



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 02:57 PM EDT

PDB ID : 5BUT
Title : Crystal structure of inactive conformation of KtrAB K⁺ transporter
Authors : Vieira-Pires, R.S.; Morais-Cabral, J.H.
Deposited on : 2015-06-04
Resolution : 5.97 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

<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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

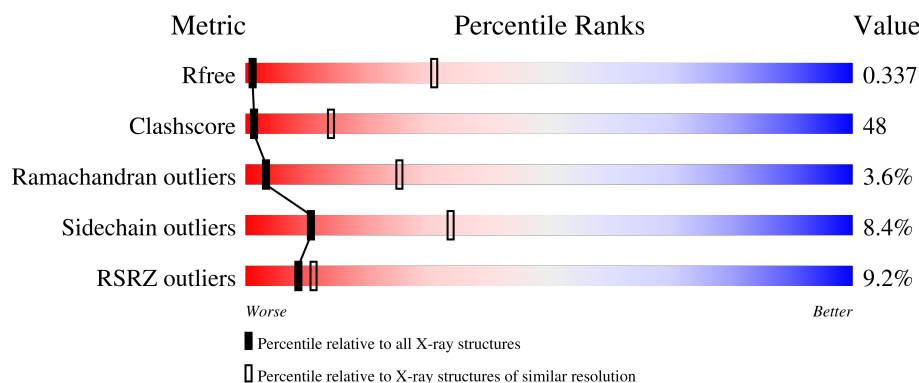
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.97 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}	130704	1000 (8.00-3.88)
Clashscore	141614	1049 (8.00-3.90)
Ramachandran outliers	138981	1016 (8.00-3.86)
Sidechain outliers	138945	1017 (8.00-3.82)
RSRZ outliers	127900	1014 (8.00-3.78)

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	288	<div> <div>12%</div> <div>38%</div> <div>47%</div> <div>8%</div> <div>7%</div> </div>
1	C	288	<div> <div>5%</div> <div>37%</div> <div>48%</div> <div>8%</div> <div>7%</div> </div>
1	E	288	<div> <div>9%</div> <div>40%</div> <div>45%</div> <div>8%</div> <div>7%</div> </div>
1	G	288	<div> <div>14%</div> <div>38%</div> <div>47%</div> <div>8%</div> <div>7%</div> </div>
2	I	445	<div> <div>5%</div> <div>30%</div> <div>60%</div> <div>7%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
2	J	445	<div><div></div><div>8%</div><div>31%</div><div>58%</div><div>7%</div><div></div></div>
2	K	445	<div><div></div><div>12%</div><div>27%</div><div>62%</div><div>7%</div><div></div></div>
2	L	445	<div><div></div><div>7%</div><div>29%</div><div>60%</div><div>7%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21476 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 Ktr system potassium uptake protein A, Ktr system potassium uptake protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2096	1336	362	394	4			
1	C	268	Total	C	N	O	S	0	0	0
			2096	1336	362	394	4			
1	E	268	Total	C	N	O	S	0	0	0
			2096	1336	362	394	4			
1	G	268	Total	C	N	O	S	0	0	0
			2096	1336	362	394	4			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	145	LEU	-	linker	UNP O32080
A	146	GLU	-	linker	UNP O32080
A	147	GLY	-	linker	UNP O32080
A	148	SER	-	linker	UNP O32080
A	283	LEU	-	expression tag	UNP O32080
A	284	GLU	-	expression tag	UNP O32080
A	285	LEU	-	expression tag	UNP O32080
A	286	VAL	-	expression tag	UNP O32080
A	287	PRO	-	expression tag	UNP O32080
A	288	ARG	-	expression tag	UNP O32080
A	22	VAL	CYS	engineered mutation	UNP O32080
C	145	LEU	-	linker	UNP O32080
C	146	GLU	-	linker	UNP O32080
C	147	GLY	-	linker	UNP O32080
C	148	SER	-	linker	UNP O32080
C	283	LEU	-	expression tag	UNP O32080
C	284	GLU	-	expression tag	UNP O32080
C	285	LEU	-	expression tag	UNP O32080
C	286	VAL	-	expression tag	UNP O32080
C	287	PRO	-	expression tag	UNP O32080

