



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 25, 2016 – 12:25 PM GMT

PDB ID : 4RO0
Title : Crystal structure of MthK gating ring in a ligand-free form
Authors : Dong, W.; Guo, R.; Chai, H.; Chen, Z.; Cui, H.; Ren, Z.; Li, Y.; Ye, S.
Deposited on : 2014-10-27
Resolution : 3.18 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

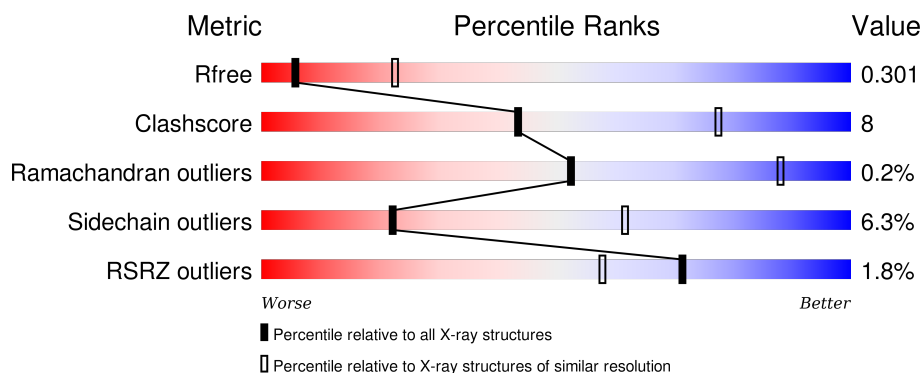
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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.













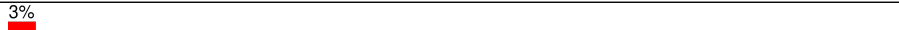

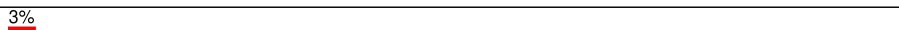
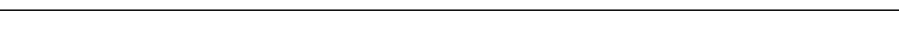



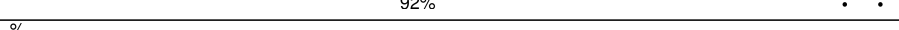






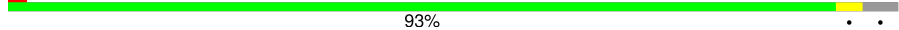
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1115 (3.22-3.14)
Clashscore	102246	1125 (3.20-3.16)
Ramachandran outliers	100387	1105 (3.20-3.16)
Sidechain outliers	100360	1104 (3.20-3.16)
RSRZ outliers	91569	1120 (3.22-3.14)

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	230	<div> <div>2%</div> <div>60% 34% . .</div> </div>
1	B	230	<div> <div>2%</div> <div>64% 31% . .</div> </div>
1	C	230	<div> <div>%</div> <div>63% 28% 5% .</div> </div>
1	D	230	<div> <div></div> <div>67% 25% . .</div> </div>
1	E	230	<div> <div>%</div> <div>60% 31% 5% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	230	
1	G	230	
1	H	230	
1	I	230	
1	J	230	
1	K	230	
1	L	230	
1	M	230	
1	N	230	
1	O	230	
1	P	230	
1	Q	230	
1	R	230	
1	S	230	
1	T	230	
1	a	230	
1	b	230	
1	c	230	
1	d	230	
1	e	230	
1	f	230	
1	g	230	
1	h	230	
1	i	230	
1	j	230	

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Mol	Chain	Length	Quality of chain
1	k	230	<div><div><div></div><div></div><div></div></div><div>%</div><div>90%</div><div>6%</div><div>.</div></div>
1	l	230	<div><div><div></div><div></div><div></div></div><div>90%</div><div>6%</div><div>.</div></div>
1	m	230	<div><div><div></div><div></div><div></div></div><div>2%</div><div>93%</div><div>.</div><div>.</div></div>
1	n	230	<div><div><div></div><div></div><div></div></div><div>%</div><div>90%</div><div>5%</div><div>.</div></div>
1	o	230	<div><div><div></div><div></div><div></div></div><div>89%</div><div>7%</div><div>.</div></div>
1	p	230	<div><div><div></div><div></div><div></div></div><div>%</div><div>90%</div><div>6%</div><div>.</div></div>
1	q	230	<div><div><div></div><div></div><div></div></div><div>8%</div><div>93%</div><div>.</div><div>.</div></div>
1	r	230	<div><div><div></div><div></div><div></div></div><div>3%</div><div>90%</div><div>7%</div><div>.</div></div>
1	s	230	<div><div><div></div><div></div><div></div></div><div>90%</div><div>6%</div><div>.</div></div>
1	t	230	<div><div><div></div><div></div><div></div></div><div>3%</div><div>91%</div><div>5%</div><div>.</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 68748 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 Calcium-gated potassium channel MthK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	a	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	B	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	b	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	C	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	c	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	D	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	d	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	E	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	e	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	F	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	f	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	G	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	g	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	H	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	h	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	i	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	J	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	j	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	K	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	k	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	L	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	l	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	M	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	m	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	N	221	Total	C	N	O	S	0	0	0
			1713	1066	302	338	7			
1	n	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	O	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	o	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	P	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	p	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	Q	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	q	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	R	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	r	221	Total	C	N	O	S	0	0	0
			1713	1066	302	338	7			
1	S	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			

