



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:17 PM GMT

PDB ID : 4RES
Title : Crystal structure of the Na,K-ATPase E2P-bufalin complex with bound potassium
Authors : Laursen, M.; Yatime, L.; Gregersen, J.L.; Nissen, P.; Fedosova, N.U.
Deposited on : 2014-09-23
Resolution : 3.41 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

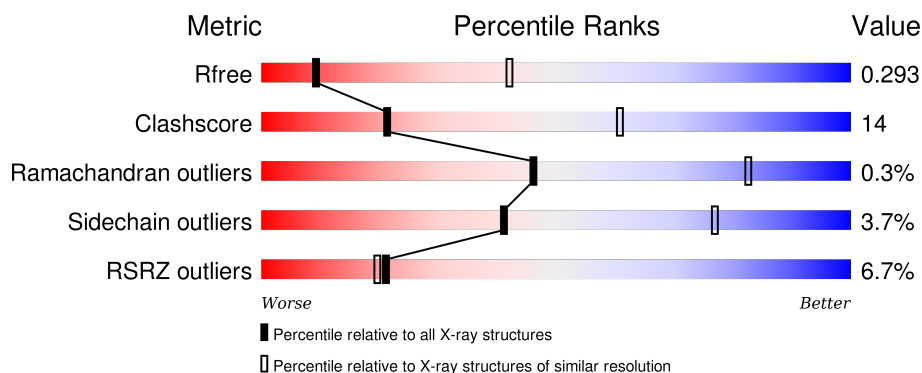
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	1021	<div> <div>6%</div> <div>67%</div> <div>29%</div> <div>..</div> </div>
1	C	1021	<div> <div>7%</div> <div>67%</div> <div>29%</div> <div>..</div> </div>
2	B	303	<div> <div>6%</div> <div>56%</div> <div>36%</div> <div>• 5%</div> </div>
2	D	303	<div> <div>6%</div> <div>54%</div> <div>37%</div> <div>• 6%</div> </div>
3	E	65	<div> <div>3%</div> <div>40%</div> <div>9%</div> <div>51%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	65	

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
5	CLR	A	2002	-	-	-	X
9	17F	G	1001	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 20881 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 Sodium/potassium-transporting ATPase subunit alpha-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	996	Total	C	N	O	P	S	0	0	0
			7730	4922	1301	1459	1	47			
1	C	996	Total	C	N	O	P	S	0	0	0
			7730	4922	1301	1459	1	47			

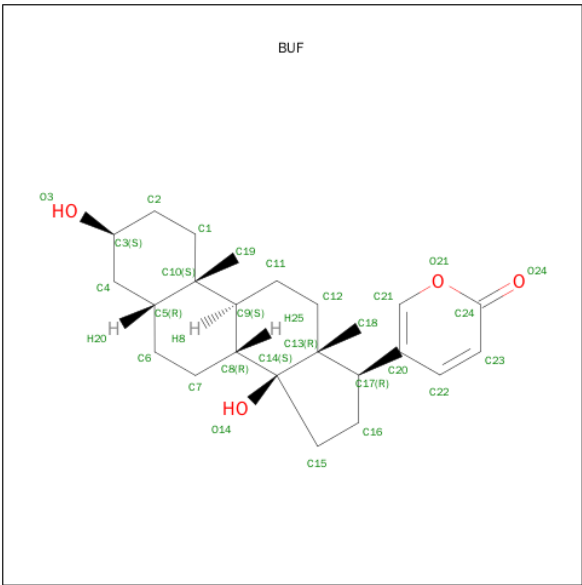
- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	288	Total	C	N	O	S	0	0	0
			2357	1525	385	434	13			
2	D	285	Total	C	N	O	S	0	0	0
			2327	1504	380	430	13			

- Molecule 3 is a protein called Na⁺/K⁺ ATPase gamma subunit transcript variant a.