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Chain	Residue	Modelled	Actual	Comment	Reference
C	288	ARG	-	expression tag	UNP O32080
C	22	VAL	CYS	engineered mutation	UNP O32080
E	145	LEU	-	linker	UNP O32080
E	146	GLU	-	linker	UNP O32080
E	147	GLY	-	linker	UNP O32080
E	148	SER	-	linker	UNP O32080
E	283	LEU	-	expression tag	UNP O32080
E	284	GLU	-	expression tag	UNP O32080
E	285	LEU	-	expression tag	UNP O32080
E	286	VAL	-	expression tag	UNP O32080
E	287	PRO	-	expression tag	UNP O32080
E	288	ARG	-	expression tag	UNP O32080
E	22	VAL	CYS	engineered mutation	UNP O32080
G	145	LEU	-	linker	UNP O32080
G	146	GLU	-	linker	UNP O32080
G	147	GLY	-	linker	UNP O32080
G	148	SER	-	linker	UNP O32080
G	283	LEU	-	expression tag	UNP O32080
G	284	GLU	-	expression tag	UNP O32080
G	285	LEU	-	expression tag	UNP O32080
G	286	VAL	-	expression tag	UNP O32080
G	287	PRO	-	expression tag	UNP O32080
G	288	ARG	-	expression tag	UNP O32080
G	22	VAL	CYS	engineered mutation	UNP O32080

- Molecule 2 is a protein called Ktr system potassium uptake protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	431	Total	C	N	O	S	0	0	0
			3272	2180	507	570	15			
2	J	431	Total	C	N	O	S	0	0	0
			3272	2180	507	570	15			
2	K	431	Total	C	N	O	S	0	0	0
			3272	2180	507	570	15			
2	L	431	Total	C	N	O	S	0	0	0
			3272	2180	507	570	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	103	ALA	GLY	conflict	UNP O32081
I	104	ALA	LYS	conflict	UNP O32081

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Chain	Residue	Modelled	Actual	Comment	Reference
I	105	ALA	LYS	conflict	UNP O32081
I	218	GLN	ASN	conflict	UNP O32081
I	229	ALA	LYS	conflict	UNP O32081
I	261	ALA	HIS	conflict	UNP O32081
I	262	ALA	ILE	conflict	UNP O32081
I	429	ALA	LYS	conflict	UNP O32081
J	103	ALA	GLY	conflict	UNP O32081
J	104	ALA	LYS	conflict	UNP O32081
J	105	ALA	LYS	conflict	UNP O32081
J	218	GLN	ASN	conflict	UNP O32081
J	229	ALA	LYS	conflict	UNP O32081
J	261	ALA	HIS	conflict	UNP O32081
J	262	ALA	ILE	conflict	UNP O32081
J	429	ALA	LYS	conflict	UNP O32081
K	103	ALA	GLY	conflict	UNP O32081
K	104	ALA	LYS	conflict	UNP O32081
K	105	ALA	LYS	conflict	UNP O32081
K	218	GLN	ASN	conflict	UNP O32081
K	229	ALA	LYS	conflict	UNP O32081
K	261	ALA	HIS	conflict	UNP O32081
K	262	ALA	ILE	conflict	UNP O32081
K	429	ALA	LYS	conflict	UNP O32081
L	103	ALA	GLY	conflict	UNP O32081
L	104	ALA	LYS	conflict	UNP O32081
L	105	ALA	LYS	conflict	UNP O32081
L	218	GLN	ASN	conflict	UNP O32081
L	229	ALA	LYS	conflict	UNP O32081
L	261	ALA	HIS	conflict	UNP O32081
L	262	ALA	ILE	conflict	UNP O32081
L	429	ALA	LYS	conflict	UNP O32081

