



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:38 AM UTC

PDB ID : 3UKN / pdb_00003ukn
Title : Structure of the C-linker/CNBHD of zELK channels in C 2 2 21 space group
Authors : Brelidze, T.I.
Deposited on : 2011-11-09
Resolution : 2.20 Å(reported)

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

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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

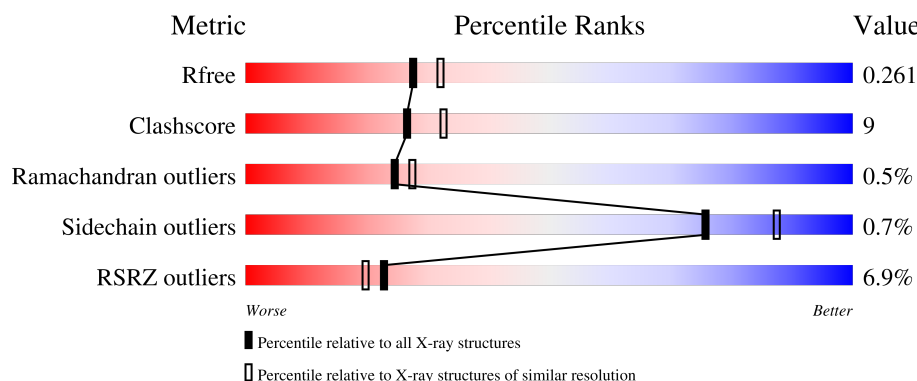
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 ≥ 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	212	0% 81% 11% 8%
1	B	212	3% 75% 18% 7%
1	C	212	15% 65% 22% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4726 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 Novel protein similar to vertebrate potassium voltage-gated channel, subfamily H (Eag-related) family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1520	972	252	288	8			
1	B	198	Total	C	N	O	S	0	0	0
			1530	982	256	284	8			
1	C	186	Total	C	N	O	S	0	0	0
			1346	869	220	249	8			

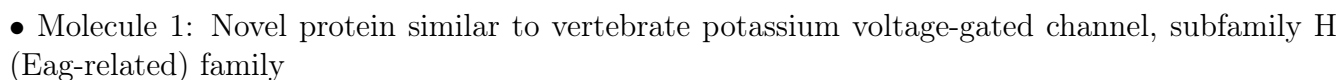
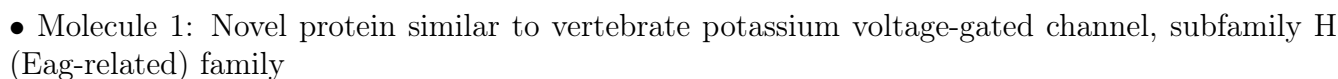
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	539	GLY	-	expression tag	UNP A8WHX9
A	540	ALA	-	expression tag	UNP A8WHX9
A	541	MET	-	expression tag	UNP A8WHX9
A	542	ASP	-	expression tag	UNP A8WHX9
B	539	GLY	-	expression tag	UNP A8WHX9
B	540	ALA	-	expression tag	UNP A8WHX9
B	541	MET	-	expression tag	UNP A8WHX9
B	542	ASP	-	expression tag	UNP A8WHX9
C	539	GLY	-	expression tag	UNP A8WHX9
C	540	ALA	-	expression tag	UNP A8WHX9
C	541	MET	-	expression tag	UNP A8WHX9
C	542	ASP	-	expression tag	UNP A8WHX9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	158	Total	O	0	0
			158	158		
2	B	105	Total	O	0	0
			105	105		
2	C	67	Total	O	0	0
			67	67		

- Molecule 1: Novel protein similar to vertebrate potassium voltage-gated channel, subfamily H (Eag-related) family



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	57.98Å 95.48Å 241.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.56 – 2.20 49.56 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.56-2.20) 97.2 (49.56-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.212 , 0.254 (Not available) , 0.261	Depositor DCC
R_{free} test set	1679 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 66.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.038 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.049 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4726	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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	0.58	0/1544	0.83	0/2091
1	B	0.52	0/1555	0.82	3/2105 (0.1%)
1	C	0.39	0/1363	0.81	2/1849 (0.1%)
All	All	0.51	0/4462	0.82	5/6045 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	642	ALA	CA-C-N	6.77	128.30	119.84
1	C	642	ALA	C-N-CA	6.77	128.30	119.84
1	B	723	TYR	CA-C-N	5.37	125.44	119.32
1	B	723	TYR	C-N-CA	5.37	125.44	119.32
1	B	670	ASP	CB-CA-C	-5.12	110.69	116.63

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	1520	0	1509	21	0
1	B	1530	0	1526	28	0
1	C	1346	0	1267	34	0
2	A	158	0	0	4	0
2	B	105	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	67	0	0	6	0
All	All	4726	0	4302	81	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 9.