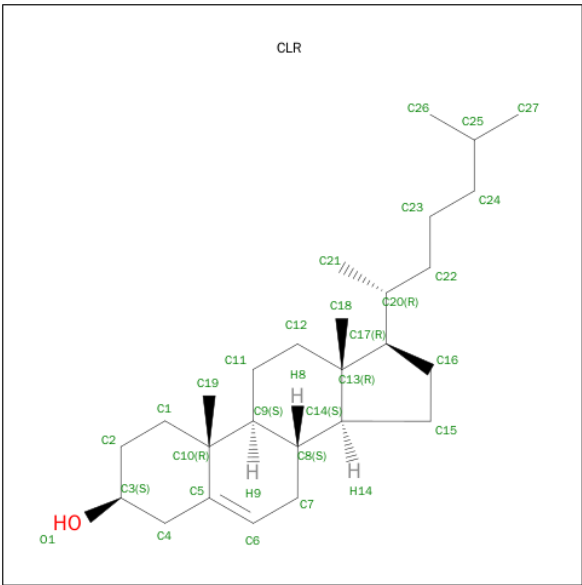
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	32	Total	C	N	O	0	0	0
			255	174	37	44			
3	E	32	Total	C	N	O	0	0	0
			255	174	37	44			

- Molecule 4 is BUFALIN (three-letter code: BUF) (formula: C₂₄H₃₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			28	24	4		
4	C	1	Total	C	O	0	0
			28	24	4		

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			28	27	1		
5	E	1	Total	C	O	0	0
			28	27	1		

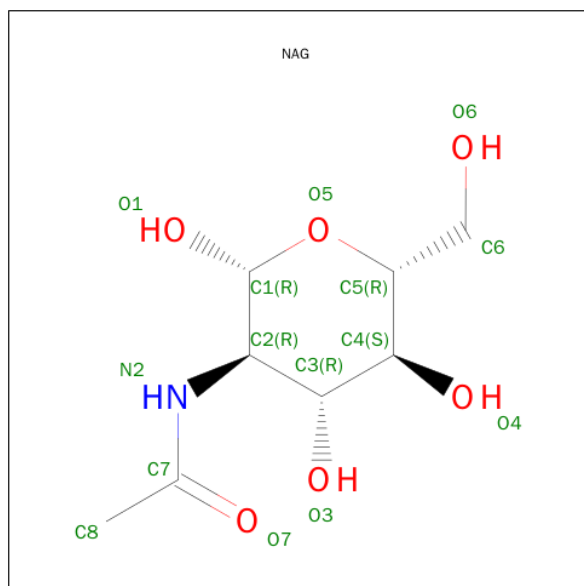
- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	K	0	0
			3	3		
6	C	3	Total	K	0	0
			3	3		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

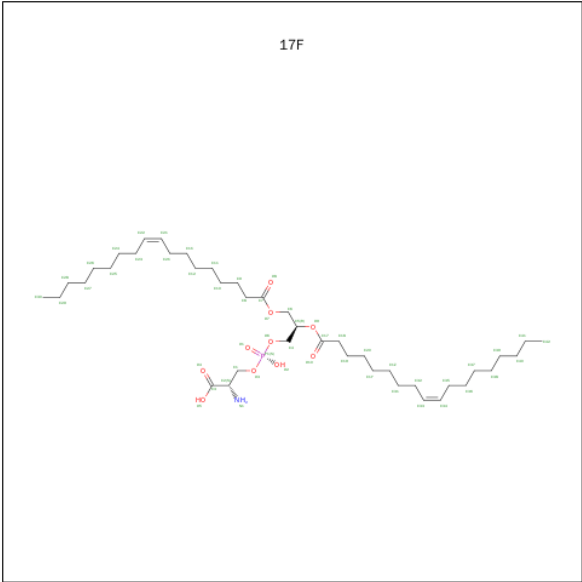
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