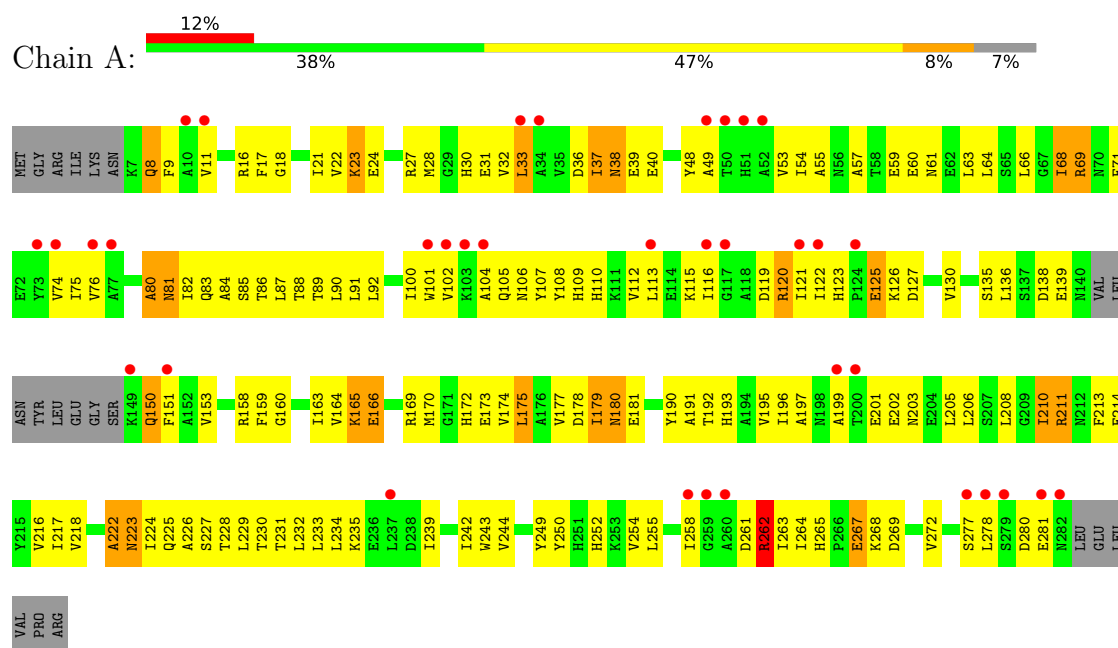
- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	1	Total K 1 1	0	0
3	J	1	Total K 1 1	0	0
3	K	1	Total K 1 1	0	0
3	L	1	Total K 1 1	0	0

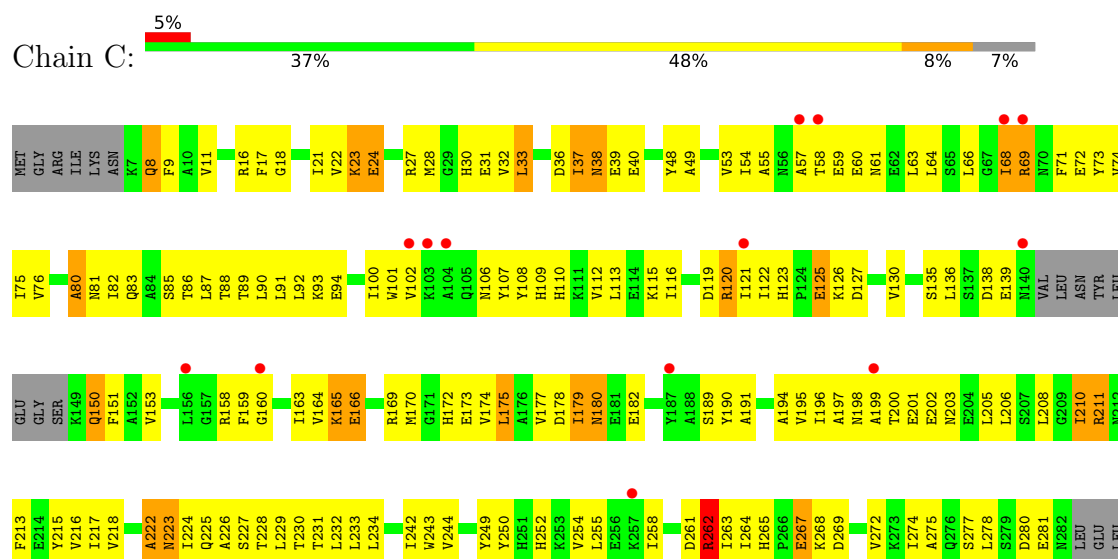
3 Residue-property plots

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.