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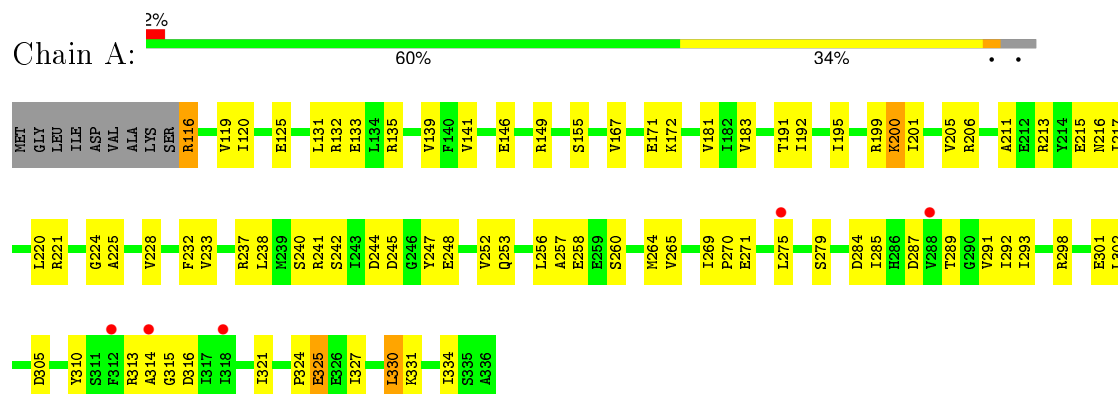
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	s	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	T	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			
1	t	221	Total	C	N	O	S	0	0	0
			1719	1069	305	338	7			

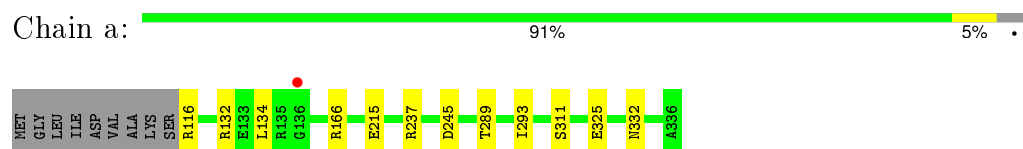
3 Residue-property plots

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.

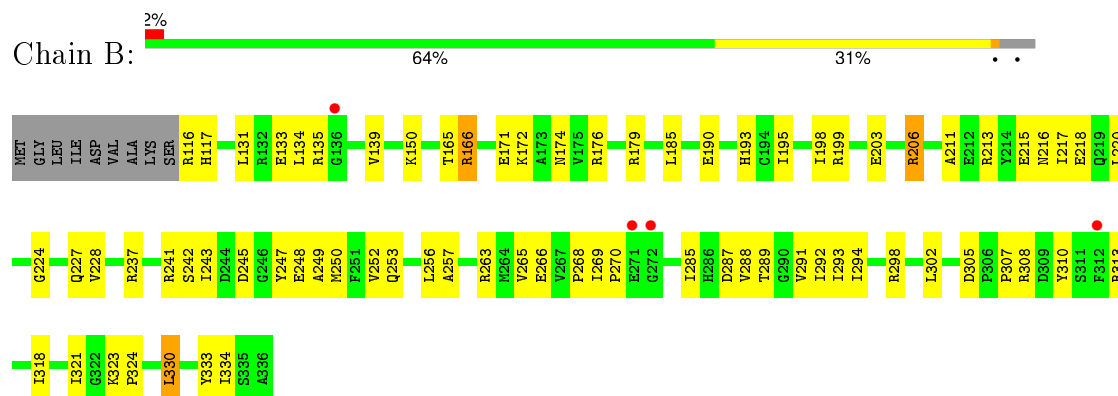
- Molecule 1: Calcium-gated potassium channel MthK