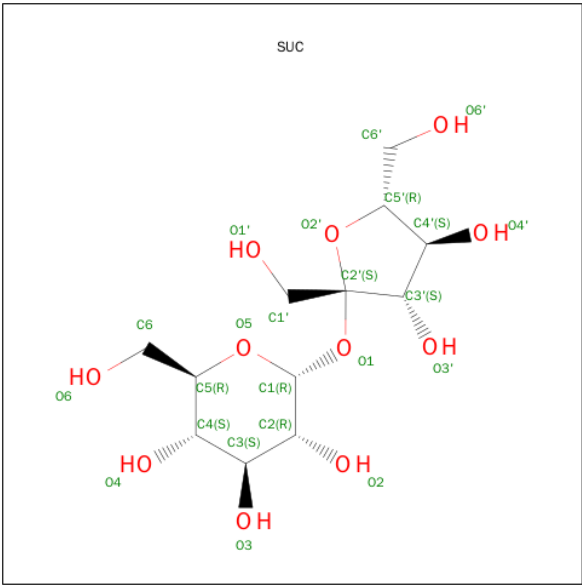
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is O-[(S)-({(2R)-2,3-BIS[(9Z)-OCTADEC-9-ENOYLOXY]PROPYL}OXY)(HYDROXY)PHOSPHORYL]-L-SERINE (three-letter code: 17F) (formula: C₄₂H₇₈NO₁₀P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	G	1	19	8	1	9	1	0	0

- Molecule 10 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	C	1	23	12	11	0	0
10	C	1	23	12	11	0	0

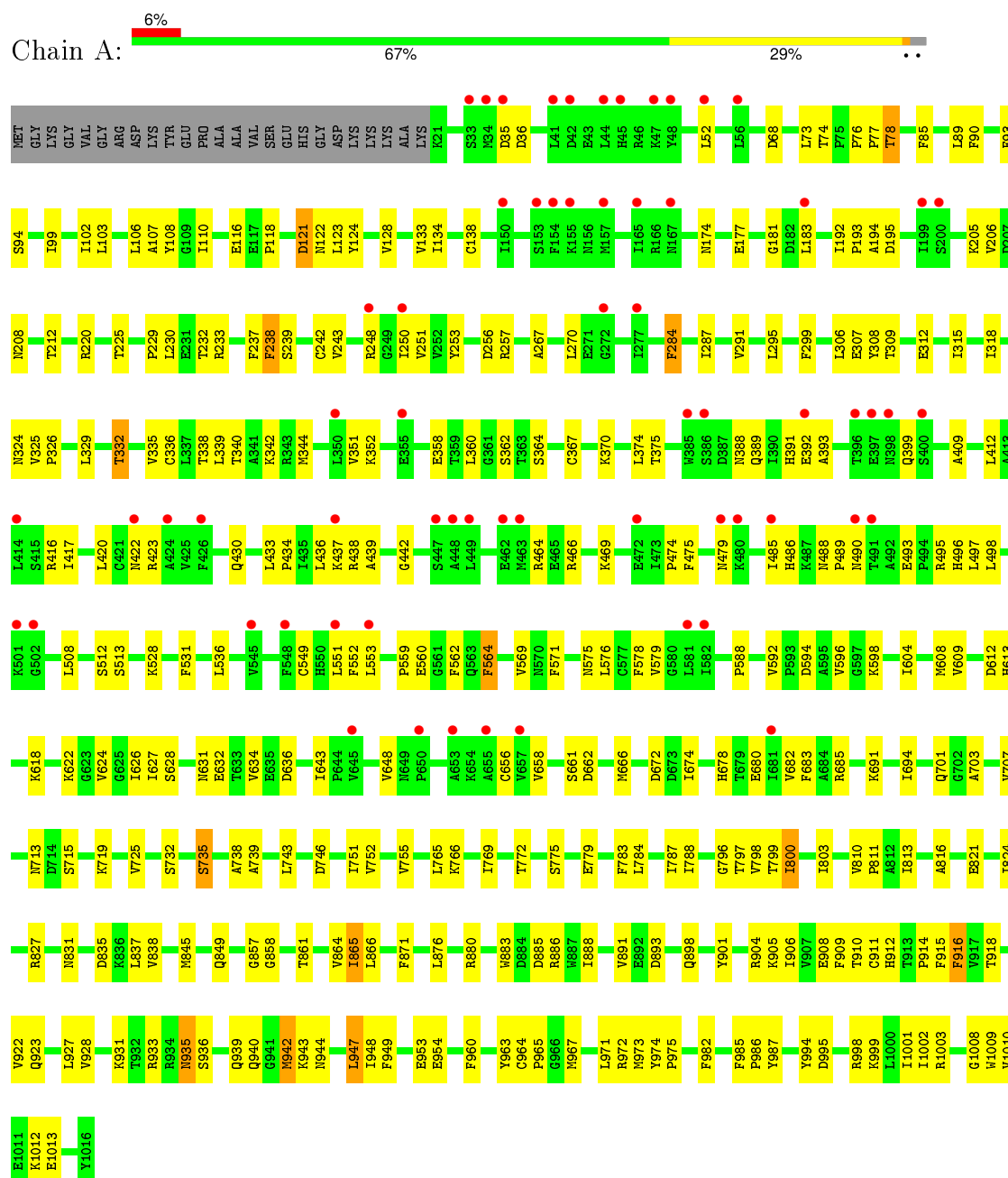
- Molecule 11 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	2	Total	C	N	O	0	0
			28	16	2	10		