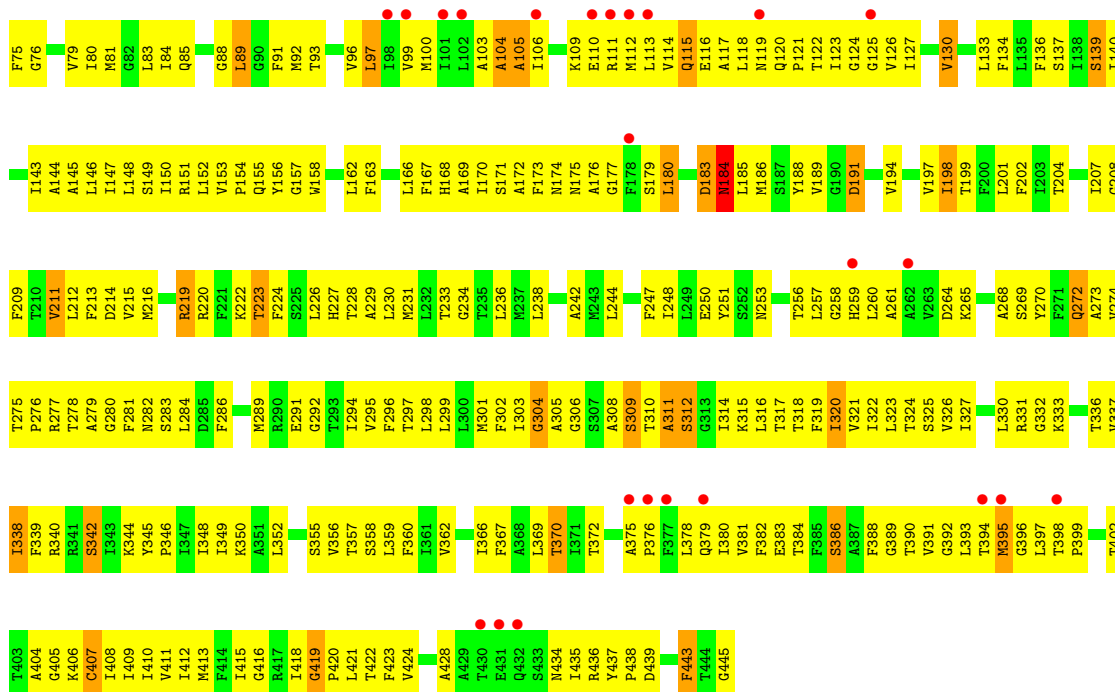
- Molecule 1: Ktr system potassium uptake protein A, Ktr system potassium uptake protein A



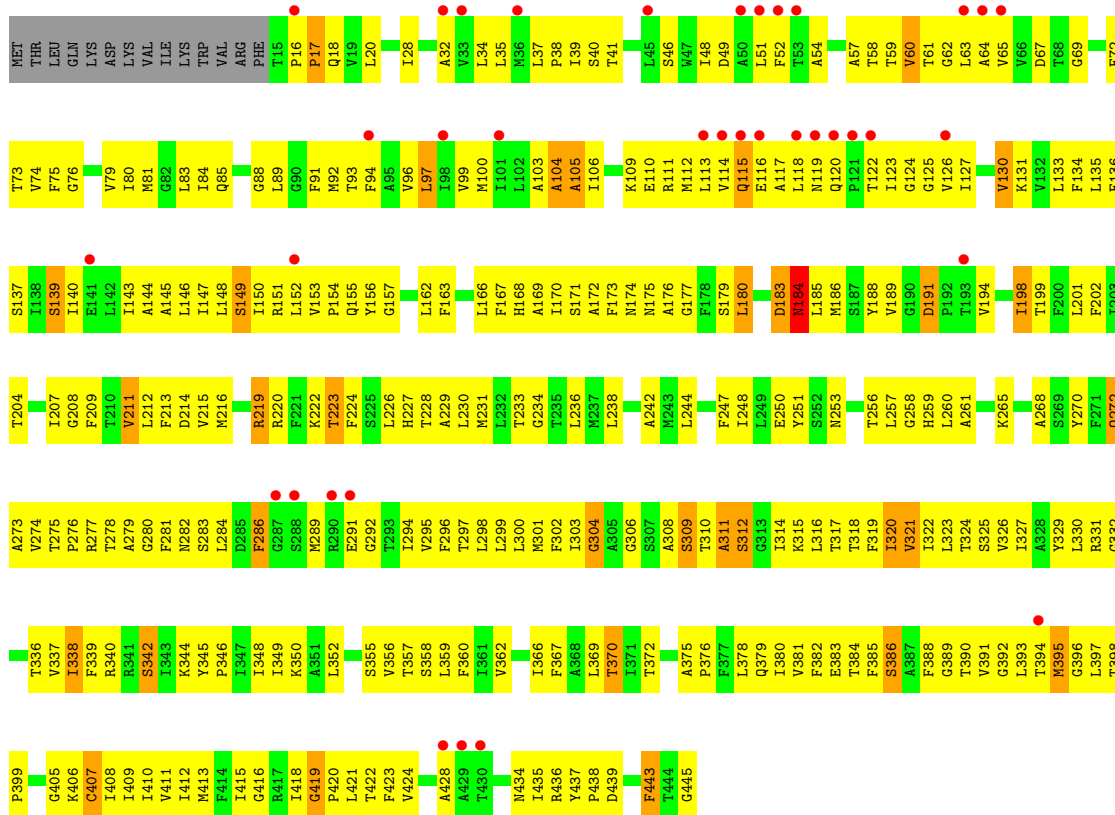
- Molecule 1: Ktr system potassium uptake protein A, Ktr system potassium uptake protein A