- Molecule 1: Calcium-gated potassium channel MthK

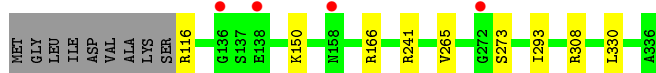


- Molecule 1: Calcium-gated potassium channel MthK

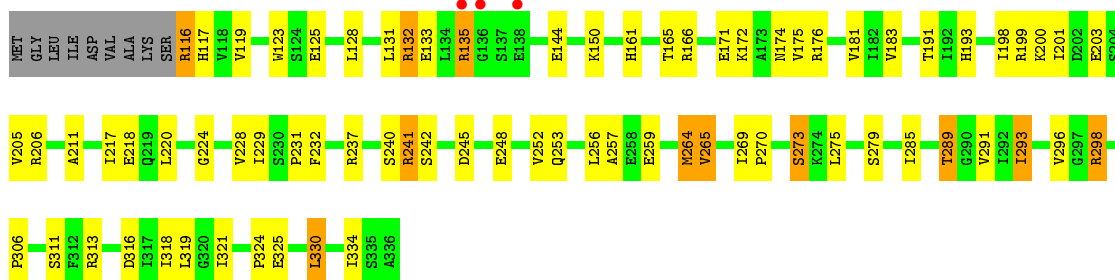


- Molecule 1: Calcium-gated potassium channel MthK

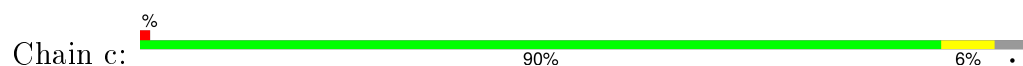




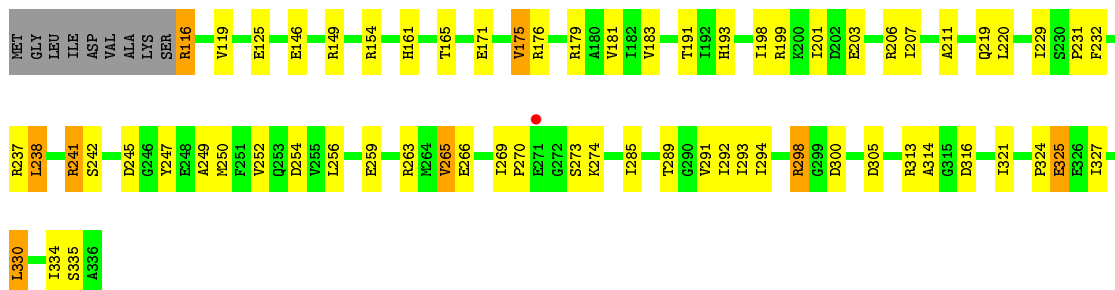
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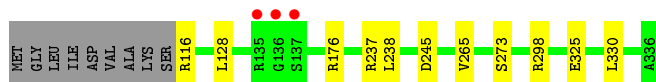
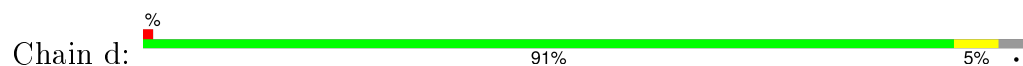
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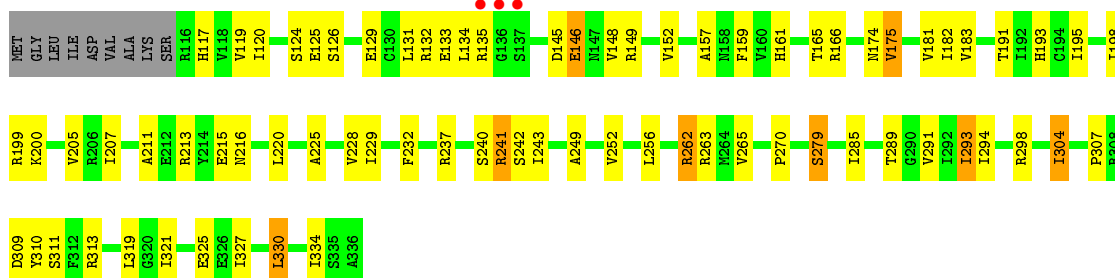


- Molecule 1: Calcium-gated potassium channel MthK





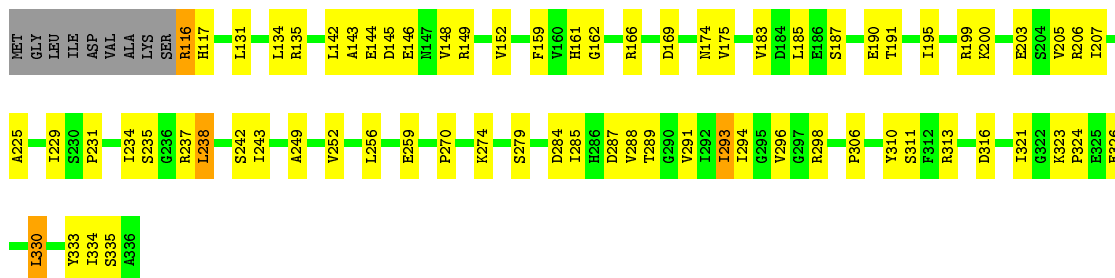
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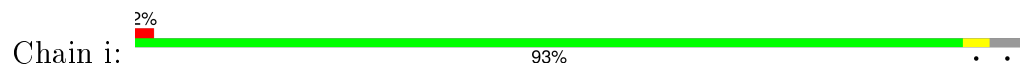
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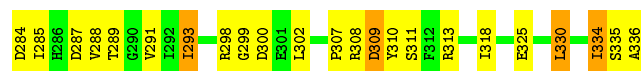