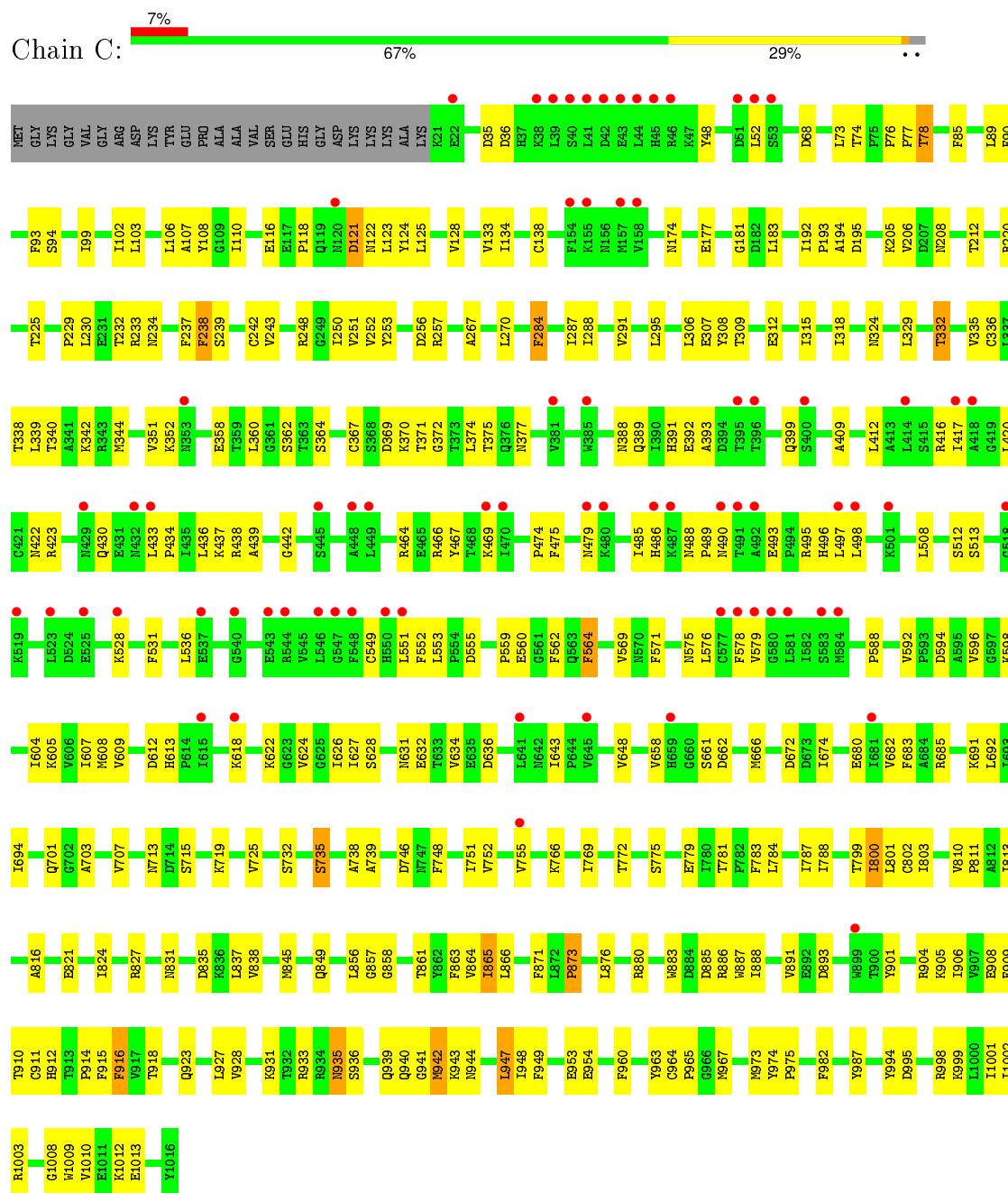
3 Residue-property plots

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.

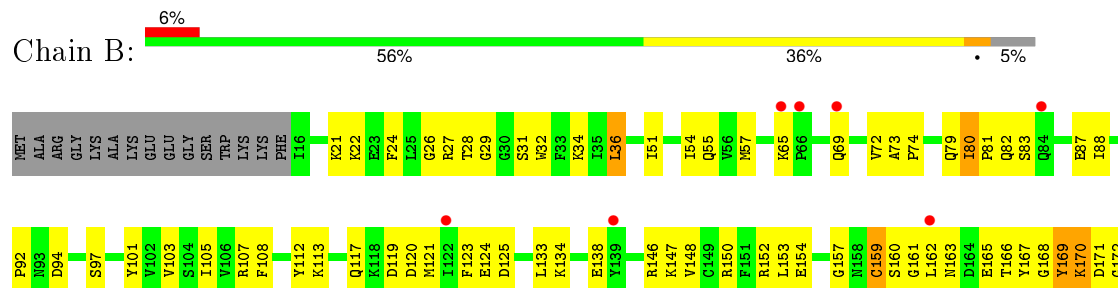
- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

