wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:53 PM BST

PDB ID	:	3JAC
EMDB ID:	:	EMD-6343
Title	:	Cryo-EM study of a channel
Authors	:	Ge, J.; Li, W.; Zhao, Q.; Li, N.; Xiao, B.; Gao, N.; Yang, M.
Deposited on	:	2015-06-05
Resolution	:	4.80 Å(reported)
Based on PDB ID	:	4RAX

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

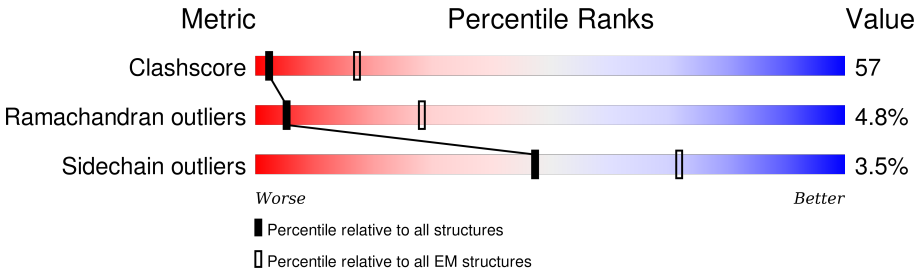
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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%

Mol	Chain	Length	Quality of chain
1	A	2553	23% 9% • 64%
1	B	2553	22% 10% • 64%
1	C	2553	23% 9% • 64%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15741 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Piezo-type mechanosensitive ion channel component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	918	Total	C	N	O	S	0	0
			5247	3208	995	1038	6		
1	B	918	Total	C	N	O	S	0	0
			5247	3208	995	1038	6		
1	C	918	Total	C	N	O	S	0	0
			5247	3208	995	1038	6		

There are 18 discrepancies between the modelled and reference sequences:

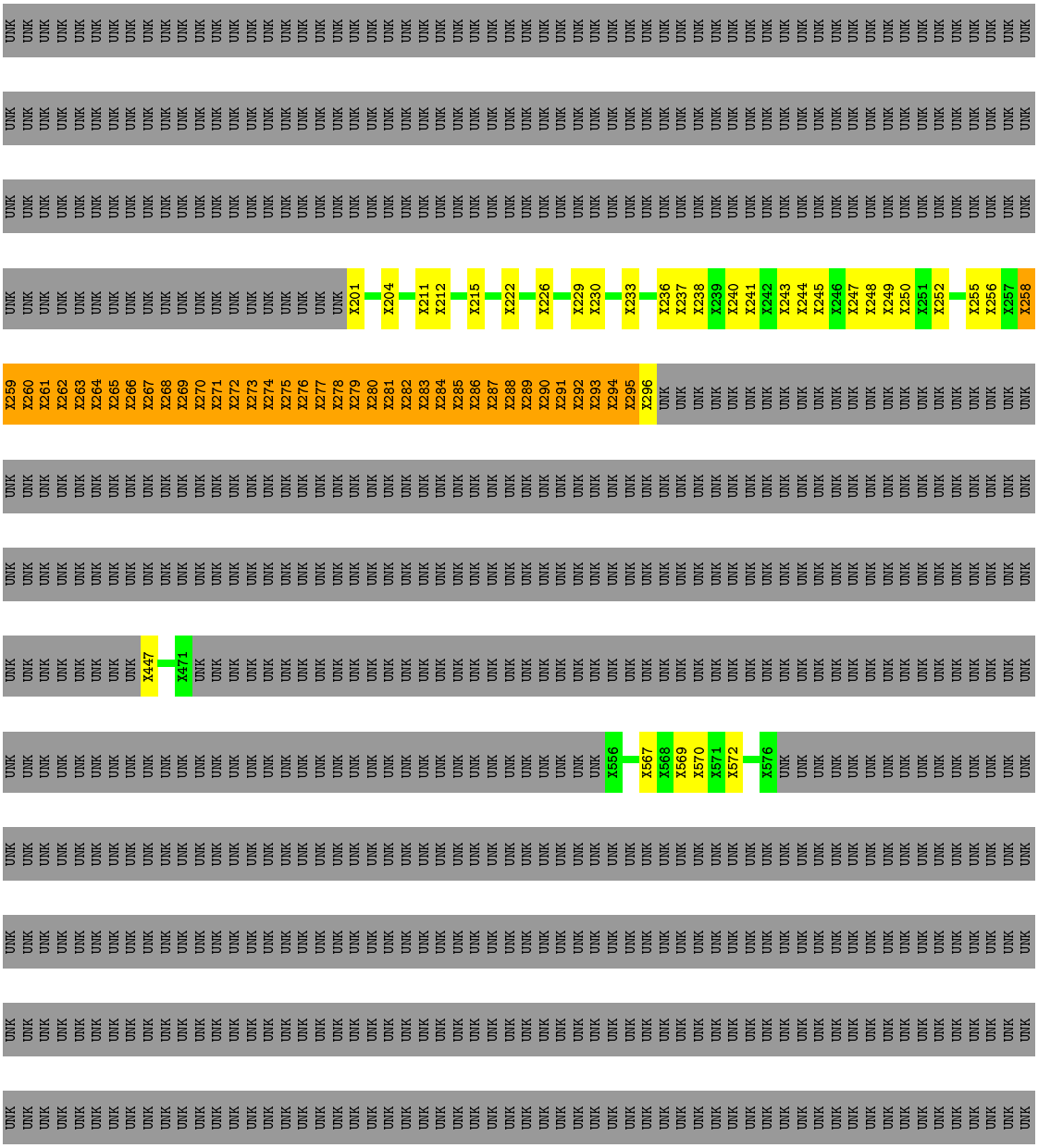
Chain	Residue	Modelled	Actual	Comment	Reference
A	2548	LEU	-	EXPRESSION TAG	UNP E2JF22
A	2549	GLU	-	EXPRESSION TAG	UNP E2JF22
A	2550	VAL	-	EXPRESSION TAG	UNP E2JF22
A	2551	LEU	-	EXPRESSION TAG	UNP E2JF22
A	2552	PHE	-	EXPRESSION TAG	UNP E2JF22
A	2553	GLN	-	EXPRESSION TAG	UNP E2JF22
B	2548	LEU	-	EXPRESSION TAG	UNP E2JF22
B	2549	GLU	-	EXPRESSION TAG	UNP E2JF22
B	2550	VAL	-	EXPRESSION TAG	UNP E2JF22
B	2551	LEU	-	EXPRESSION TAG	UNP E2JF22
B	2552	PHE	-	EXPRESSION TAG	UNP E2JF22
B	2553	GLN	-	EXPRESSION TAG	UNP E2JF22
C	2548	LEU	-	EXPRESSION TAG	UNP E2JF22
C	2549	GLU	-	EXPRESSION TAG	UNP E2JF22
C	2550	VAL	-	EXPRESSION TAG	UNP E2JF22
C	2551	LEU	-	EXPRESSION TAG	UNP E2JF22
C	2552	PHE	-	EXPRESSION TAG	UNP E2JF22
C	2553	GLN	-	EXPRESSION TAG	UNP E2JF22