- Molecule 1: Calcium-gated potassium channel MthK

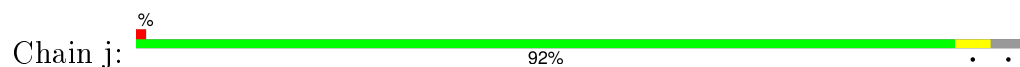


- Molecule 1: Calcium-gated potassium channel MthK





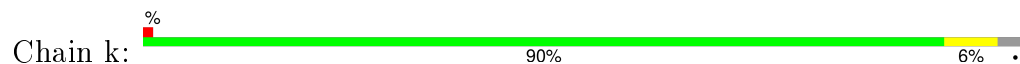
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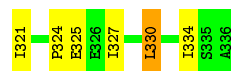
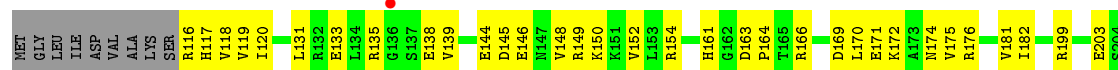
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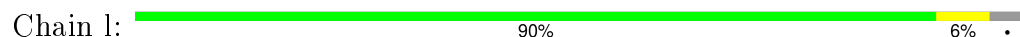
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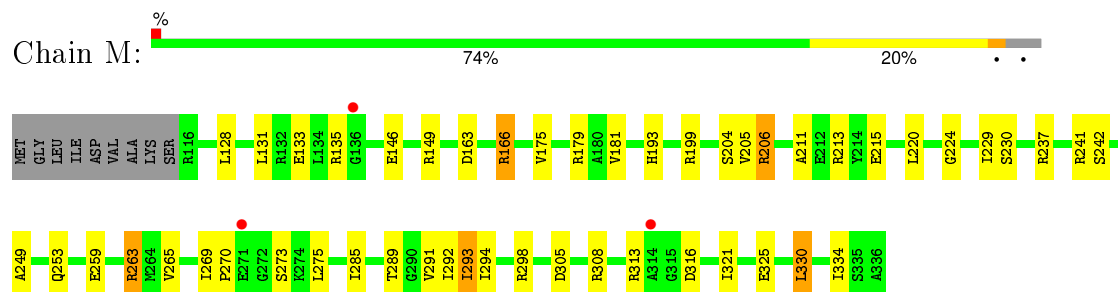
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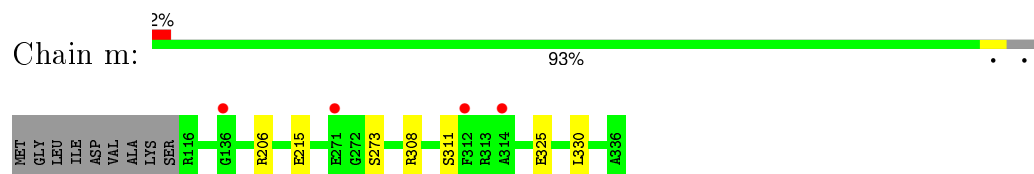
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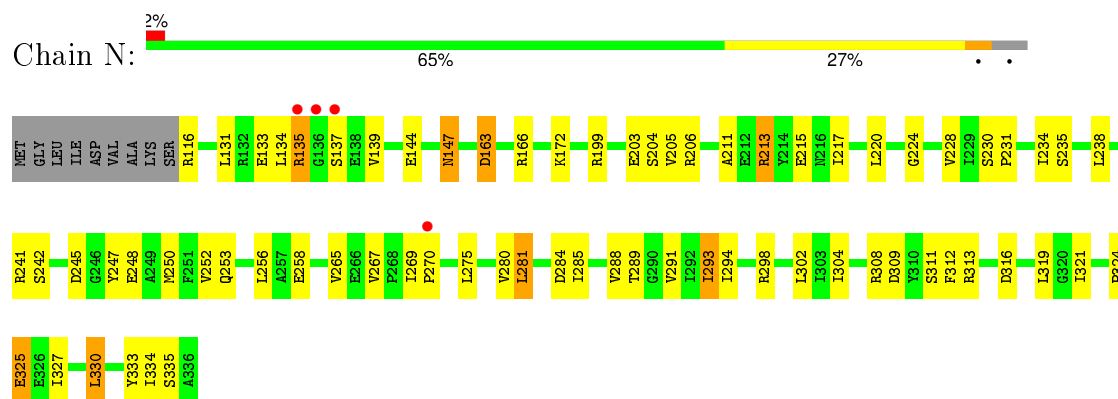
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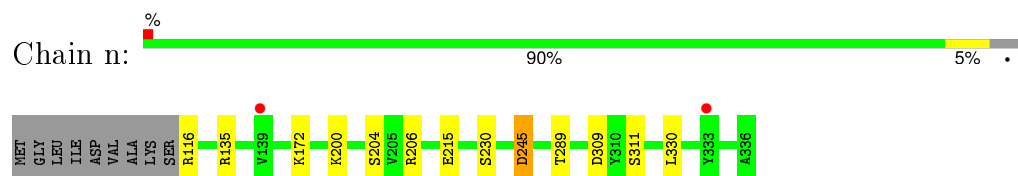
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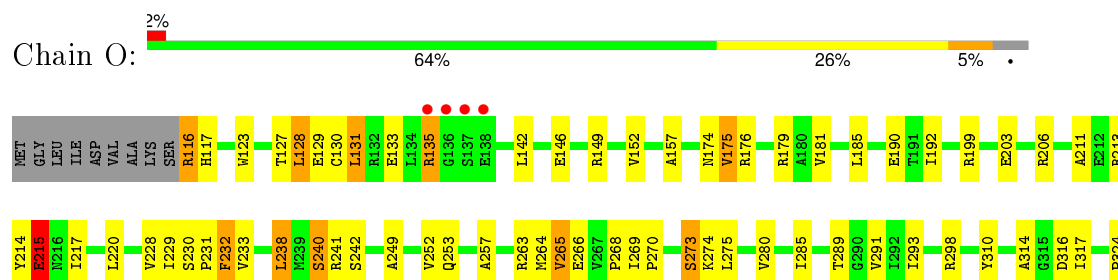
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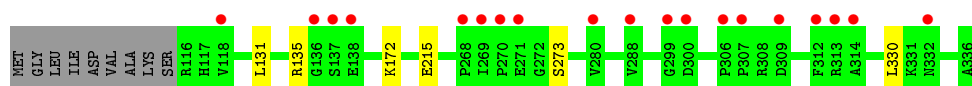
- Molecule 1: Calcium-gated potassium channel MthK