All (81) 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:690:LYS:HB2	1:B:691:GLU:HA	1.17	1.14
1:B:690:LYS:HB2	1:B:691:GLU:CA	2.04	0.84
1:A:630:ARG:HD2	2:A:191:HOH:O	1.77	0.84
1:B:690:LYS:CB	1:B:691:GLU:HA	2.07	0.76
1:B:690:LYS:HG3	2:B:159:HOH:O	1.89	0.72
1:B:638:THR:HG22	1:B:709:GLN:HG2	1.71	0.71
1:A:574:GLN:HG3	2:A:261:HOH:O	1.92	0.70
1:C:551:LEU:HD12	1:C:586:VAL:HG13	1.74	0.69
1:C:579:CYS:O	1:C:583:THR:HG22	1.91	0.69
1:C:555:ARG:HB3	1:C:580:PHE:CZ	2.31	0.66
1:A:728:GLN:OE1	2:A:174:HOH:O	2.13	0.65
1:B:558:ASP:OD1	2:B:280:HOH:O	2.15	0.64
1:C:586:VAL:HB	1:C:647:LEU:HD12	1.80	0.62
1:C:555:ARG:HB3	1:C:580:PHE:HZ	1.63	0.62
1:C:692:GLN:HA	1:C:693:VAL:C	2.25	0.61
1:B:621:PHE:HB3	1:B:629:LEU:HD21	1.84	0.60
1:B:668:LEU:CD2	1:B:673:VAL:HG22	2.31	0.60
1:C:735:GLN:HA	1:C:738:LEU:HB3	1.84	0.59
1:A:555:ARG:HB3	1:A:580:PHE:HZ	1.68	0.59
1:C:704:THR:HG22	1:C:705:TYR:N	2.16	0.59
1:B:595:LEU:O	2:B:206:HOH:O	2.15	0.59
1:A:646:PHE:CZ	1:A:701:LYS:HD2	2.37	0.58
1:B:586:VAL:HB	1:B:647:LEU:HD12	1.86	0.57
1:C:624:ALA:HA	1:C:726:TYR:CD1	2.40	0.57
1:C:638:THR:HG22	1:C:709:GLN:HG2	1.86	0.56
1:B:548:ARG:HA	2:B:192:HOH:O	2.05	0.55
1:B:548:ARG:N	2:B:192:HOH:O	2.40	0.54
1:B:565:VAL:HG23	1:B:566:HIS:ND1	2.23	0.53
1:A:647:LEU:HG	1:A:648:ILE:HD13	1.90	0.53
1:C:704:THR:CG2	1:C:705:TYR:N	2.70	0.53
1:C:638:THR:HA	1:C:708:LEU:O	2.09	0.53
1:B:729:LYS:O	1:B:733:GLU:HG2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:637:LYS:O	1:C:709:GLN:HA	2.09	0.52
1:A:647:LEU:O	1:A:648:ILE:HD12	2.10	0.52
1:A:566:HIS:CD2	1:B:611:LEU:HD22	2.44	0.52
1:B:574:GLN:O	1:B:578:GLU:HG2	2.11	0.51
1:B:669:LYS:HB2	1:B:674:LEU:HD11	1.93	0.51
1:B:548:ARG:CA	2:B:192:HOH:O	2.58	0.50
1:B:718:GLU:HG3	1:B:721:ARG:HH21	1.76	0.50
1:A:728:GLN:NE2	2:A:195:HOH:O	2.44	0.50
1:C:565:VAL:HG23	1:C:566:HIS:ND1	2.27	0.49
1:C:564:ARG:NE	2:C:303:HOH:O	2.38	0.49
1:B:744:GLU:OE1	2:B:260:HOH:O	2.20	0.49
1:B:595:LEU:HB2	2:B:293:HOH:O	2.13	0.49
1:C:734:ILE:CA	2:C:227:HOH:O	2.61	0.49
1:B:740:TYR:HE2	1:B:742:LEU:HD23	1.78	0.48
1:A:647:LEU:HG	1:A:648:ILE:CD1	2.42	0.48
1:A:729:LYS:O	1:A:733:GLU:HG2	2.12	0.48
1:C:592:VAL:O	1:C:592:VAL:HG22	2.14	0.47
1:C:734:ILE:N	2:C:227:HOH:O	2.48	0.46
1:A:638:THR:HG22	1:A:709:GLN:HG2	1.98	0.46
1:B:587:ASN:HA	1:B:658:TYR:OH	2.16	0.46
1:C:615:LEU:HD23	1:C:615:LEU:O	2.15	0.46
1:C:625:SER:HB2	1:C:628:CYS:HB2	1.97	0.46
1:B:661:CYS:SG	1:B:709:GLN:HG3	2.56	0.45
1:C:724:PRO:HA	1:C:727:ALA:HB3	1.99	0.45
1:C:643:PRO:HD3	1:C:705:TYR:CD1	2.51	0.45
1:C:643:PRO:HD3	1:C:705:TYR:CE1	2.52	0.45
1:B:641:CYS:HB3	1:B:706:CYS:HB2	1.98	0.45
1:C:561:ASP:O	1:C:565:VAL:HG22	2.17	0.45
1:A:559:LEU:O	1:A:563:ILE:HG13	2.17	0.45
1:C:712:SER:HB2	2:C:199:HOH:O	2.15	0.45
1:B:637:LYS:HB2	1:B:710:TYR:CZ	2.52	0.44
1:C:665:MET:O	1:C:676:ILE:HG23	2.18	0.44
1:A:647:LEU:HD13	1:A:708:LEU:HD13	2.00	0.43
1:B:550:SER:N	1:C:609:MET:HE1	2.34	0.43
1:C:615:LEU:HD23	1:C:615:LEU:C	2.43	0.43
1:C:649:ARG:NH2	2:C:200:HOH:O	2.50	0.43
1:A:587:ASN:HA	1:A:658:TYR:OH	2.18	0.43
1:A:688:LEU:HD22	1:A:713:LEU:HD22	2.00	0.43
1:A:647:LEU:C	1:A:648:ILE:HD12	2.42	0.43
1:C:646:PHE:CZ	1:C:701:LYS:HD2	2.54	0.42
1:B:632:LEU:O	1:B:636:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:ARG:HB3	1:A:580:PHE:CZ	2.52	0.41
1:C:636:ILE:HG12	1:C:711:ILE:HG12	2.01	0.41
1:C:627:GLY:N	2:C:157:HOH:O	2.52	0.41
1:A:586:VAL:O	1:A:590:ILE:HG23	2.20	0.41
1:A:595:LEU:HD23	1:A:595:LEU:HA	1.93	0.41
1:C:584:TRP:CG	1:C:585:SER:N	2.90	0.40
1:C:654:LEU:HD23	1:C:694:ILE:HG21	2.04	0.40
1:A:647:LEU:HD11	1:A:658:TYR:CD1	2.56	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	194/212 (92%)	190 (98%)	4 (2%)	0	100	100
1	B	196/212 (92%)	189 (96%)	6 (3%)	1 (0%)	24	27
1	C	178/212 (84%)	163 (92%)	13 (7%)	2 (1%)	11	10
All	All	568/636 (89%)	542 (95%)	23 (4%)	3 (0%)	24	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	679	LYS
1	C	693	VAL
1	B	690	LYS