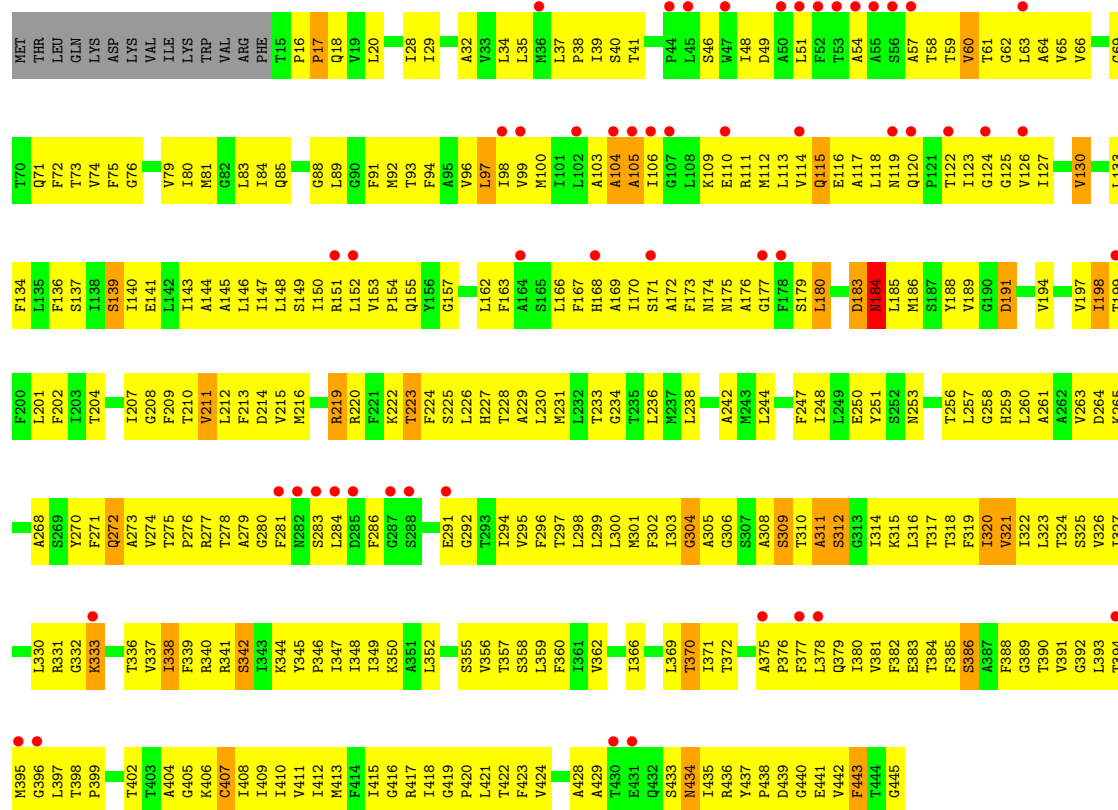
MET	THR	LEU	GLN	LYS	ASP	LYS	LYS	VAL	ILE	LYS	TRP	VAL	ARG	PHE	TIS	T15	T16	P17	T18	T19	T20	T21	T22	T23	T24	T25	T26	T27	T28	T29	T30	T31	T32	T33	T34	T35	T36	T37	T38	T39	T40	T41	T42	T43	T44	T45	T46	T47	T48	T49	T50	T51	T52	T53	T54	T55	T56	T57	T58	T59	T60	T61	T62	T63	T64	T65	T66	T67	T68	T69	T70	T71	T72	T73	T74	T75	T76	T77	T78	T79	T80	T81	T82	T83	T84	T85	T86	T87	T88	T89	T90	T91	T92	T93	T94	T95	T96	T97	T98	T99	T100	T101	T102	T103	T104	T105	T106	T107	T108	T109	T110	T111	T112	T113	T114	T115	T116	T117	T118	T119	T120	T121	T122	T123	T124	T125	T126	T127	T128	T129	T130	T131	T132	T133	T134	T135	T136	T137	T138	T139	T140	T141	T142	T143	T144	T145	T146	T147	T148	T149	T150	T151	T152	T153	T154	T155	T156	T157	T158	T159	T160	T161	T162	T163	T164	T165	T166	T167	T168	T169	T170	T171	T172	T173	T174	T175	T176	T177	T178	T179	T180	T181	T182	T183	T184	T185	T186	T187	T188	T189	T190	T191	T192	T193	T194	T195	T196	T197	T198	T199	T200	T201	T202	T203	T204	T205	T206	T207	T208	T209	T210	T211	T212	T213	T214	T215	T216	T217	T218	T219	T220	T221	T222	T223	T224	T225	T226	T227	T228	T229	T230	T231	T232	T233	T234	T235	T236	T237	T238	T239	T240	T241	T242	T243	T244	T245	T246	T247	T248	T249	T250	T251	T252	T253	T254	T255	T256	T257	T258	T259	T260	T261	T262	T263	T264	T265	T266	T267	T268	T269	T270	T271	T272	T273	T274	T275	T276	T277	T278	T279	T280	T281	T282	