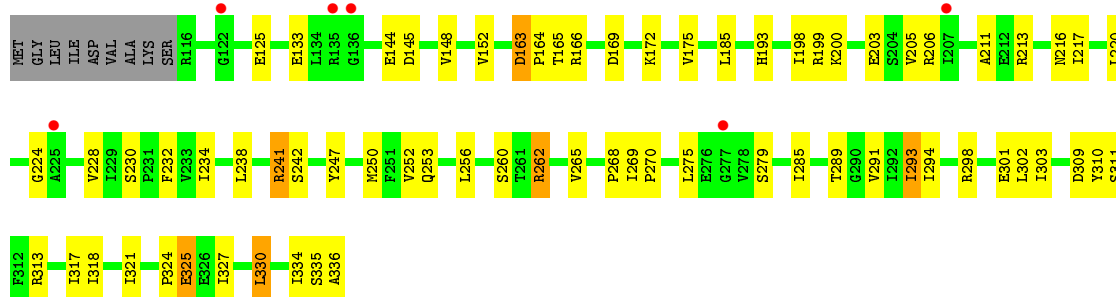
- Molecule 1: Calcium-gated potassium channel MthK



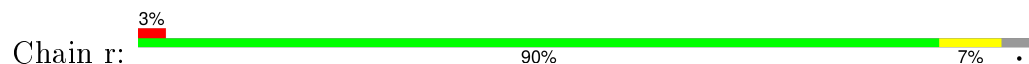




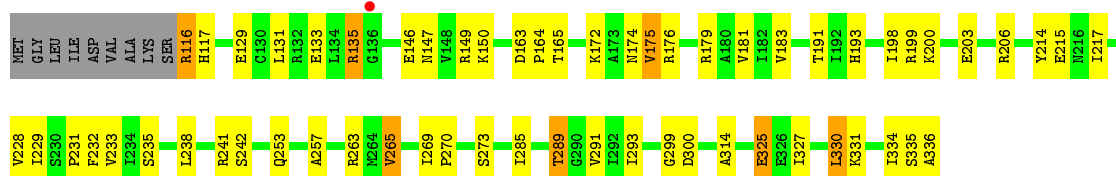
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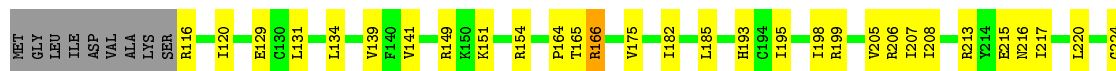
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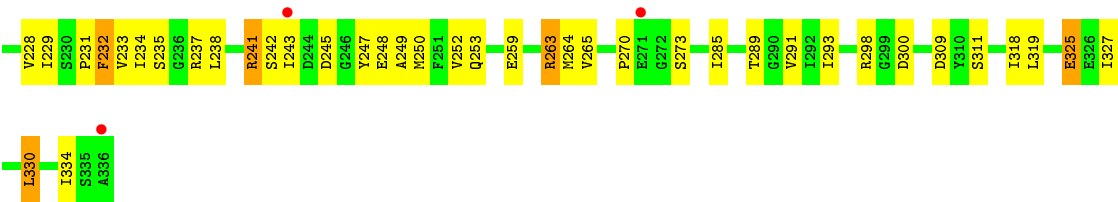


- Molecule 1: Calcium-gated potassium channel MthK

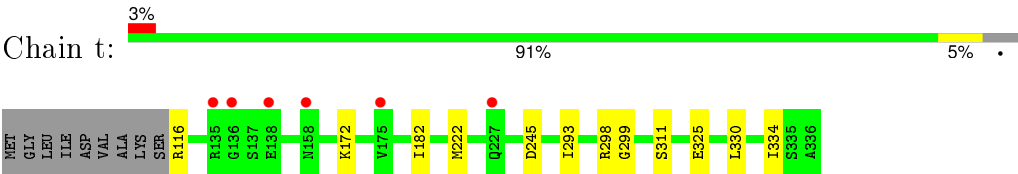


- Molecule 1: Calcium-gated potassium channel MthK





● Molecule 1: Calcium-gated potassium channel MthK



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	166.34Å 231.68Å 197.98Å 90.00° 94.58° 90.00°	Depositor
Resolution (Å)	49.26 – 3.18 49.21 – 3.18	Depositor EDS
% Data completeness (in resolution range)	92.2 (49.26-3.18) 92.2 (49.21-3.18)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.263 , 0.301 0.263 , 0.301	Depositor DCC
R_{free} test set	2303 reflections (1.01%)	DCC
Wilson B-factor (Å ²)	68.2	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	4 of 229682 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	68748	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.89 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.4248e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 ⓘ

