



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:18 PM GMT

PDB ID : 4L76
Title : Ca²⁺-bound E212Q mutant MthK RCK domain
Authors : Smith, F.J.; Rothberg, B.S.
Deposited on : 2013-06-13
Resolution : 2.99 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

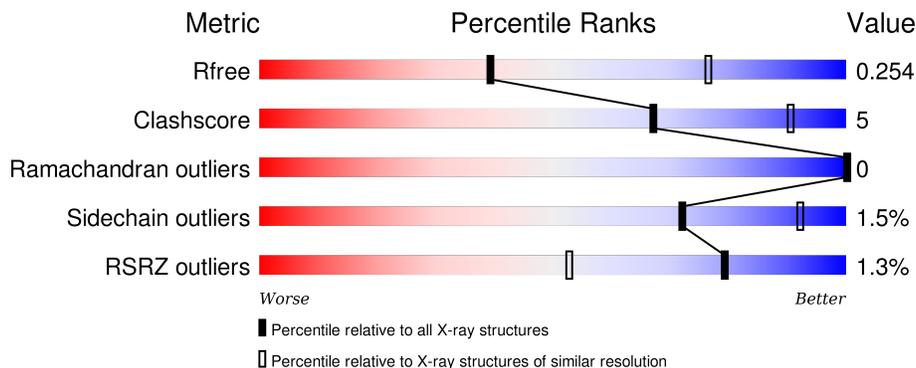
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	242	
1	B	242	
1	C	242	
1	D	242	
1	E	242	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	242	 <p>%</p> <p>76% 16% 8%</p>

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
2	CA	D	404	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10218 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
			Total	C	N	O	S			
1	A	227	Total 1712	C 1072	N 299	O 334	S 7	0	0	0
1	B	224	Total 1715	C 1068	N 308	O 332	S 7	0	0	0
1	C	221	Total 1693	C 1057	N 297	O 332	S 7	0	0	0
1	D	222	Total 1684	C 1051	N 305	O 321	S 7	0	0	0
1	E	223	Total 1705	C 1064	N 302	O 332	S 7	0	0	0
1	F	223	Total 1693	C 1056	N 300	O 330	S 7	0	0	0

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	212	GLN	GLU	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
A	341	GLY	-	EXPRESSION TAG	UNP O27564
A	342	SER	-	EXPRESSION TAG	UNP O27564
A	343	HIS	-	EXPRESSION TAG	UNP O27564
A	344	HIS	-	EXPRESSION TAG	UNP O27564
A	345	HIS	-	EXPRESSION TAG	UNP O27564
A	346	HIS	-	EXPRESSION TAG	UNP O27564
A	347	HIS	-	EXPRESSION TAG	UNP O27564
A	348	HIS	-	EXPRESSION TAG	UNP O27564
B	212	GLN	GLU	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	340	ARG	-	EXPRESSION TAG	UNP O27564
B	341	GLY	-	EXPRESSION TAG	UNP O27564
B	342	SER	-	EXPRESSION TAG	UNP O27564
B	343	HIS	-	EXPRESSION TAG	UNP O27564
B	344	HIS	-	EXPRESSION TAG	UNP O27564
B	345	HIS	-	EXPRESSION TAG	UNP O27564
B	346	HIS	-	EXPRESSION TAG	UNP O27564
B	347	HIS	-	EXPRESSION TAG	UNP O27564
B	348	HIS	-	EXPRESSION TAG	UNP O27564
C	212	GLN	GLU	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
C	341	GLY	-	EXPRESSION TAG	UNP O27564
C	342	SER	-	EXPRESSION TAG	UNP O27564
C	343	HIS	-	EXPRESSION TAG	UNP O27564
C	344	HIS	-	EXPRESSION TAG	UNP O27564
C	345	HIS	-	EXPRESSION TAG	UNP O27564
C	346	HIS	-	EXPRESSION TAG	UNP O27564
C	347	HIS	-	EXPRESSION TAG	UNP O27564
C	348	HIS	-	EXPRESSION TAG	UNP O27564
D	212	GLN	GLU	ENGINEERED MUTATION	UNP O27564
D	337	LEU	-	EXPRESSION TAG	UNP O27564
D	338	VAL	-	EXPRESSION TAG	UNP O27564
D	339	PRO	-	EXPRESSION TAG	UNP O27564
D	340	ARG	-	EXPRESSION TAG	UNP O27564
D	341	GLY	-	EXPRESSION TAG	UNP O27564
D	342	SER	-	EXPRESSION TAG	UNP O27564
D	343	HIS	-	EXPRESSION TAG	UNP O27564
D	344	HIS	-	EXPRESSION TAG	UNP O27564
D	345	HIS	-	EXPRESSION TAG	UNP O27564
D	346	HIS	-	EXPRESSION TAG	UNP O27564
D	347	HIS	-	EXPRESSION TAG	UNP O27564
D	348	HIS	-	EXPRESSION TAG	UNP O27564
E	212	GLN	GLU	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
E	341	GLY	-	EXPRESSION TAG	UNP O27564
E	342	SER	-	EXPRESSION TAG	UNP O27564