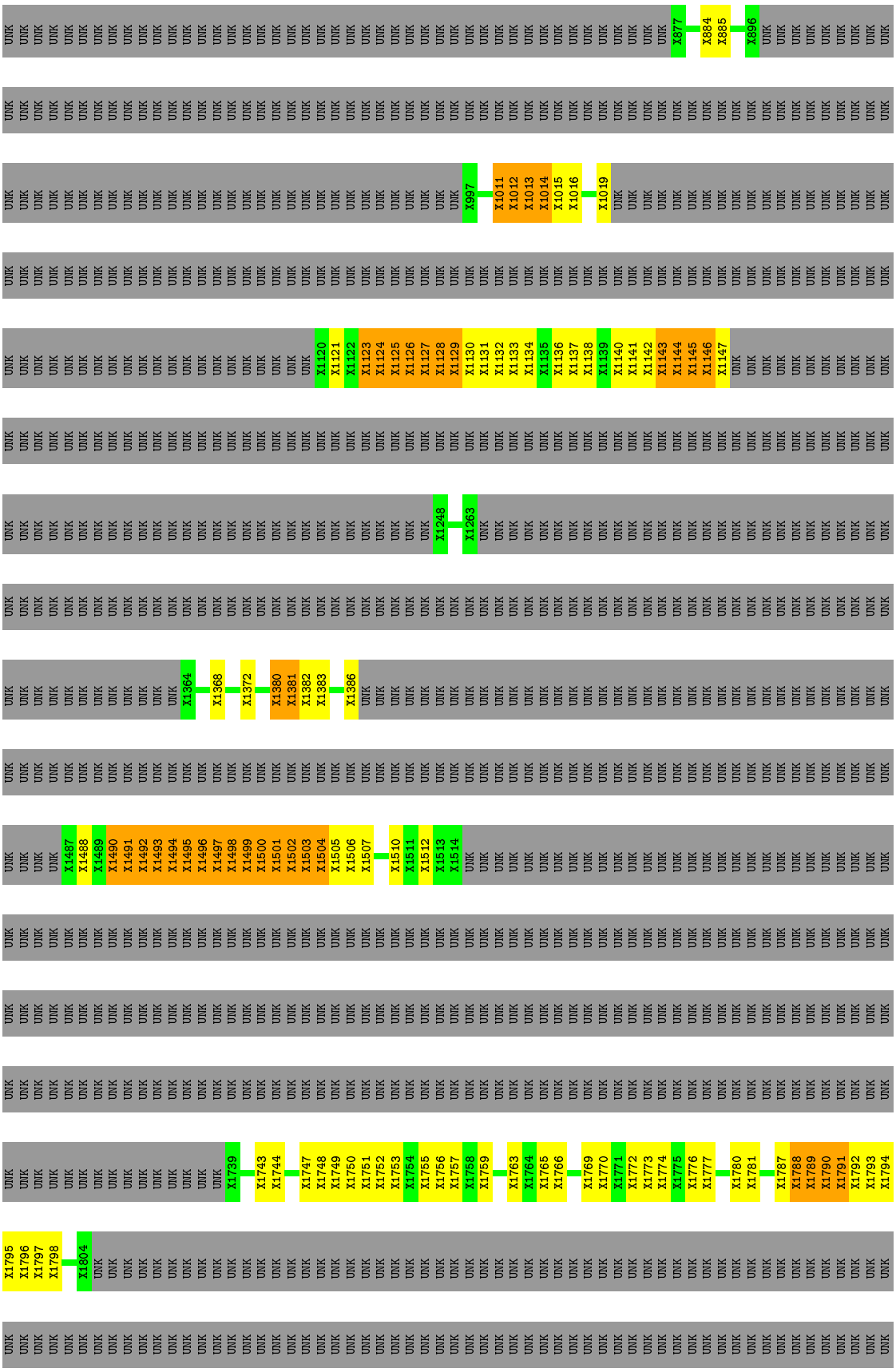
3 Residue-property plots (i)