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 >5	RMSZ	# Z >5
1	A	0.39	0/1740	0.61	0/2347
1	B	0.39	1/1740 (0.1%)	0.57	1/2347 (0.0%)
1	C	0.38	0/1740	0.60	0/2347
1	D	0.39	0/1740	0.60	0/2347
1	E	0.40	0/1740	0.61	0/2347
1	F	0.39	0/1740	0.59	0/2347
1	G	0.41	0/1740	0.60	1/2347 (0.0%)
1	H	0.39	0/1740	0.59	0/2347
1	I	0.35	0/1740	0.57	0/2347
1	J	0.38	0/1740	0.61	0/2347
1	K	0.37	0/1740	0.59	0/2347
1	L	0.43	0/1740	0.61	1/2347 (0.0%)
1	M	0.36	0/1740	0.56	0/2347
1	N	0.38	0/1734	0.59	0/2340
1	O	0.43	0/1740	0.63	1/2347 (0.0%)
1	P	0.35	0/1740	0.58	0/2347
1	Q	0.36	1/1740 (0.1%)	0.55	0/2347
1	R	0.38	0/1740	0.59	0/2347
1	S	0.37	0/1740	0.57	0/2347
1	T	0.37	0/1740	0.59	0/2347
1	a	0.40	0/1740	0.62	0/2347
1	b	0.36	0/1740	0.56	0/2347
1	c	0.39	0/1740	0.60	1/2347 (0.0%)
1	d	0.41	0/1740	0.64	0/2347
1	e	0.39	0/1740	0.60	0/2347
1	f	0.41	0/1740	0.61	0/2347
1	g	0.46	0/1740	0.64	1/2347 (0.0%)
1	h	0.37	0/1740	0.57	0/2347
1	i	0.39	0/1740	0.60	0/2347
1	j	0.40	0/1740	0.57	1/2347 (0.0%)
1	k	0.40	0/1740	0.63	0/2347
1	l	0.39	0/1740	0.60	0/2347
1	m	0.37	0/1740	0.57	0/2347
1	n	0.38	0/1740	0.63	1/2347 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	o	0.41	0/1740	0.61	0/2347
1	p	0.36	0/1740	0.57	0/2347
1	q	0.35	0/1740	0.54	0/2347
1	r	0.36	0/1734	0.58	0/2340
1	s	0.38	0/1740	0.59	0/2347
1	t	0.35	0/1740	0.56	0/2347
All	All	0.39	2/69588 (0.0%)	0.59	8/93866 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	266	GLU	CD-OE1	-5.19	1.20	1.25
1	Q	171	GLU	CD-OE1	-5.08	1.20	1.25

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	266	GLU	OE1-CD-OE2	-5.75	116.41	123.30
1	n	245	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	266	GLU	OE1-CD-OE2	-5.55	116.64	123.30
1	j	276	GLU	OE1-CD-OE2	-5.48	116.72	123.30
1	g	328	GLU	OE1-CD-OE2	-5.39	116.83	123.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1719	0	1726	81	0
1	B	1719	0	1726	46	0
1	C	1719	0	1726	76	0
1	D	1719	0	1726	64	0
1	E	1719	0	1726	73	0
1	F	1719	0	1726	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1719	0	1726	56	0
1	H	1719	0	1726	69	0
1	I	1719	0	1726	47	0
1	J	1719	0	1726	75	0
1	K	1719	0	1726	48	0
1	L	1719	0	1726	56	0
1	M	1719	0	1726	45	0
1	N	1713	0	1715	64	0
1	O	1719	0	1726	65	0
1	P	1719	0	1726	50	0
1	Q	1719	0	1726	52	0
1	R	1719	0	1726	59	0
1	S	1719	0	1726	53	0
1	T	1719	0	1726	47	0
1	a	1719	0	1726	0	0
1	b	1719	0	1726	0	0
1	c	1719	0	1726	0	0
1	d	1719	0	1726	0	0
1	e	1719	0	1726	0	0
1	f	1719	0	1726	0	0
1	g	1719	0	1726	0	0
1	h	1719	0	1726	0	0
1	i	1719	0	1726	0	0
1	j	1719	0	1726	0	0
1	k	1719	0	1726	0	0
1	l	1719	0	1726	0	0
1	m	1719	0	1726	0	0
1	n	1719	0	1726	0	0
1	o	1719	0	1726	0	0
1	p	1719	0	1726	0	0
1	q	1719	0	1726	0	0
1	r	1713	0	1715	0	0
1	s	1719	0	1726	0	0
1	t	1719	0	1726	0	0
All	All	68748	0	69018	1117	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 8.

The worst 5 of 1117 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:I:324:PRO:HB2	1:S:325:GLU:HG2	36.68	1.12
1:M:298:ARG:HH22	1:M:313:ARG:HB2	1.94	1.12
1:A:116:ARG:HG2	1:A:116:ARG:HH21	2.96	1.08
1:O:116:ARG:HG3	1:O:116:ARG:HH21	1.51	1.07
1:J:298:ARG:HH22	1:J:313:ARG:HB2	1.15	1.06

