163	5			
1	B	128	Total	C	N	O	S	0	0	0
			897	579	149	164	5			
1	C	119	Total	C	N	O	S	0	0	0
			811	523	131	153	4			
1	D	129	Total	C	N	O	S	0	0	0
			916	591	153	168	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	307	TRP	ARG	engineered mutation	UNP Q98GN8
B	307	TRP	ARG	engineered mutation	UNP Q98GN8
C	307	TRP	ARG	engineered mutation	UNP Q98GN8
D	307	TRP	ARG	engineered mutation	UNP Q98GN8

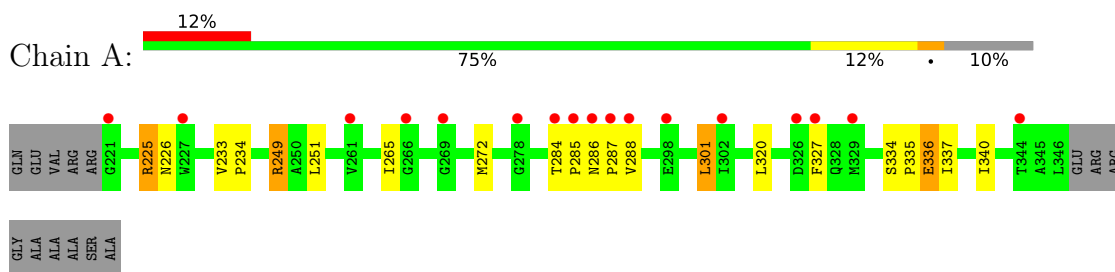
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	O	0	0
			4	4		
2	B	3	Total	O	0	0
			3	3		
2	C	1	Total	O	0	0
			1	1		
2	D	1	Total	O	0	0
			1	1		

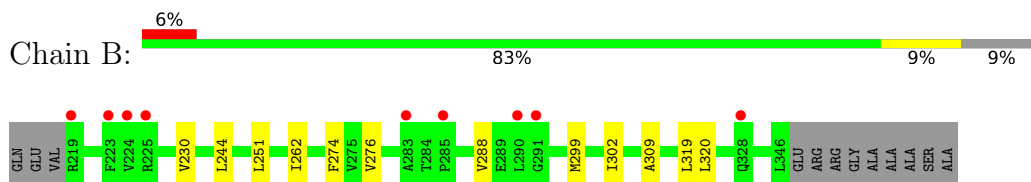
3 Residue-property plots

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

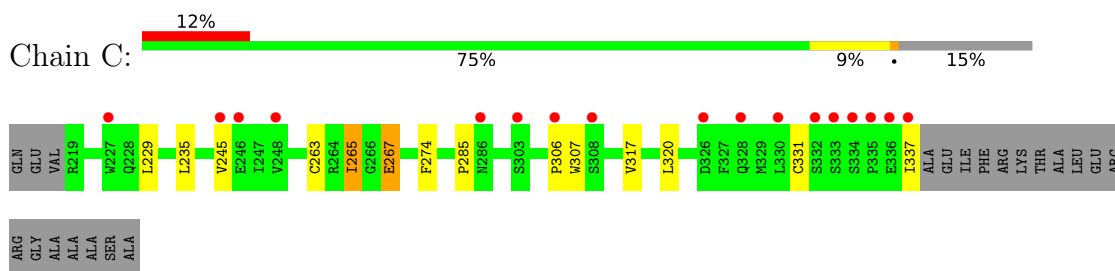
- Molecule 1: Mlotik1 ion channel protein



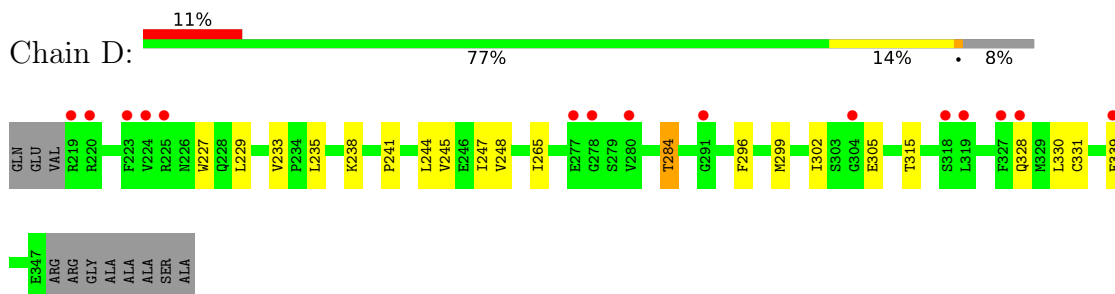
- Molecule 1: Mlotik1 ion channel protein



