wwPDB X-ray Structure Validation Summary Report (i)

Feb 15, 2024 – 06:03 PM EST

PDB ID	:	3RBX
Title	:	MthK RCK domain D184N mutant, Ca2+-bound
Authors	:	Samakai, E.; Rothberg, B.S.
Deposited on	:	2011-03-30
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

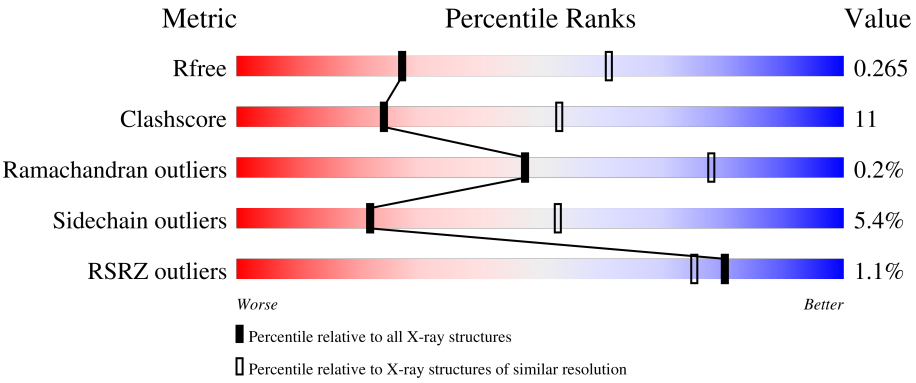
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	234	71% 21% • 6%
1	B	234	70% 21% • 6%
1	C	234	5% 73% 20% • 6%
1	D	234	70% 22% • 6%
1	E	234	% 69% 24% • 6%

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Mol	Chain	Length	Quality of chain
1	F	234	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10055 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
			1689	1055	297	330	7			
1	B	221	Total	C	N	O	S	0	0	0
			1689	1053	301	328	7			
1	C	220	Total	C	N	O	S	0	0	0
			1653	1034	288	324	7			
1	D	219	Total	C	N	O	S	0	0	0
			1672	1044	296	325	7			
1	E	220	Total	C	N	O	S	0	0	0
			1678	1049	293	329	7			
1	F	219	Total	C	N	O	S	0	0	0
			1662	1039	293	323	7			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	ASN	ASP	engineered mutation	UNP O27564
A	337	LEU	-	expression tag	UNP O27564
A	338	VAL	-	expression tag	UNP O27564
A	339	PRO	-	expression tag	UNP O27564
A	340	ARG	-	expression tag	UNP O27564
B	184	ASN	ASP	engineered mutation	UNP O27564
B	337	LEU	-	expression tag	UNP O27564
B	338	VAL	-	expression tag	UNP O27564
B	339	PRO	-	expression tag	UNP O27564
B	340	ARG	-	expression tag	UNP O27564
C	184	ASN	ASP	engineered mutation	UNP O27564
C	337	LEU	-	expression tag	UNP O27564
C	338	VAL	-	expression tag	UNP O27564
C	339	PRO	-	expression tag	UNP O27564
C	340	ARG	-	expression tag	UNP O27564
D	184	ASN	ASP	engineered mutation	UNP O27564
D	337	LEU	-	expression tag	UNP O27564

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Chain	Residue	Modelled	Actual	Comment	Reference
D	338	VAL	-	expression tag	UNP O27564
D	339	PRO	-	expression tag	UNP O27564
D	340	ARG	-	expression tag	UNP O27564
E	184	ASN	ASP	engineered mutation	UNP O27564
E	337	LEU	-	expression tag	UNP O27564
E	338	VAL	-	expression tag	UNP O27564
E	339	PRO	-	expression tag	UNP O27564
E	340	ARG	-	expression tag	UNP O27564
F	184	ASN	ASP	engineered mutation	UNP O27564
F	337	LEU	-	expression tag	UNP O27564
F	338	VAL	-	expression tag	UNP O27564
F	339	PRO	-	expression tag	UNP O27564
F	340	ARG	-	expression tag	UNP O27564

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

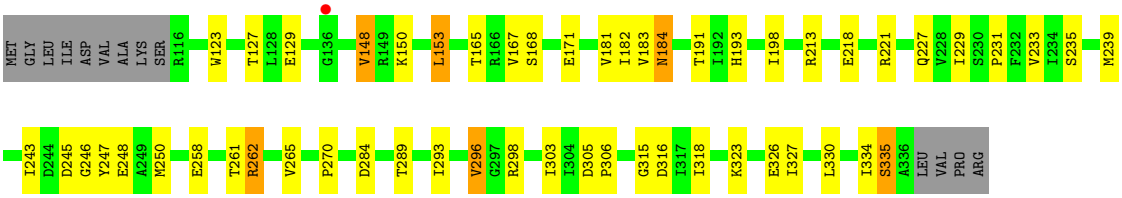
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0
2	B	2	Total Ca 2 2	0	0
2	C	4	Total Ca 4 4	0	0
2	E	2	Total Ca 2 2	0	0
2	F	2	Total Ca 2 2	0	0

3 Residue-property plots (i)

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.