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	343	HIS	-	EXPRESSION TAG	UNP O27564
E	344	HIS	-	EXPRESSION TAG	UNP O27564
E	345	HIS	-	EXPRESSION TAG	UNP O27564
E	346	HIS	-	EXPRESSION TAG	UNP O27564
E	347	HIS	-	EXPRESSION TAG	UNP O27564
E	348	HIS	-	EXPRESSION TAG	UNP O27564
F	212	GLN	GLU	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
F	341	GLY	-	EXPRESSION TAG	UNP O27564
F	342	SER	-	EXPRESSION TAG	UNP O27564
F	343	HIS	-	EXPRESSION TAG	UNP O27564
F	344	HIS	-	EXPRESSION TAG	UNP O27564
F	345	HIS	-	EXPRESSION TAG	UNP O27564
F	346	HIS	-	EXPRESSION TAG	UNP O27564
F	347	HIS	-	EXPRESSION TAG	UNP O27564
F	348	HIS	-	EXPRESSION TAG	UNP O27564

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	3	Total Ca 3 3	0	0
2	E	3	Total Ca 3 3	0	0
2	B	2	Total Ca 2 2	0	0
2	C	2	Total Ca 2 2	0	0
2	A	2	Total Ca 2 2	0	0
2	F	1	Total Ca 1 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0

Continued on next page...

Continued from previous page...

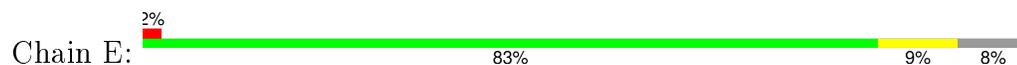
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Na 1 1	0	0

- Molecule 4 is water.

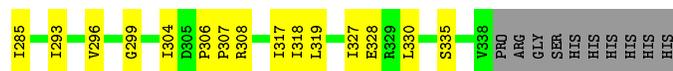
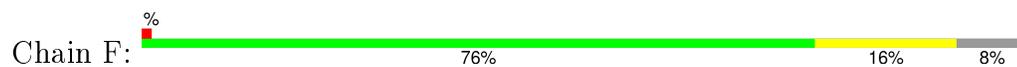
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total O 1 1	0	0



- 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 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	118.88Å 118.88Å 356.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.56 – 2.99 44.56 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.8 (44.56-2.99) 90.3 (44.56-2.99)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.01Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.217 , 0.263 0.211 , 0.254	Depositor DCC
R_{free} test set	1805 reflections (6.45%)	DCC
Wilson B-factor (Å ²)	78.8	Xtrriage
Anisotropy	0.336	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.7	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Outliers	5 of 30788 reflections (0.016%)	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10218	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.73 % 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 3.0302e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 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	0.36	0/1734	0.55	0/2350
1	B	0.39	0/1736	0.53	0/2346
1	C	0.32	0/1714	0.49	0/2317
1	D	0.34	0/1705	0.50	0/2307
1	E	0.33	0/1726	0.51	0/2333
1	F	0.37	0/1714	0.55	0/2320
All	All	0.35	0/10329	0.52	0/13973

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	1712	0	1695	18	0
1	B	1715	0	1712	17	0
1	C	1693	0	1689	21	0
1	D	1684	0	1678	28	0
1	E	1705	0	1700	14	0
1	F	1693	0	1674	24	0
2	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	D	1	0	0	1	0
All	All	10218	0	10148	97	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 5.