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	163/186 (88%)	163 (100%)	0	100	100
1	B	162/186 (87%)	161 (99%)	1 (1%)	78	89
1	C	125/186 (67%)	123 (98%)	2 (2%)	55	71
All	All	450/558 (81%)	447 (99%)	3 (1%)	76	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	582	THR
1	C	568	LEU
1	C	665	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	617	GLN
1	B	736	HIS
1	C	610	HIS
1	C	617	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	196/212 (92%)	-0.10	2 (1%) 79 77	15, 33, 63, 93	0
1	B	198/212 (93%)	0.07	7 (3%) 47 44	25, 40, 70, 125	0
1	C	186/212 (87%)	1.03	31 (16%) 4 3	39, 66, 116, 146	0
All	All	580/636 (91%)	0.32	40 (6%) 23 20	15, 45, 100, 146	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	737	ASP	5.7
1	C	689	THR	5.2
1	B	671	ASN	4.2
1	C	626	ARG	3.7
1	B	670	ASP	3.4
1	C	736	HIS	3.4
1	C	725	GLU	3.3
1	C	743	ARG	3.1
1	C	686	ASP	3.1
1	B	640	PHE	3.0
1	C	729	LYS	3.0
1	C	694	ILE	2.9
1	C	734	ILE	2.9
1	B	691	GLU	2.8
1	C	735	GLN	2.7
1	C	595	LEU	2.6
1	C	693	VAL	2.6
1	C	687	SER	2.6
1	C	669	LYS	2.6
1	C	722	LEU	2.5
1	B	692	GLN	2.5
1	C	643	PRO	2.5
1	C	673	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	652	ASP	2.4
1	C	724	PRO	2.4
1	C	625	SER	2.3
1	C	716	LEU	2.3
1	C	675	ALA	2.3
1	A	549	ARG	2.2
1	A	692	GLN	2.2
1	B	668	LEU	2.2
1	C	612	ASN	2.2
1	C	717	ARG	2.1
1	C	740	TYR	2.1
1	C	741	ASN	2.1
1	C	688	LEU	2.1
1	C	698	ALA	2.0
1	B	595	LEU	2.0
1	C	703	LEU	2.0
1	C	699	ASN	2.0

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.