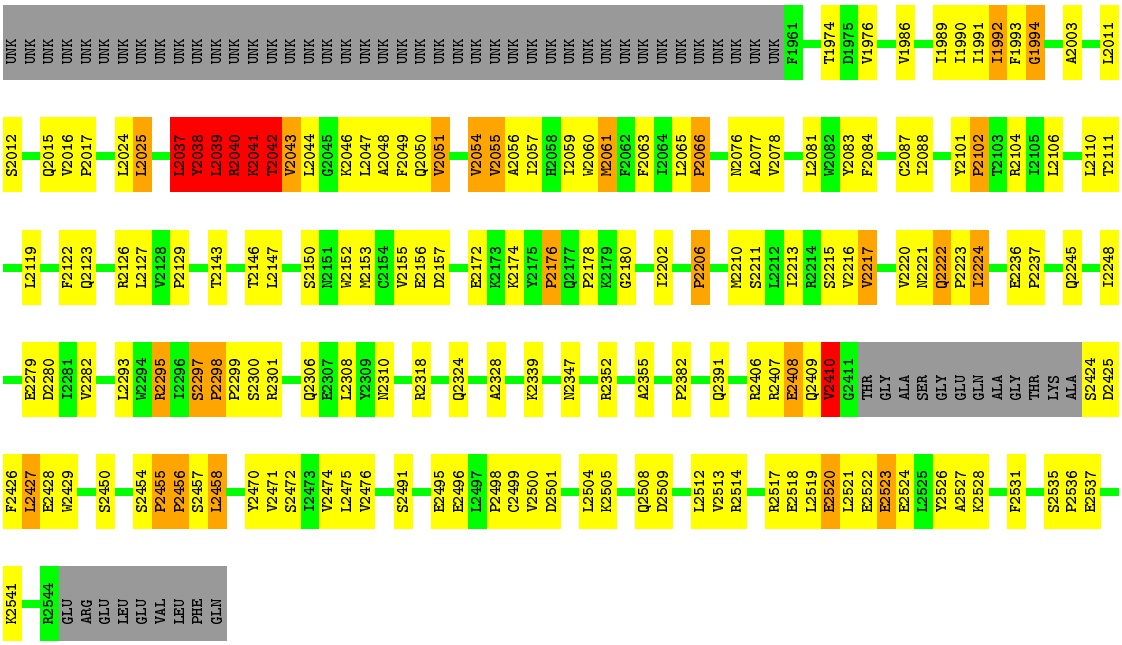
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. 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: Piezo-type mechanosensitive ion channel component 1

Chain A:

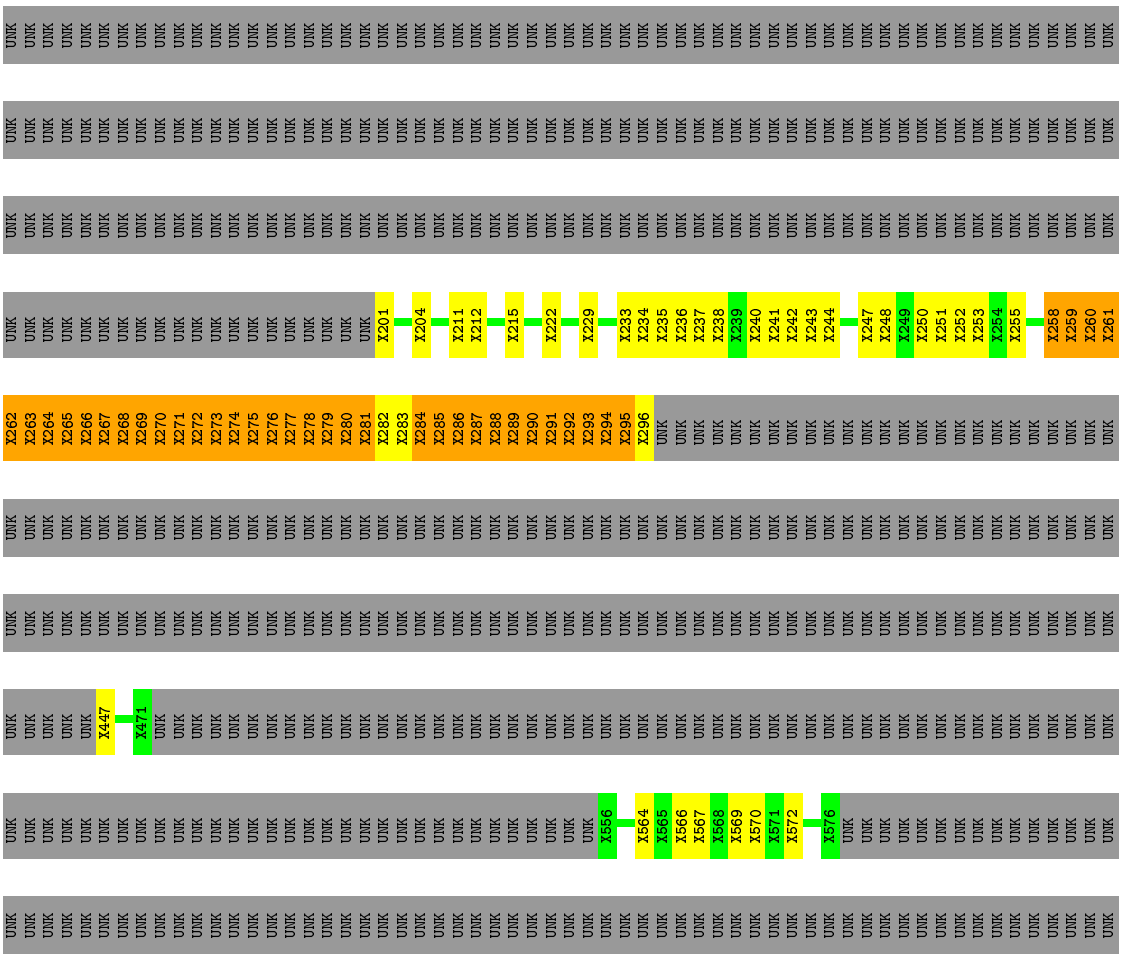


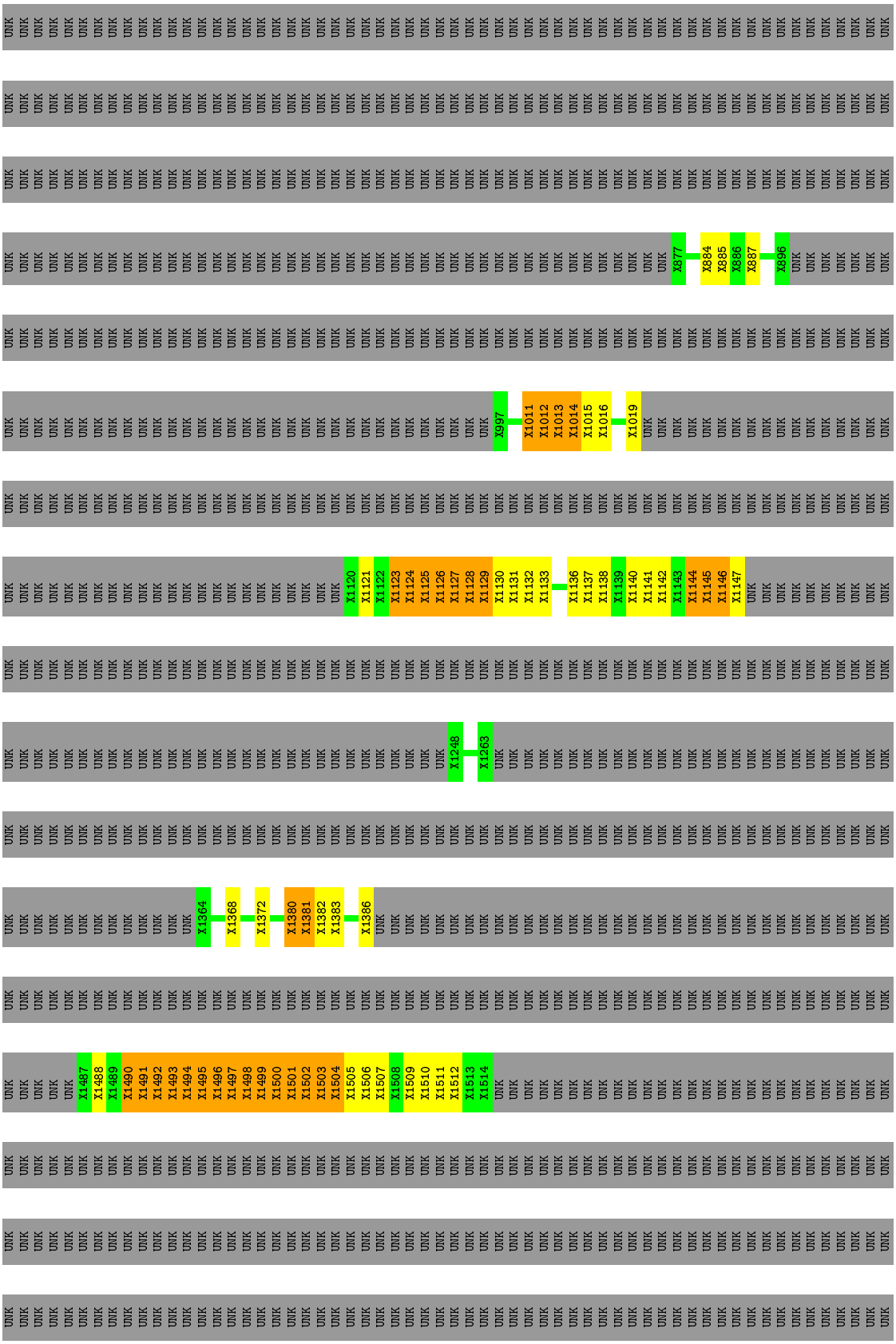

UNK X877 X884 X885 X896
UNK X997 X1011 X1012 X1013 X1014 X1015 X1016 X1019
UNK X1120 X1121 X1122 X1123 X1124 X1125 X1126 X1127 X1128 X1129 X1130 X1131 X1132 X1133 X1134 X1135 X1136 X1137 X1138 X1139 X1140 X1141 X1142 X1143 X1144 X1145 X1146 X1147
UNK X1248 X1263
UNK X1364 X1368 X1372 X1380 X1381 X1382 X1383 X1386
UNK X1487 X1488 X1489 X1490 X1491 X1492 X1493 X1494 X1495 X1496 X1497 X1498 X1499 X1500 X1501 X1502 X1503 X1504 X1505 X1506 X1507 X1510 X1511 X1512 X1513 X1514
UNK X1739 X1743 X1744 X1747 X1748 X1749 X1750 X1751 X1752 X1753 X1754 X1755 X1756 X1757 X1758 X1759 X1763 X1764 X1765 X1766 X1769 X1770 X1771 X1772 X1773 X1774 X1775 X1776 X1777 X1780 X1781 X1787 X1788 X1789 X1790 X1791 X1792 X1793 X1794
X1795 X1796 X1797 X1798 X1804



- Molecule 1: Piezo-type mechanosensitive ion channel component 1

Chain B:

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X1016
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X1121
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X1123
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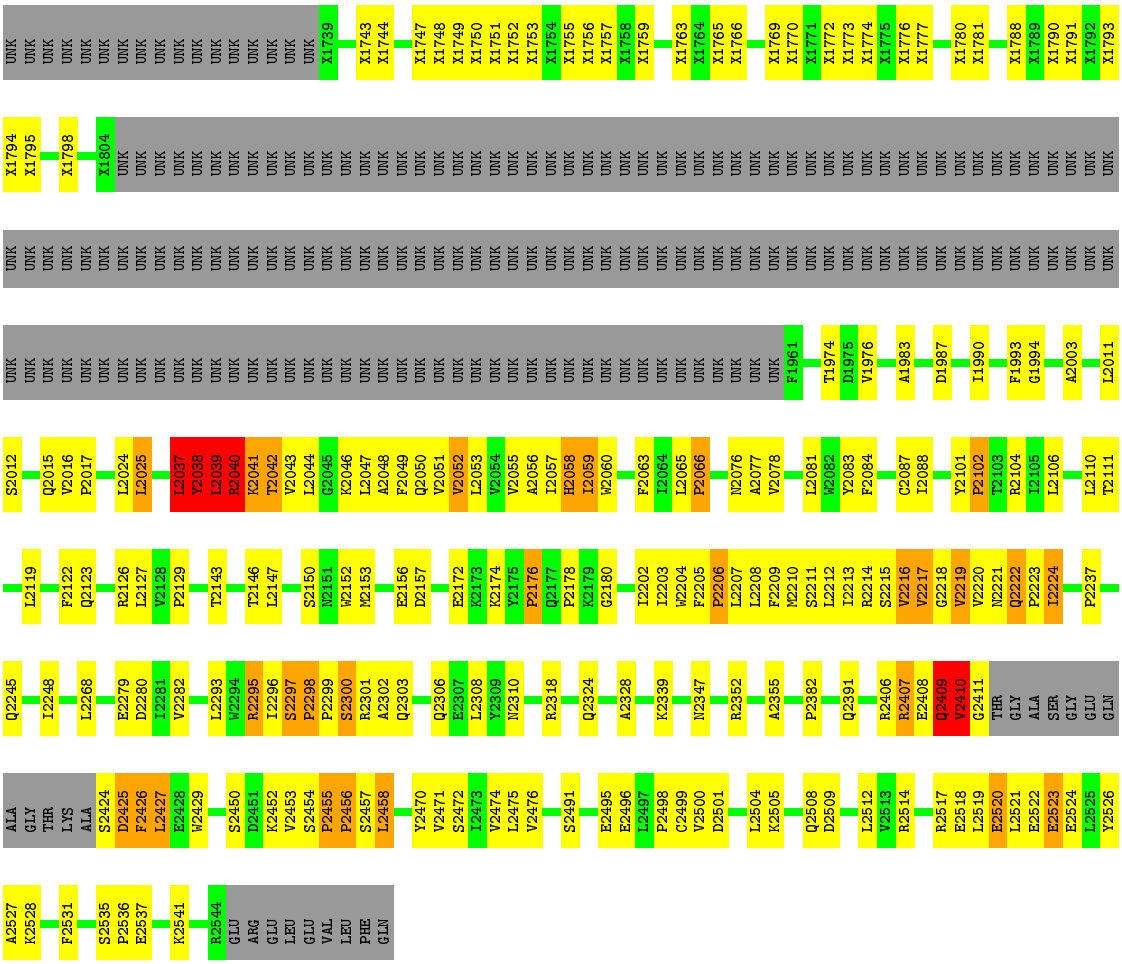
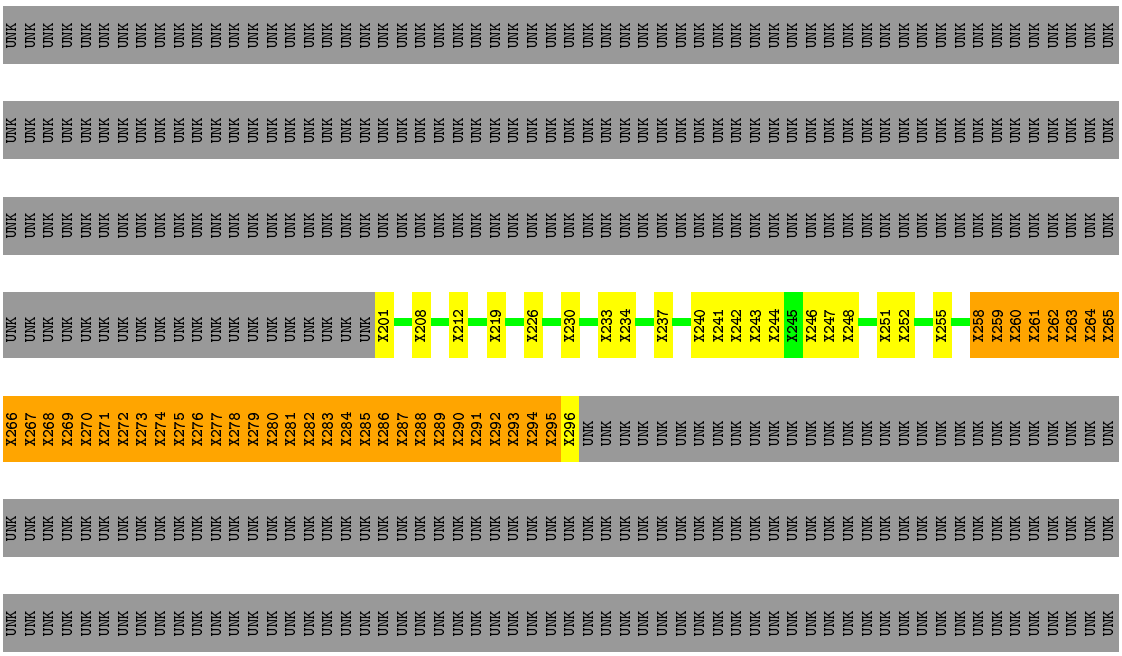
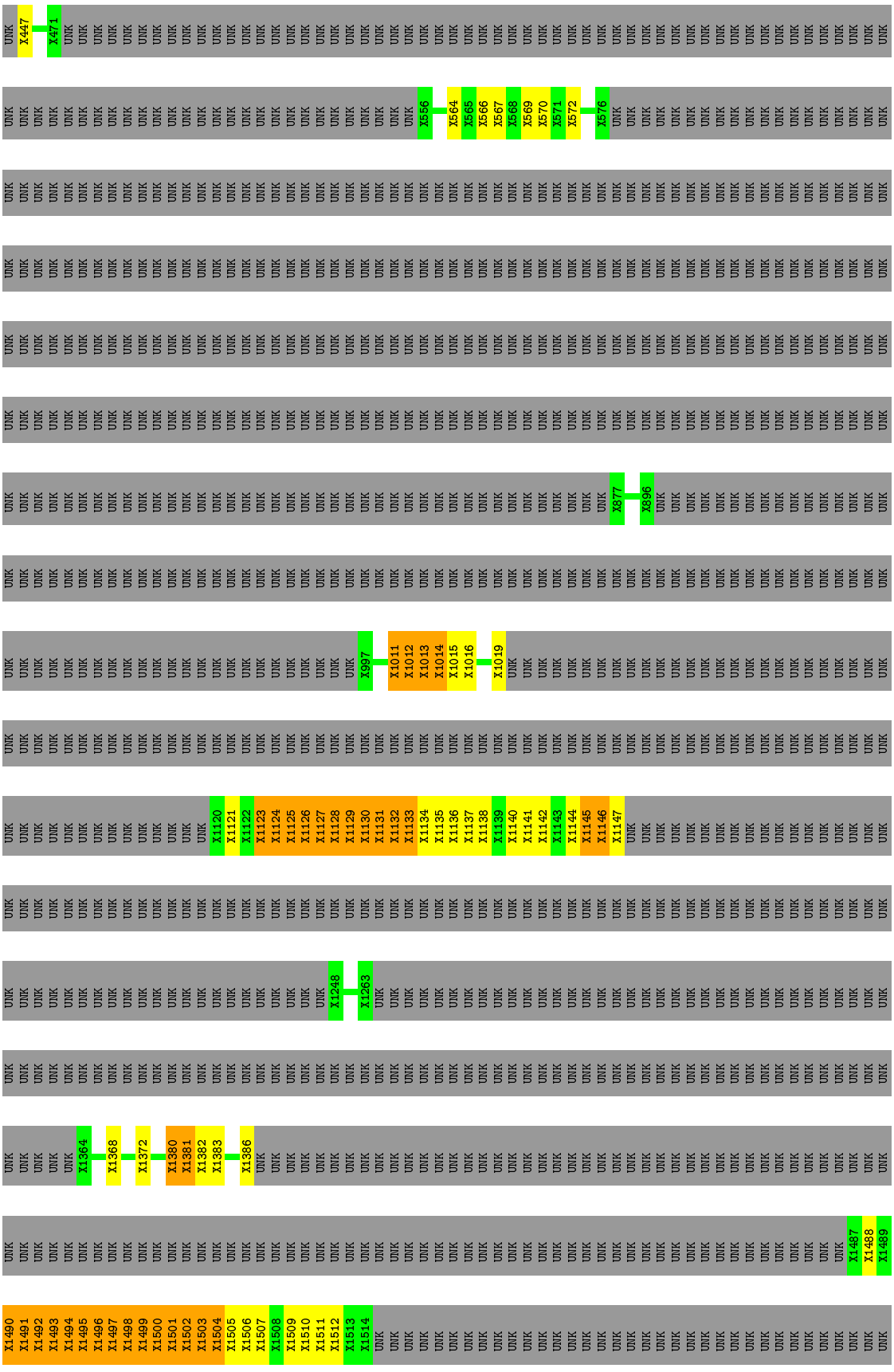
X1514