- Molecule 1: Mlotik1 ion channel protein



- Molecule 1: Mlotik1 ion channel protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	111.47Å 132.35Å 39.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.03 – 2.90 41.03 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (41.03-2.90) 99.3 (41.03-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.48Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.261 , 0.306 0.263 , 0.305	Depositor DCC
R_{free} test set	1075 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	3519	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% 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 [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	0.46	0/904	0.90	2/1237 (0.2%)
1	B	0.49	0/916	0.90	0/1256
1	C	0.51	0/830	0.93	1/1143 (0.1%)
1	D	0.49	0/936	0.90	4/1282 (0.3%)
All	All	0.49	0/3586	0.91	7/4918 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	265	ILE	CB-CG1-CD1	7.94	130.47	113.80
1	A	284	THR	CA-C-N	7.23	128.87	119.84
1	A	284	THR	C-N-CA	7.23	128.87	119.84
1	D	233	VAL	CA-C-N	5.23	125.28	119.32
1	D	233	VAL	C-N-CA	5.23	125.28	119.32
1	D	284	THR	CA-C-N	5.19	126.33	119.84
1	D	284	THR	C-N-CA	5.19	126.33	119.84

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	886	0	852	12	0
1	B	897	0	863	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	811	0	754	7	0
1	D	916	0	890	12	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	3519	0	3359	33	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 5.

All (33) 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:249:ARG:HH21	1:A:249:ARG:HG2	1.33	0.94
1:A:249:ARG:HH21	1:A:249:ARG:CG	1.88	0.85
1:A:249:ARG:HG2	1:A:249:ARG:NH2	1.96	0.78
1:B:274:PHE:HB2	1:B:320:LEU:HB2	1.83	0.61
1:C:331:CYS:SG	1:C:337:ILE:HG12	2.40	0.61
1:A:233:VAL:HG11	1:A:272:MET:HE1	1.82	0.60
1:D:227:TRP:HH2	1:D:241:PRO:HA	1.66	0.59
1:A:327:PHE:CE1	1:A:337:ILE:HD12	2.41	0.56
1:B:262:ILE:HG23	1:B:319:LEU:HD11	1.88	0.56
1:D:339:GLU:HA	1:D:339:GLU:OE1	2.06	0.55
1:A:225:ARG:NH1	1:A:226:ASN:OD1	2.43	0.51
1:C:267:GLU:O	1:C:306:PRO:HA	2.11	0.50
1:D:227:TRP:CH2	1:D:241:PRO:HA	2.45	0.50
1:D:328:GLN:NE2	1:D:331:CYS:SG	2.85	0.50
1:B:251:LEU:HD13	1:B:320:LEU:HD13	1.94	0.50
1:C:245:VAL:HG21	1:D:245:VAL:CG2	2.42	0.49
1:D:227:TRP:C	1:D:227:TRP:CD1	2.90	0.49
1:C:274:PHE:HB2	1:C:320:LEU:HB2	1.95	0.48
1:B:230:VAL:HG12	1:B:244:LEU:HD22	1.98	0.46
1:D:235:LEU:HD21	1:D:302:ILE:HD11	1.98	0.45
1:B:299:MET:SD	1:B:299:MET:N	2.87	0.44
1:C:245:VAL:HG21	1:D:245:VAL:HG21	2.00	0.44
1:A:251:LEU:HD13	1:A:320:LEU:HD13	1.98	0.43
1:A:272:MET:HB2	1:A:301:LEU:HG	2.00	0.43
1:A:288:VAL:HA	1:D:296:PHE:HB3	2.00	0.43
1:B:309:ALA:HB2	1:C:285:PRO:HB2	2.00	0.43
1:D:328:GLN:C	1:D:330:LEU:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:LEU:O	1:D:248:VAL:HG23	2.18	0.42
1:D:299:MET:HB3	1:D:305:GLU:HG3	2.00	0.42
1:C:263:CYS:HB2	1:C:307:TRP:CD2	2.55	0.42
1:A:233:VAL:HA	1:A:234:PRO:HD2	1.86	0.41
1:A:334:SER:HA	1:A:335:PRO:HD2	1.86	0.41
1:A:336:GLU:O	1:A:340:ILE:HG12	2.21	0.40