T283	T284	T285	T286	T287	T288	T289	T290	T291	T292	T293	T294	T295	T296	T297	T298	T299	T300	T301	T302	T303	T304	T305	T306	T307	T308	T309	T310	T311	T312	T313	T314	T315	T316	T317	T318	T319	T320	T321	T322	T323	T324	T325	T326	T327	T328	T329	T330	T331	T332	T333	T334	T335	T336	T337	T338	T339	T340	T341	T342	T343	T344	T345	T346	T347	T348	T349	T350	T351	T352	T353	T354	T355	T356	T357	T358	T359	T360	T361	T362	T363	T364	T365	T366	T367	T368	T369	T370	T371	T372	T373	T374	T375	T376	T377	T378	T379	T380	T381	T382	T383	T384	T385	T386	T387	T388	T389	T390	T391	T392	T393	T394	T395	T396	T397	T398	T399	T400	T401	T402	T403	T404	T405	T406	T407	T408	T409	T410	T411	T412	T413	T414	T415	T416	T417	T418	T419	T420	T421	T422	T423	T424	T425	T426	T427	T428	T429	T430	T431	T432	T433	T434	T435	T436	T437	T438	T439	T440	T441	T442	T443	T444	T445	T446	T447	T448	T449	T450	T451	T452	T453	T454	T455	T456	T457	T458	T459	T460	T461	T462	T463	T464	T465	T466	T467	T468	T469	T470	T471	T472	T473	T474	T475	T476	T477	T478	T479	T480	T481	T482	T483	T484	T485	T486	T487	T488	T489	T490	T491	T492	T493	T494	T495	T496	T497	T498	T499	T500	T501	T502	T503	T504	T505	T506	T507	T508	T509	T510	T511	T512	T513	T514	T515	T516	T517	T518	T519	T520	T521	T522	T523</
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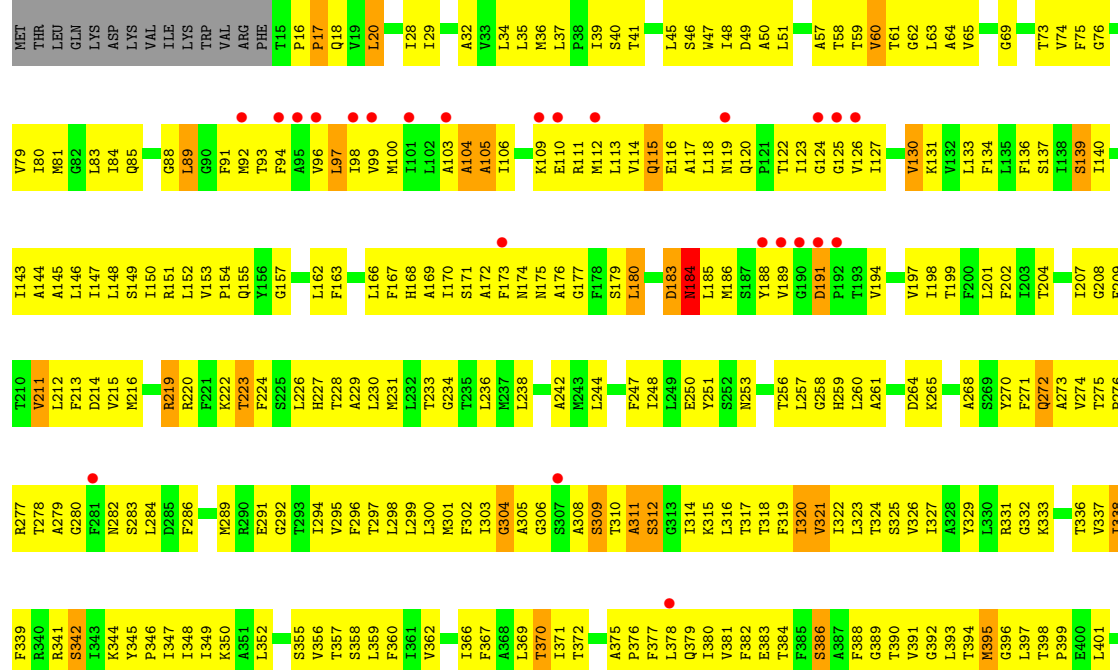
• Molecule 2: Ktr system potassium uptake protein B