- Molecule 1: Piezo-type mechanosensitive ion channel component 1

Chain C:




X447
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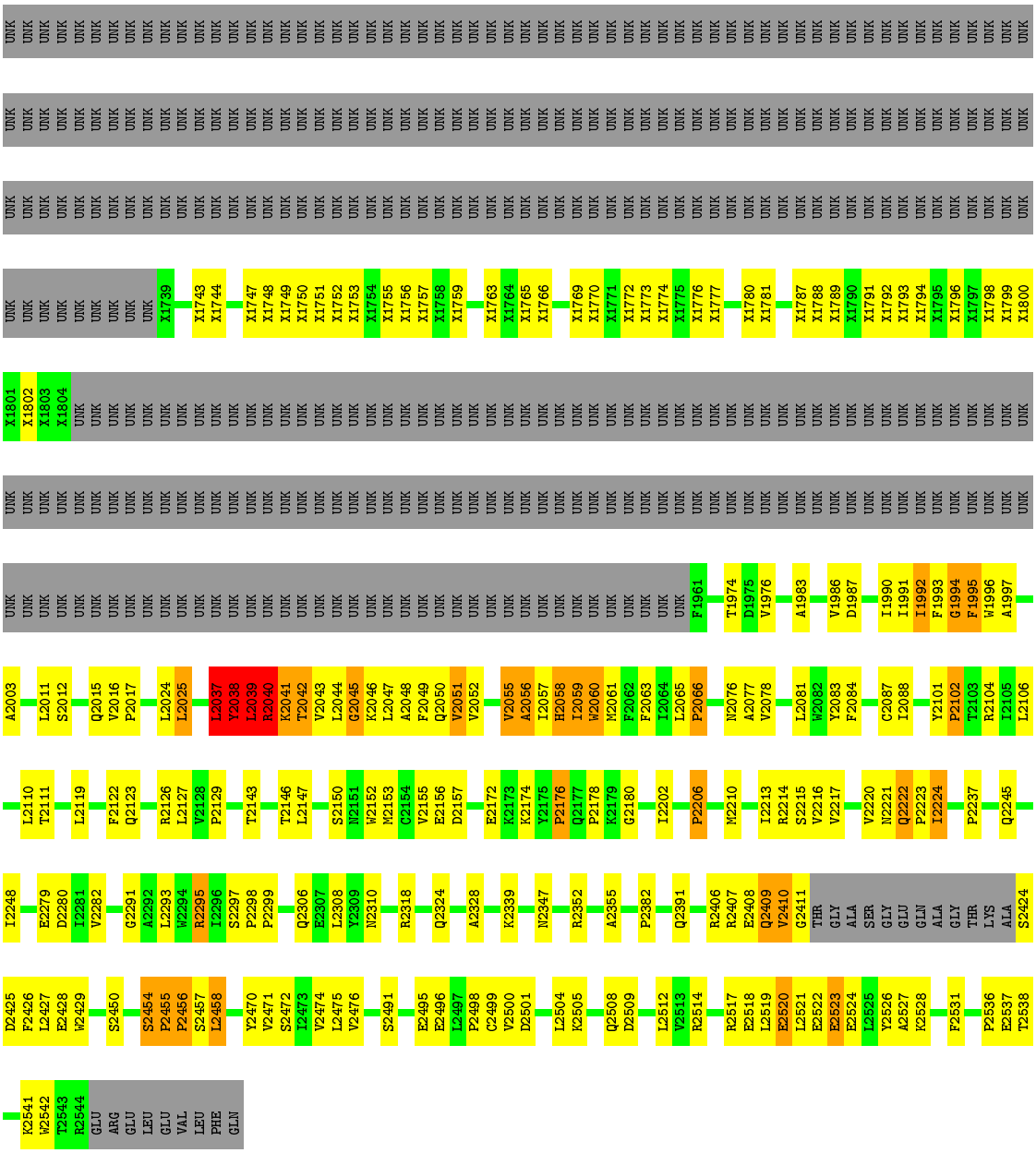