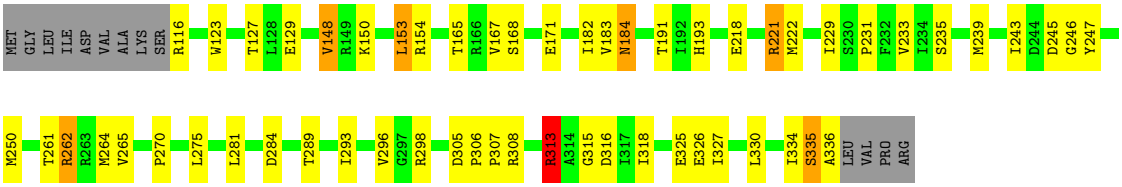
• Molecule 1: Calcium-gated potassium channel mthK

Chain A:



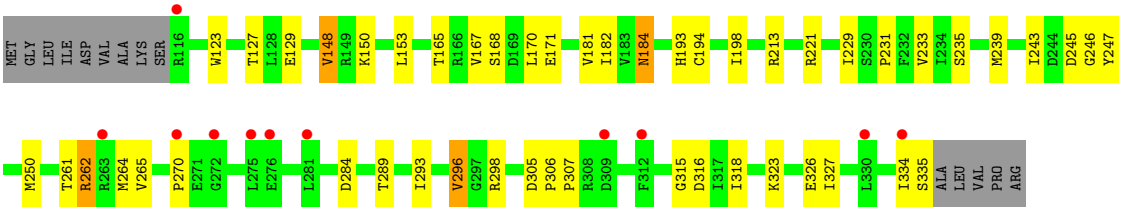
• Molecule 1: Calcium-gated potassium channel mthK

Chain B:



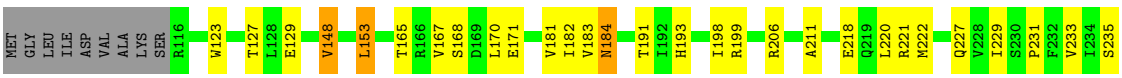
• Molecule 1: Calcium-gated potassium channel mthK

Chain C:



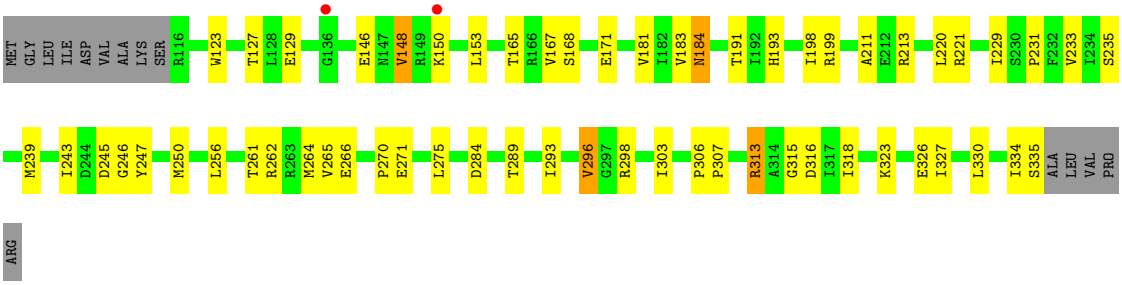
• Molecule 1: Calcium-gated potassium channel mthK

Chain D:



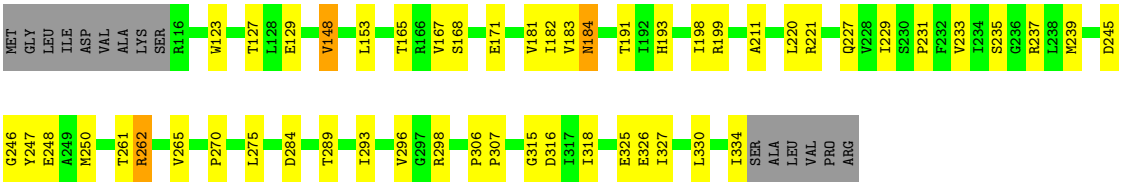
• Molecule 1: Calcium-gated potassium channel mthK

Chain E:



• Molecule 1: Calcium-gated potassium channel mthK

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	119.12Å 119.12Å 351.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.49 – 2.80 49.49 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.49-2.80) 99.4 (49.49-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.240 , 0.274 0.234 , 0.265	Depositor DCC
R_{free} test set	1855 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	55.9	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10055	wwPDB-VP
Average B, all atoms (Å^2)	55.0	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 50.98 % 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 5.9904e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.45	0/1710	0.57	0/2312
1	B	0.46	0/1710	0.61	1/2313 (0.0%)
1	C	0.41	0/1674	0.54	0/2267
1	D	0.42	0/1693	0.56	0/2291
1	E	0.43	0/1699	0.57	0/2298
1	F	0.39	0/1683	0.54	0/2279
All	All	0.43	0/10169	0.56	1/13760 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	313	ARG	NE-CZ-NH1	5.15	122.88	120.30

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	1689	0	1685	47	0
1	B	1689	0	1681	50	0
1	C	1653	0	1621	41	0
1	D	1672	0	1660	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1678	0	1669	45	0
1	F	1662	0	1645	36	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	4	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
All	All	10055	0	9961	221	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 11.

The worst 5 of 221 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:E:298:ARG:HD3	1:E:313:ARG:HH21	1.27	0.98
1:C:239:MET:HG3	1:D:229:ILE:HD12	1.46	0.96
1:B:313:ARG:HG3	1:B:313:ARG:HH11	1.39	0.85
1:A:239:MET:HG3	1:B:229:ILE:HD12	1.59	0.85
1:E:229:ILE:HD12	1:F:239:MET:HG3	1.58	0.84

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	219/234 (94%)	209 (95%)	9 (4%)	1 (0%)	29 61
1	B	219/234 (94%)	209 (95%)	9 (4%)	1 (0%)	29 61
1	C	218/234 (93%)	209 (96%)	9 (4%)	0	100 100
1	D	217/234 (93%)	209 (96%)	8 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	218/234 (93%)	209 (96%)	9 (4%)	0	100	100
1	F	217/234 (93%)	210 (97%)	7 (3%)	0	100	100
All	All	1308/1404 (93%)	1255 (96%)	51 (4%)	2 (0%)	47	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	SER
1	B	335	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/200 (92%)	173 (94%)	10 (6%)	21	52
1	B	182/200 (91%)	173 (95%)	9 (5%)	25	57
1	C	175/200 (88%)	165 (94%)	10 (6%)	20	50
1	D	180/200 (90%)	172 (96%)	8 (4%)	28	61
1	E	182/200 (91%)	170 (93%)	12 (7%)	16	44
1	F	178/200 (89%)	169 (95%)	9 (5%)	24	55
All	All	1080/1200 (90%)	1022 (95%)	58 (5%)	22	53

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	296	VAL
1	F	284	ASP
1	D	284	ASP
1	F	262	ARG
1	F	148	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 12 ligands modelled in this entry, 12 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	221/234 (94%)	-0.24	1 (0%) 91 88	22, 45, 85, 126	0
1	B	221/234 (94%)	-0.39	0 100 100	23, 41, 74, 123	0
1	C	220/234 (94%)	0.09	11 (5%) 28 19	24, 56, 127, 178	0
1	D	219/234 (93%)	-0.20	0 100 100	25, 50, 90, 135	0
1	E	220/234 (94%)	-0.19	2 (0%) 84 80	22, 47, 92, 152	0
1	F	219/234 (93%)	-0.06	0 100 100	29, 58, 100, 133	0
All	All	1320/1404 (94%)	-0.17	14 (1%) 80 75	22, 49, 100, 178	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	330	LEU	6.1
1	C	275	LEU	5.8
1	C	312	PHE	3.6
1	C	270	PRO	3.1
1	C	309	ASP	3.0

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 monosaccharides in this entry.

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. The B-factors column lists the minimum, median, 95^{th} 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
2	CA	C	341	1/1	0.46	0.14	108,108,108,108	0
2	CA	A	600	1/1	0.69	0.07	59,59,59,59	0
2	CA	C	601	1/1	0.72	0.11	75,75,75,75	0
2	CA	F	600	1/1	0.76	0.15	82,82,82,82	0
2	CA	E	600	1/1	0.83	0.13	71,71,71,71	0
2	CA	E	601	1/1	0.85	0.09	57,57,57,57	0
2	CA	C	342	1/1	0.88	0.07	65,65,65,65	0
2	CA	B	600	1/1	0.90	0.11	76,76,76,76	0
2	CA	C	600	1/1	0.92	0.08	69,69,69,69	0
2	CA	A	601	1/1	0.95	0.09	31,31,31,31	0
2	CA	B	601	1/1	0.96	0.10	43,43,43,43	0
2	CA	F	601	1/1	0.97	0.16	56,56,56,56	0

6.5 Other polymers

There are no such residues in this entry.