• Molecule 2: Ktr system potassium uptake protein B



• Molecule 2: Ktr system potassium uptake protein B



A404	A405	A406	A407	A408	A409	A410	A411	A412	A413	A414	A415	A416	A417	A418	A419	A420	A421	A422	A423	A424	A425	A426	A427	A428	A429	A430	A431	A432	A433	A434	A435	A436	A437	A438	A439	A440	A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	307.06Å 79.41Å 205.65Å 90.00° 98.10° 90.00°	Depositor
Resolution (Å)	200.00 – 5.97 58.35 – 5.97	Depositor EDS
% Data completeness (in resolution range)	96.7 (200.00-5.97) 98.1 (58.35-5.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 6.17Å)	Xtriage
Refinement program	CNS DENR	Depositor
R, R_{free}	0.325 , 0.339 0.338 , 0.337	Depositor DCC
R_{free} test set	2336 reflections (9.90%)	wwPDB-VP
Wilson B-factor (Å ²)	316.7	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 272.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	21476	wwPDB-VP
Average B, all atoms (Å ²)	342.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.94% 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](#)

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

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	0.23	0/2130	0.52	4/2882 (0.1%)
1	C	0.25	0/2130	0.75	5/2882 (0.2%)
1	E	0.23	0/2130	0.52	4/2882 (0.1%)
1	G	0.25	0/2130	0.75	5/2882 (0.2%)
2	I	0.28	0/3343	0.50	0/4550
2	J	0.28	0/3343	0.50	0/4550
2	K	0.28	0/3343	0.50	0/4550
2	L	0.28	0/3343	0.50	0/4550
All	All	0.27	0/21892	0.56	18/29728 (0.1%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	120	ARG	NE-CZ-NH1	-21.01	109.80	120.30
1	G	120	ARG	NE-CZ-NH1	-20.98	109.81	120.30
1	C	120	ARG	NE-CZ-NH2	19.76	130.18	120.30
1	G	120	ARG	NE-CZ-NH2	19.75	130.18	120.30
1	C	120	ARG	CD-NE-CZ	9.78	137.29	123.60

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	2096	0	2120	181	0
1	C	2096	0	2120	177	0
1	E	2096	0	2120	145	0
1	G	2096	0	2120	156	0
2	I	3272	0	3442	384	0
2	J	3272	0	3442	379	0
2	K	3272	0	3442	405	0
2	L	3272	0	3442	386	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
All	All	21476	0	22248	2100	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 48.