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	30021	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	CTFFIND	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	16	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor

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	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	A	0.42	2/3562 (0.1%)	0.67	19/4908 (0.4%)
1	B	0.43	2/3562 (0.1%)	0.66	19/4908 (0.4%)
1	C	0.40	1/3562 (0.0%)	0.61	16/4908 (0.3%)
All	All	0.41	5/10686 (0.0%)	0.65	54/14724 (0.4%)

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	A	0	80
1	B	0	72
1	C	0	76
All	All	0	228

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2298	PRO	N-CD	5.23	1.55	1.47
1	B	2410	VAL	CA-CB	5.17	1.65	1.54
1	C	2455	PRO	N-CD	5.02	1.54	1.47
1	B	2455	PRO	N-CD	5.02	1.54	1.47
1	A	2455	PRO	N-CD	5.01	1.54	1.47

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2410	VAL	CB-CA-C	8.86	128.24	111.40
1	B	2410	VAL	CG1-CB-CG2	-8.19	97.79	110.90
1	B	2037	LEU	O-C-N	-8.16	109.65	122.70
1	C	2037	LEU	O-C-N	-8.15	109.65	122.70
1	A	2037	LEU	O-C-N	-8.14	109.67	122.70

There are no chirality outliers.

5 of 228 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	258	UNK	Mainchain
1	A	259	UNK	Mainchain
1	A	260	UNK	Mainchain
1	A	261	UNK	Mainchain
1	A	262	UNK	Mainchain

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	5247	0	2895	498	0
1	B	5247	0	2893	538	0
1	C	5247	0	2898	527	0
All	All	15741	0	8686	1389	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 57.

The worst 5 of 1389 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:C:2410:VAL:HG21	1:C:2426:PHE:CD2	1.22	1.67
1:C:2410:VAL:HG21	1:C:2426:PHE:CE2	1.16	1.62
1:C:2409:GLN:CA	1:C:2410:VAL:HG22	1.28	1.60
1:C:230:UNK:HA	1:C:259:UNK:CB	1.19	1.58
1:B:201:UNK:HA	1:B:288:UNK:CB	1.18	1.57

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 PDB entries followed by that with respect to all EM entries.

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	568/2553 (22%)	512 (90%)	31 (6%)	25 (4%)	3 34
1	B	568/2553 (22%)	513 (90%)	27 (5%)	28 (5%)	3 31
1	C	568/2553 (22%)	513 (90%)	27 (5%)	28 (5%)	3 31
All	All	1704/7659 (22%)	1538 (90%)	85 (5%)	81 (5%)	5 32

5 of 81 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1992	ILE
1	A	1993	PHE
1	A	2025	LEU
1	A	2043	VAL
1	A	2051	VAL

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 PDB entries followed by that with respect to all EM entries.

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	200/522 (38%)	194 (97%)	6 (3%)	48 78
1	B	200/522 (38%)	190 (95%)	10 (5%)	30 67
1	C	200/522 (38%)	195 (98%)	5 (2%)	55 82
All	All	600/1566 (38%)	579 (96%)	21 (4%)	47 76

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2300	SER
1	B	2407	ARG
1	C	2295	ARG
1	B	2297	SER
1	C	2391	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2245	GLN
1	A	2409	GLN
1	B	2245	GLN
1	B	2409	GLN
1	C	2245	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 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.