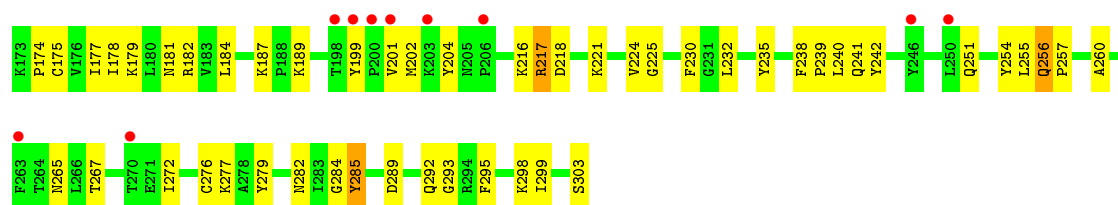


• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

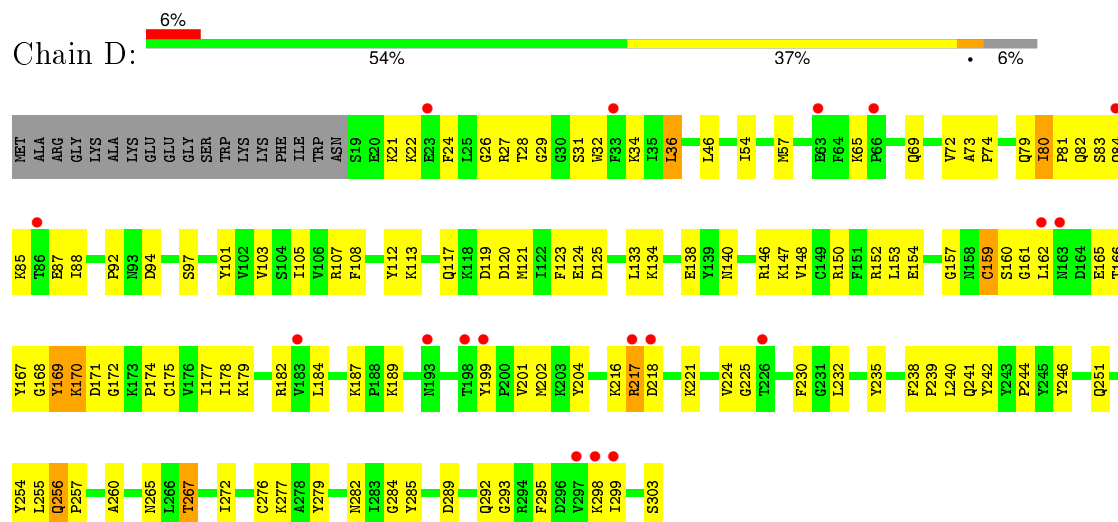


• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

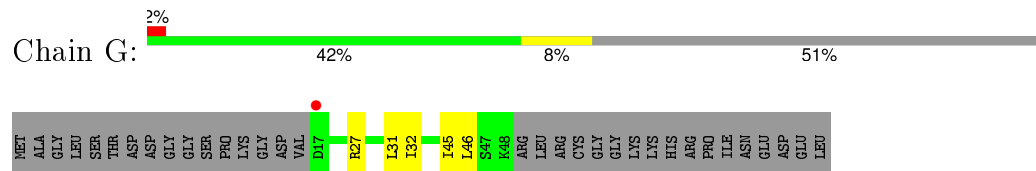




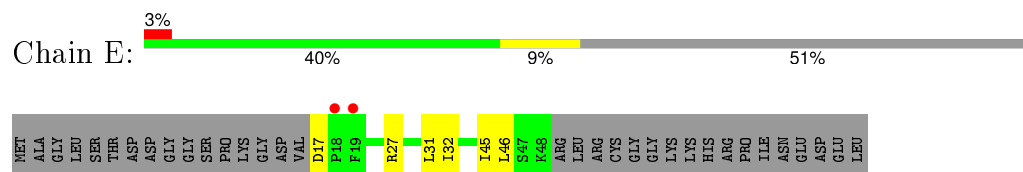
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



• Molecule 3: Na⁺/K⁺ ATPase gamma subunit transcript variant a



• Molecule 3: Na⁺/K⁺ ATPase gamma subunit transcript variant a



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.91Å 240.27Å 152.70Å 90.00° 102.28° 90.00°	Depositor
Resolution (Å)	49.90 – 3.41 54.59 – 3.41	Depositor EDS
% Data completeness (in resolution range)	49.9 (49.90-3.41) 50.2 (54.59-3.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.245 , 0.288 0.254 , 0.293	Depositor DCC
R_{free} test set	1634 reflections (5.43%)	DCC
Wilson B-factor (Å ²)	92.8	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.2	EDS
Estimated twinning fraction	0.368 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 31754 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	20881	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: MG, SUC, NAG, 17F, K, PHD, BUF, CLR

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	0.34	0/7867	0.54	0/10674
1	C	0.34	0/7867	0.54	0/10674
2	B	0.36	0/2419	0.59	0/3263
2	D	0.35	0/2387	0.59	0/3218
3	E	0.36	0/261	0.51	0/354
3	G	0.33	0/261	0.52	0/354
All	All	0.34	0/21062	0.55	0/28537

There are no bond length outliers.

There are no bond angle outliers.

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	7730	0	7776	211	0
1	C	7730	0	7776	219	0
2	B	2357	0	2328	83	0
2	D	2327	0	2301	83	0
3	E	255	0	259	5	0
3	G	255	0	259	4	0
4	A	28	0	34	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	28	0	34	4	0
5	A	28	0	46	4	0
5	E	28	0	46	4	0
6	A	3	0	0	0	0
6	C	3	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	14	0	13	1	0
9	G	19	0	10	0	0
10	C	46	0	44	5	0
11	D	28	0	25	1	0
All	All	20881	0	20951	595	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 14.