The worst 5 of 2100 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:J:28:ILE:HG12	2:J:58:THR:HG21	1.37	1.05
2:K:28:ILE:HG12	2:K:58:THR:HG21	1.38	1.04
1:C:194:ALA:O	2:K:438:PRO:HD3	1.63	0.99
2:J:227:HIS:HA	2:J:230:LEU:HD12	1.46	0.96
2:L:133:LEU:HD12	2:L:134:PHE:H	1.29	0.96

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	264/288 (92%)	228 (86%)	32 (12%)	4 (2%)	10 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	264/288 (92%)	232 (88%)	28 (11%)	4 (2%)	10	45
1	E	264/288 (92%)	230 (87%)	30 (11%)	4 (2%)	10	45
1	G	264/288 (92%)	231 (88%)	29 (11%)	4 (2%)	10	45
2	I	429/445 (96%)	323 (75%)	84 (20%)	22 (5%)	2	19
2	J	429/445 (96%)	330 (77%)	78 (18%)	21 (5%)	2	20
2	K	429/445 (96%)	329 (77%)	80 (19%)	20 (5%)	2	21
2	L	429/445 (96%)	325 (76%)	83 (19%)	21 (5%)	2	20
All	All	2772/2932 (94%)	2228 (80%)	444 (16%)	100 (4%)	3	25

5 of 100 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	223	ASN
1	C	81	ASN
1	C	223	ASN
1	E	81	ASN

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	222/240 (92%)	200 (90%)	22 (10%)	8	26
1	C	222/240 (92%)	198 (89%)	24 (11%)	6	24
1	E	222/240 (92%)	199 (90%)	23 (10%)	7	25
1	G	222/240 (92%)	197 (89%)	25 (11%)	6	22
2	I	354/368 (96%)	328 (93%)	26 (7%)	14	39
2	J	354/368 (96%)	329 (93%)	25 (7%)	14	39
2	K	354/368 (96%)	330 (93%)	24 (7%)	16	41
2	L	354/368 (96%)	329 (93%)	25 (7%)	14	39
All	All	2304/2432 (95%)	2110 (92%)	194 (8%)	11	34

5 of 194 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	386	SER
2	J	439	ASP
2	I	443	PHE
2	J	184	ASN
2	K	130	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	195	ASN
2	K	119	ASN
2	I	239	ASN
2	J	175	ASN
2	K	379	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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	268/288 (93%)	0.58	35 (13%) 3 7	343, 343, 343, 343	0
1	C	268/288 (93%)	0.25	14 (5%) 27 27	343, 343, 343, 343	0
1	E	268/288 (93%)	0.65	27 (10%) 7 9	343, 343, 343, 343	0
1	G	268/288 (93%)	0.65	40 (14%) 2 5	343, 343, 343, 343	0
2	I	431/445 (96%)	0.39	24 (5%) 24 24	343, 343, 343, 343	0
2	J	431/445 (96%)	0.34	36 (8%) 11 13	343, 343, 343, 343	0
2	K	431/445 (96%)	0.54	52 (12%) 4 8	343, 343, 343, 343	0
2	L	431/445 (96%)	0.28	29 (6%) 17 17	343, 343, 343, 343	0
All	All	2796/2932 (95%)	0.44	257 (9%) 9 11	343, 343, 343, 343	0

The worst 5 of 257 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	105	ALA	7.1
2	J	119	ASN	7.0
2	I	431	GLU	6.3
2	K	104	ALA	5.8
1	A	281	GLU	5.5

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 monosaccharides 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. 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	B-factors(Å ²)	Q<0.9
3	K	I	501	1/1	0.88	0.46	342,342,342,342	0
3	K	K	501	1/1	0.89	0.24	342,342,342,342	0
3	K	L	501	1/1	0.92	0.25	342,342,342,342	0
3	K	J	501	1/1	0.94	0.34	342,342,342,342	0

6.5 Other polymers [i](#)

There are no such residues in this entry.