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	219/230 (95%)	209 (95%)	9 (4%)	1 (0%)	34	77
1	B	219/230 (95%)	209 (95%)	10 (5%)	0	100	100
1	C	219/230 (95%)	210 (96%)	8 (4%)	1 (0%)	34	77
1	D	219/230 (95%)	209 (95%)	10 (5%)	0	100	100
1	E	219/230 (95%)	208 (95%)	11 (5%)	0	100	100
1	F	219/230 (95%)	209 (95%)	10 (5%)	0	100	100
1	G	219/230 (95%)	206 (94%)	13 (6%)	0	100	100
1	H	219/230 (95%)	209 (95%)	9 (4%)	1 (0%)	34	77
1	I	219/230 (95%)	212 (97%)	7 (3%)	0	100	100
1	J	219/230 (95%)	208 (95%)	9 (4%)	2 (1%)	21	66
1	K	219/230 (95%)	210 (96%)	8 (4%)	1 (0%)	34	77
1	L	219/230 (95%)	208 (95%)	11 (5%)	0	100	100
1	M	219/230 (95%)	205 (94%)	14 (6%)	0	100	100
1	N	219/230 (95%)	208 (95%)	10 (5%)	1 (0%)	34	77
1	O	219/230 (95%)	209 (95%)	9 (4%)	1 (0%)	34	77
1	P	219/230 (95%)	212 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	219/230 (95%)	211 (96%)	8 (4%)	0	100	100
1	R	219/230 (95%)	205 (94%)	14 (6%)	0	100	100
1	S	219/230 (95%)	206 (94%)	12 (6%)	1 (0%)	34	77
1	T	219/230 (95%)	211 (96%)	8 (4%)	0	100	100
1	a	219/230 (95%)	211 (96%)	8 (4%)	0	100	100
1	b	219/230 (95%)	210 (96%)	9 (4%)	0	100	100
1	c	219/230 (95%)	207 (94%)	12 (6%)	0	100	100
1	d	219/230 (95%)	207 (94%)	12 (6%)	0	100	100
1	e	219/230 (95%)	207 (94%)	12 (6%)	0	100	100
1	f	219/230 (95%)	205 (94%)	13 (6%)	1 (0%)	34	77
1	g	219/230 (95%)	209 (95%)	9 (4%)	1 (0%)	34	77
1	h	219/230 (95%)	210 (96%)	9 (4%)	0	100	100
1	i	219/230 (95%)	210 (96%)	9 (4%)	0	100	100
1	j	219/230 (95%)	206 (94%)	12 (6%)	1 (0%)	34	77
1	k	219/230 (95%)	208 (95%)	10 (5%)	1 (0%)	34	77
1	l	219/230 (95%)	205 (94%)	14 (6%)	0	100	100
1	m	219/230 (95%)	209 (95%)	10 (5%)	0	100	100
1	n	219/230 (95%)	209 (95%)	10 (5%)	0	100	100
1	o	219/230 (95%)	208 (95%)	10 (5%)	1 (0%)	34	77
1	p	219/230 (95%)	208 (95%)	11 (5%)	0	100	100
1	q	219/230 (95%)	210 (96%)	9 (4%)	0	100	100
1	r	219/230 (95%)	207 (94%)	12 (6%)	0	100	100
1	s	219/230 (95%)	208 (95%)	10 (5%)	1 (0%)	34	77
1	t	219/230 (95%)	209 (95%)	9 (4%)	1 (0%)	34	77
All	All	8760/9200 (95%)	8337 (95%)	407 (5%)	16 (0%)	52	88

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	k	135	ARG
1	o	135	ARG
1	s	135	ARG
1	O	215	GLU
1	A	244	ASP

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	189/196 (96%)	178 (94%)	11 (6%)	25	65
1	B	189/196 (96%)	181 (96%)	8 (4%)	36	75
1	C	189/196 (96%)	173 (92%)	16 (8%)	13	46
1	D	189/196 (96%)	179 (95%)	10 (5%)	28	68
1	E	189/196 (96%)	170 (90%)	19 (10%)	9	35
1	F	189/196 (96%)	174 (92%)	15 (8%)	15	51
1	G	189/196 (96%)	177 (94%)	12 (6%)	22	62
1	H	189/196 (96%)	176 (93%)	13 (7%)	19	58
1	I	189/196 (96%)	182 (96%)	7 (4%)	41	78
1	J	189/196 (96%)	171 (90%)	18 (10%)	11	38
1	K	189/196 (96%)	176 (93%)	13 (7%)	19	58
1	L	189/196 (96%)	177 (94%)	12 (6%)	22	62
1	M	189/196 (96%)	179 (95%)	10 (5%)	28	68
1	N	188/196 (96%)	174 (93%)	14 (7%)	17	55
1	O	189/196 (96%)	173 (92%)	16 (8%)	13	46
1	P	189/196 (96%)	181 (96%)	8 (4%)	36	75
1	Q	189/196 (96%)	178 (94%)	11 (6%)	25	65
1	R	189/196 (96%)	179 (95%)	10 (5%)	28	68
1	S	189/196 (96%)	177 (94%)	12 (6%)	22	62
1	T	189/196 (96%)	175 (93%)	14 (7%)	17	55
1	a	189/196 (96%)	177 (94%)	12 (6%)	22	62
1	b	189/196 (96%)	180 (95%)	9 (5%)	31	72
1	c	189/196 (96%)	176 (93%)	13 (7%)	19	58
1	d	189/196 (96%)	178 (94%)	11 (6%)	25	65
1	e	189/196 (96%)	177 (94%)	12 (6%)	22	62
1	f	189/196 (96%)	178 (94%)	11 (6%)	25	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	g	189/196 (96%)	178 (94%)	11 (6%)	25	65
1	h	189/196 (96%)	178 (94%)	11 (6%)	25	65
1	i	189/196 (96%)	181 (96%)	8 (4%)	36	75
1	j	189/196 (96%)	180 (95%)	9 (5%)	31	72
1	k	189/196 (96%)	177 (94%)	12 (6%)	22	62
1	l	189/196 (96%)	175 (93%)	14 (7%)	17	55
1	m	189/196 (96%)	182 (96%)	7 (4%)	41	78
1	n	189/196 (96%)	176 (93%)	13 (7%)	19	58
1	o	189/196 (96%)	173 (92%)	16 (8%)	13	46
1	p	189/196 (96%)	175 (93%)	14 (7%)	17	55
1	q	189/196 (96%)	183 (97%)	6 (3%)	46	81
1	r	188/196 (96%)	173 (92%)	15 (8%)	15	51
1	s	189/196 (96%)	176 (93%)	13 (7%)	19	58
1	t	189/196 (96%)	178 (94%)	11 (6%)	25	65
All	All	7558/7840 (96%)	7081 (94%)	477 (6%)	22	62