The worst 5 of 595 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)
2:B:80:ILE:HG13	2:B:81:PRO:HD3	1.44	0.97
2:D:80:ILE:HG13	2:D:81:PRO:HD3	1.45	0.97
2:B:79:GLN:HB3	2:B:295:PHE:HZ	1.33	0.93
2:D:79:GLN:HB3	2:D:295:PHE:HZ	1.34	0.91
2:D:80:ILE:HD12	2:D:105:ILE:HD12	1.52	0.91

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 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	993/1021 (97%)	939 (95%)	53 (5%)	1 (0%)	56 89

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	993/1021 (97%)	937 (94%)	55 (6%)	1 (0%)	56 89
2	B	286/303 (94%)	265 (93%)	18 (6%)	3 (1%)	19 63
2	D	283/303 (93%)	263 (93%)	17 (6%)	3 (1%)	17 61
3	E	30/65 (46%)	30 (100%)	0	0	100 100
3	G	30/65 (46%)	30 (100%)	0	0	100 100
All	All	2615/2778 (94%)	2464 (94%)	143 (6%)	8 (0%)	46 82

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	170	LYS
2	B	217	ARG
2	D	170	LYS
2	D	217	ARG
1	A	78	THR

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	846/864 (98%)	819 (97%)	27 (3%)	46 80
1	C	846/864 (98%)	818 (97%)	28 (3%)	45 80
2	B	258/269 (96%)	245 (95%)	13 (5%)	30 69
2	D	255/269 (95%)	242 (95%)	13 (5%)	29 69
3	E	26/52 (50%)	25 (96%)	1 (4%)	40 76
3	G	26/52 (50%)	25 (96%)	1 (4%)	40 76
All	All	2257/2370 (95%)	2174 (96%)	83 (4%)	41 77

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	272	ILE

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Mol	Chain	Res	Type
1	C	220	ARG
2	D	204	TYR
2	B	285	TYR
1	C	36	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	898	GLN
2	B	181	ASN
1	C	488	ASN
1	A	889	ASN
1	C	399	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	PHD	A	369	1,7	8,11,12	1.24	1 (12%)	9,15,17	1.57	2 (22%)
1	PHD	C	369	1,7	8,11,12	1.24	1 (12%)	9,15,17	1.59	2 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PHD	A	369	1,7	-	0/7/11/13	0/0/0/0
1	PHD	C	369	1,7	-	0/7/11/13	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	369	PHD	CB-CA	-2.48	1.48	1.53
1	A	369	PHD	CB-CA	-2.39	1.48	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	369	PHD	OD2-CG-CB	-3.08	117.62	124.69
1	A	369	PHD	OD2-CG-CB	-3.06	117.66	124.69
1	C	369	PHD	O-C-CA	-2.40	119.22	125.49
1	A	369	PHD	O-C-CA	-2.39	119.27	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	369	PHD	1	0

5.5 Carbohydrates ⓘ

2 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	NAG	D	1001	11,2	14,14,15	0.52	0	15,19,21	0.43	0
11	NAG	D	1002	11	14,14,15	0.33	0	15,19,21	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	D	1001	11,2	-	0/6/23/26	0/1/1/1
11	NAG	D	1002	11	-	0/6/23/26	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	1001	NAG	1	0

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BUF	A	2001	6	29,32,32	1.48	5 (17%)	46,52,52	1.54	7 (15%)
5	CLR	A	2002	-	31,31,31	2.31	10 (32%)	48,48,48	2.56	21 (43%)
8	NAG	B	1001	2	14,14,15	0.40	0	15,19,21	0.43	0
10	SUC	C	1101	-	24,24,24	0.44	0	36,36,36	1.27	3 (8%)
4	BUF	C	1102	6	29,32,32	1.54	7 (24%)	46,52,52	1.63	6 (13%)
10	SUC	C	1103	-	24,24,24	0.44	0	36,36,36	1.16	2 (5%)
5	CLR	E	101	-	31,31,31	2.28	9 (29%)	48,48,48	2.59	19 (39%)
9	17F	G	1001	-	15,18,53	1.64	3 (20%)	14,24,60	2.46	2 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BUF	A	2001	6	-	0/4/68/68	0/5/5/5
5	CLR	A	2002	-	-	0/10/68/68	0/4/4/4
8	NAG	B	1001	2	-	0/6/23/26	0/1/1/1
10	SUC	C	1101	-	-	0/12/51/51	0/2/2/2
4	BUF	C	1102	6	-	0/4/68/68	0/5/5/5
10	SUC	C	1103	-	-	0/12/51/51	0/2/2/2
5	CLR	E	101	-	-	0/10/68/68	0/4/4/4
9	17F	G	1001	-	-	0/17/21/59	0/0/0/0