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	124/140 (89%)	116 (94%)	5 (4%)	3 (2%)	4	18
1	B	126/140 (90%)	120 (95%)	6 (5%)	0	100	100
1	C	117/140 (84%)	105 (90%)	11 (9%)	1 (1%)	14	41
1	D	127/140 (91%)	123 (97%)	4 (3%)	0	100	100
All	All	494/560 (88%)	464 (94%)	26 (5%)	4 (1%)	16	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	PRO
1	A	286	ASN
1	A	287	PRO
1	C	267	GLU

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	86/109 (79%)	81 (94%)	5 (6%)	18	49
1	B	88/109 (81%)	85 (97%)	3 (3%)	32	66
1	C	78/109 (72%)	74 (95%)	4 (5%)	21	53
1	D	91/109 (84%)	85 (93%)	6 (7%)	15	43
All	All	343/436 (79%)	325 (95%)	18 (5%)	21	52

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	ARG
1	A	249	ARG
1	A	265	ILE
1	A	301	LEU
1	A	336	GLU
1	B	276	VAL
1	B	288	VAL
1	B	302	ILE
1	C	229	LEU
1	C	235	LEU
1	C	265	ILE
1	C	317	VAL
1	D	229	LEU
1	D	238	LYS
1	D	247	ILE
1	D	265	ILE
1	D	284	THR
1	D	315	THR

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	323	HIS
1	D	328	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	126/140 (90%)	0.84	17 (13%) 7 5	11, 12, 13, 13	0
1	B	128/140 (91%)	0.43	9 (7%) 22 18	11, 12, 13, 15	0
1	C	119/140 (85%)	0.97	17 (14%) 6 5	12, 12, 13, 16	0
1	D	129/140 (92%)	0.79	15 (11%) 9 8	11, 12, 13, 14	0
All	All	502/560 (89%)	0.76	58 (11%) 9 8	11, 12, 13, 16	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	337	ILE	12.1
1	C	336	GLU	7.7
1	C	333	SER	6.5
1	C	332	SER	6.4
1	C	335	PRO	6.3
1	D	328	GLN	6.3
1	C	334	SER	5.9
1	A	302	ILE	4.8
1	D	223	PHE	4.7
1	A	284	THR	4.3
1	D	277	GLU	4.2
1	A	298	GLU	3.9
1	D	278	GLY	3.7
1	D	225	ARG	3.5
1	D	327	PHE	3.5
1	C	326	ASP	3.4
1	B	283	ALA	3.4
1	D	224	VAL	3.3
1	B	291	GLY	3.1
1	C	328	GLN	3.0
1	C	286	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	287	PRO	3.0
1	B	219	ARG	2.9
1	D	291	GLY	2.9
1	B	223	PHE	2.8
1	A	329	MET	2.8
1	B	225	ARG	2.7
1	B	224	VAL	2.7
1	A	221	GLY	2.7
1	C	303	SER	2.6
1	D	318	SER	2.6
1	D	280	VAL	2.6
1	D	219	ARG	2.5
1	A	286	ASN	2.5
1	C	308	SER	2.4
1	A	269	GLY	2.4
1	A	288	VAL	2.4
1	B	290	LEU	2.4
1	D	319	LEU	2.4
1	C	248	VAL	2.3
1	D	304	GLY	2.3
1	C	227	TRP	2.3
1	A	261	VAL	2.3
1	A	344	THR	2.2
1	B	285	PRO	2.2
1	A	327	PHE	2.2
1	D	339	GLU	2.2
1	A	326	ASP	2.2
1	A	285	PRO	2.1
1	B	328	GLN	2.1
1	C	330	LEU	2.1
1	C	246	GLU	2.1
1	C	306	PRO	2.1
1	A	278	GLY	2.1
1	A	266	GLY	2.0
1	D	220	ARG	2.0
1	A	227	TRP	2.0
1	C	245	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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.