5 of 477 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	241	ARG
1	L	241	ARG
1	s	133	GLU
1	J	309	ASP
1	K	245	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	147	ASN
1	j	253	GLN
1	r	147	ASN
1	I	286	HIS
1	J	216	ASN

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.

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	221/230 (96%)	-0.01	5 (2%) 64 49	36, 70, 112, 146	0
1	B	221/230 (96%)	-0.02	4 (1%) 71 58	53, 90, 142, 153	0
1	C	221/230 (96%)	-0.09	3 (1%) 78 65	49, 71, 105, 156	0
1	D	221/230 (96%)	-0.19	1 (0%) 91 87	36, 61, 89, 111	0
1	E	221/230 (96%)	0.01	3 (1%) 78 65	38, 68, 110, 128	0
1	F	221/230 (96%)	-0.12	1 (0%) 91 87	34, 61, 93, 125	0
1	G	221/230 (96%)	0.02	3 (1%) 78 65	42, 76, 120, 151	0
1	H	221/230 (96%)	-0.06	3 (1%) 78 65	48, 79, 114, 152	0
1	I	221/230 (96%)	-0.05	0 100 100	44, 76, 122, 144	0
1	J	221/230 (96%)	0.06	1 (0%) 91 87	51, 79, 118, 138	0
1	K	221/230 (96%)	-0.03	3 (1%) 78 65	43, 71, 113, 133	0
1	L	221/230 (96%)	-0.18	1 (0%) 91 87	33, 62, 90, 121	0
1	M	221/230 (96%)	0.04	3 (1%) 78 65	63, 92, 126, 149	0
1	N	221/230 (96%)	0.06	4 (1%) 71 58	53, 76, 113, 138	0
1	O	221/230 (96%)	-0.12	4 (1%) 71 58	39, 59, 89, 133	0
1	P	221/230 (96%)	0.02	6 (2%) 58 43	46, 81, 130, 161	0
1	Q	221/230 (96%)	0.53	22 (9%) 9 5	78, 115, 147, 161	0
1	R	221/230 (96%)	0.24	6 (2%) 58 43	64, 87, 118, 146	0
1	S	221/230 (96%)	-0.16	1 (0%) 91 87	45, 65, 98, 137	0
1	T	221/230 (96%)	-0.03	3 (1%) 78 65	50, 87, 133, 172	0
1	a	221/230 (96%)	-0.05	1 (0%) 91 87	47, 70, 106, 138	0
1	b	221/230 (96%)	0.08	4 (1%) 71 58	56, 92, 127, 147	0
1	c	221/230 (96%)	-0.07	2 (0%) 85 78	36, 72, 114, 130	0
1	d	221/230 (96%)	-0.14	3 (1%) 78 65	33, 57, 85, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	e	221/230 (96%)	-0.04	3 (1%) 78 65	38, 71, 118, 139	0
1	f	221/230 (96%)	-0.24	1 (0%) 91 87	35, 59, 90, 114	0
1	g	221/230 (96%)	0.07	8 (3%) 46 30	47, 71, 102, 138	0
1	h	221/230 (96%)	0.08	8 (3%) 46 30	48, 84, 115, 145	0
1	i	221/230 (96%)	-0.04	4 (1%) 71 58	50, 76, 114, 140	0
1	j	221/230 (96%)	0.03	3 (1%) 78 65	48, 85, 118, 147	0
1	k	221/230 (96%)	-0.11	3 (1%) 78 65	39, 72, 118, 148	0
1	l	221/230 (96%)	-0.16	0 100 100	37, 61, 89, 113	0
1	m	221/230 (96%)	0.21	4 (1%) 71 58	63, 99, 129, 150	0
1	n	221/230 (96%)	-0.05	2 (0%) 85 78	42, 77, 120, 136	0
1	o	221/230 (96%)	-0.21	0 100 100	40, 58, 84, 105	0
1	p	221/230 (96%)	0.07	3 (1%) 78 65	57, 84, 114, 144	0
1	q	221/230 (96%)	0.51	19 (8%) 13 7	71, 117, 152, 170	0
1	r	221/230 (96%)	0.14	7 (3%) 51 36	51, 82, 120, 149	0
1	s	221/230 (96%)	-0.20	1 (0%) 91 87	46, 62, 92, 109	0
1	t	221/230 (96%)	0.18	6 (2%) 58 43	62, 88, 119, 138	0
All	All	8840/9200 (96%)	-0.00	159 (1%) 71 58	33, 76, 124, 172	0

The worst 5 of 159 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	136	GLY	5.8
1	r	336	ALA	5.3
1	g	312	PHE	4.8
1	r	158	ASN	4.7
1	H	136	GLY	4.4

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 ⓘ

There are no carbohydrates 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.