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1102	BUF	C13-C17	-3.42	1.53	1.58
5	A	2002	CLR	C13-C17	-3.34	1.48	1.55
5	E	101	CLR	C13-C17	-3.15	1.48	1.55
4	A	2001	BUF	C13-C17	-3.11	1.54	1.58
5	E	101	CLR	C20-C17	-3.07	1.48	1.54

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2002	CLR	C4-C5-C6	-6.42	109.67	120.57
5	E	101	CLR	C4-C5-C6	-6.31	109.87	120.57
5	E	101	CLR	C7-C6-C5	-6.11	111.89	125.01
5	A	2002	CLR	C7-C6-C5	-5.83	112.48	125.01
5	E	101	CLR	C10-C5-C6	-4.83	114.00	122.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	BUF	2	0
5	A	2002	CLR	4	0
8	B	1001	NAG	1	0
10	C	1101	SUC	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1102	BUF	4	0
10	C	1103	SUC	2	0
5	E	101	CLR	4	0

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	995/1021 (97%)	0.21	64 (6%) 23 21	40, 119, 201, 295	0
1	C	995/1021 (97%)	0.31	74 (7%) 17 17	41, 124, 212, 292	0
2	B	288/303 (95%)	0.28	17 (5%) 26 23	53, 124, 205, 248	0
2	D	285/303 (94%)	0.19	18 (6%) 23 22	56, 120, 199, 326	0
3	E	32/65 (49%)	0.16	2 (6%) 23 22	51, 80, 158, 178	0
3	G	32/65 (49%)	0.28	1 (3%) 52 48	56, 86, 144, 172	0
All	All	2627/2778 (94%)	0.25	176 (6%) 21 20	40, 121, 206, 326	0

The worst 5 of 176 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	547	GLY	11.9
2	B	198	THR	11.7
1	C	491	THR	9.3
2	B	199	TYR	9.0
1	C	550	HIS	7.4

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	PHD	A	369	12/13	0.98	0.18	-	116,118,121,121	0
1	PHD	C	369	12/13	0.97	0.23	-	102,103,105,105	0

6.3 Carbohydrates ⓘ

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(Å ²)	Q<0.9
11	NAG	D	1001	14/15	0.78	0.33	-	157,166,174,177	0
11	NAG	D	1002	14/15	0.84	0.38	-	168,173,183,184	0

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
9	17F	G	1001	19/54	0.81	0.44	3.41	136,142,150,152	0
5	CLR	A	2002	28/28	0.98	0.36	2.77	40,44,51,53	0
5	CLR	E	101	28/28	0.98	0.31	1.00	56,60,65,67	0
7	MG	A	2006	1/1	1.00	0.20	0.62	71,71,71,71	0
4	BUF	C	1102	28/28	0.97	0.28	0.57	90,94,99,100	0
4	BUF	A	2001	28/28	0.96	0.25	0.36	93,97,101,102	0
6	K	A	2005	1/1	0.96	0.28	0.21	121,121,121,121	0
7	MG	C	1107	1/1	0.99	0.18	-0.05	106,106,106,106	0
6	K	A	2003	1/1	0.94	0.20	-0.76	121,121,121,121	0
6	K	C	1104	1/1	0.96	0.18	-0.84	92,92,92,92	0
10	SUC	C	1101	23/23	0.96	0.18	-0.91	110,114,117,120	0
10	SUC	C	1103	23/23	0.94	0.18	-1.15	101,105,107,109	0
6	K	C	1106	1/1	0.98	0.13	-1.37	69,69,69,69	0
6	K	C	1105	1/1	0.98	0.13	-2.38	60,60,60,60	0
6	K	A	2004	1/1	0.99	0.14	-3.70	54,54,54,54	0
8	NAG	B	1001	14/15	0.86	0.16	-	138,146,152,154	0

6.5 Other polymers ⓘ

There are no such residues in this entry.