The worst 5 of 97 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:116:ARG:HG3	1:E:179:ARG:HD2	1.70	0.73
1:F:281:LEU:HB2	1:F:308:ARG:HB2	1.76	0.67
1:D:213:ARG:NH2	1:D:215:GLU:OE1	2.28	0.67
1:F:285:ILE:HG21	1:F:293:ILE:HD11	1.77	0.66
1:A:285:ILE:HG21	1:A:293:ILE:HD11	1.79	0.64

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	225/242 (93%)	221 (98%)	4 (2%)	0	100 100
1	B	222/242 (92%)	219 (99%)	3 (1%)	0	100 100
1	C	219/242 (90%)	216 (99%)	3 (1%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	220/242 (91%)	217 (99%)	3 (1%)	0	100	100
1	E	221/242 (91%)	217 (98%)	4 (2%)	0	100	100
1	F	221/242 (91%)	219 (99%)	2 (1%)	0	100	100
All	All	1328/1452 (92%)	1309 (99%)	19 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	183/207 (88%)	182 (100%)	1 (0%)	92	98
1	B	185/207 (89%)	184 (100%)	1 (0%)	92	98
1	C	184/207 (89%)	179 (97%)	5 (3%)	52	85
1	D	179/207 (86%)	177 (99%)	2 (1%)	80	94
1	E	184/207 (89%)	181 (98%)	3 (2%)	70	92
1	F	181/207 (87%)	177 (98%)	4 (2%)	60	88
All	All	1096/1242 (88%)	1080 (98%)	16 (2%)	72	92

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	296	VAL
1	D	328	GLU
1	F	146	GLU
1	C	334	ILE
1	F	261	THR

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

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](#)

Of 15 ligands modelled in this entry, 15 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	227/242 (93%)	0.03	4 (1%) 71 43	70, 95, 125, 150	0
1	B	224/242 (92%)	0.00	1 (0%) 93 80	69, 92, 118, 164	0
1	C	221/242 (91%)	0.16	4 (1%) 71 43	81, 112, 154, 184	0
1	D	222/242 (91%)	0.03	1 (0%) 91 76	78, 101, 134, 160	0
1	E	223/242 (92%)	0.16	4 (1%) 71 43	81, 112, 151, 162	0
1	F	223/242 (92%)	0.03	3 (1%) 79 53	72, 97, 125, 148	0
All	All	1340/1452 (92%)	0.07	17 (1%) 79 53	69, 101, 140, 184	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	115	SER	3.9
1	C	136	GLY	3.5
1	E	136	GLY	3.2
1	C	312	PHE	3.0
1	A	113	ALA	2.7

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 carbohydrates 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. 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
2	CA	D	404	1/1	0.74	0.42	2.49	171,171,171,171	0
3	NA	B	403	1/1	0.67	0.22	0.65	71,71,71,71	0
3	NA	D	403	1/1	0.65	0.17	0.56	88,88,88,88	0
2	CA	B	401	1/1	0.57	0.25	0.10	140,140,140,140	0
2	CA	C	401	1/1	0.54	0.24	0.06	152,152,152,152	0
2	CA	A	401	1/1	0.33	0.20	0.00	135,135,135,135	0
2	CA	E	403	1/1	0.89	0.20	-0.33	175,175,175,175	0
2	CA	F	401	1/1	0.47	0.17	-0.47	124,124,124,124	0
2	CA	E	402	1/1	0.96	0.15	-0.48	112,112,112,112	0
2	CA	A	402	1/1	0.94	0.09	-1.95	84,84,84,84	0
2	CA	D	402	1/1	0.90	0.12	-1.97	113,113,113,113	0
2	CA	B	402	1/1	0.85	0.09	-1.98	97,97,97,97	0
2	CA	C	402	1/1	0.92	0.06	-1.99	138,138,138,138	0
2	CA	D	401	1/1	0.81	0.14	-2.23	126,126,126,126	0
2	CA	E	401	1/1	0.90	0.05	-2.34	136,136,136,136	0

6.5 Other polymers [i](#)

There are no such residues in this entry.