



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:50 AM GMT

PDB ID : 2OGU
Title : Crystal structure of the isolated MthK RCK domain
Authors : Kuo, M.M.C.; Baker, K.A.; Wong, L.; Choe, S.
Deposited on : 2007-01-08
Resolution : 3.23 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

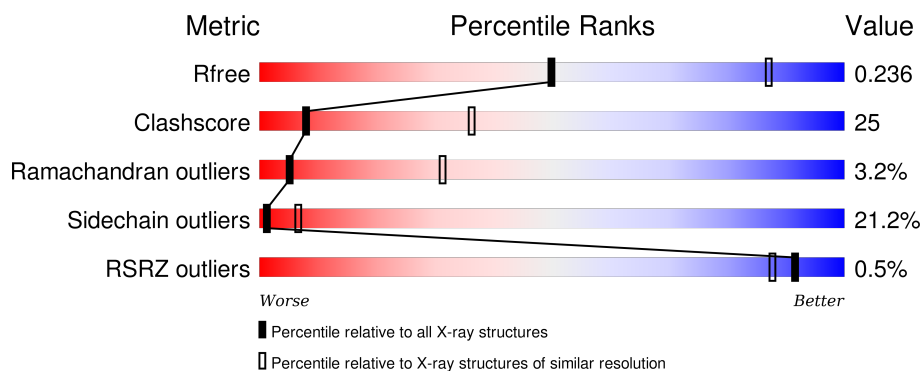
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.23 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	1092 (3.28-3.20)
Clashscore	102246	1227 (3.28-3.20)
Ramachandran outliers	100387	1204 (3.28-3.20)
Sidechain outliers	100360	1203 (3.28-3.20)
RSRZ outliers	91569	1097 (3.28-3.20)

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	233	 <div>45% 39% 9% • 5%</div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1719 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	5	0	0
			1719	1069	305	338	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	GLY	-	CLONING ARTIFACT	UNP O27564
A	105	SER	-	CLONING ARTIFACT	UNP O27564
A	106	GLY	-	CLONING ARTIFACT	UNP O27564

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	165.89Å 165.89Å 82.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.23 28.61 – 3.23	Depositor EDS
% Data completeness (in resolution range)	95.3 (30.00-3.23) 95.2 (28.61-3.23)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.77 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.232 , 0.299 0.232 , 0.236	Depositor DCC
R_{free} test set	319 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	110.5	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 103.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 6717 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1719	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.74	4/1740 (0.2%)	0.80	3/2347 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	325	GLU	CD-OE1	14.67	1.41	1.25
1	A	325	GLU	CD-OE2	10.18	1.36	1.25
1	A	328	GLU	CD-OE2	8.04	1.34	1.25
1	A	328	GLU	CD-OE1	7.92	1.34	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	ARG	CB-CG-CD	15.02	150.65	111.60
1	A	213	ARG	CG-CD-NE	10.74	134.35	111.80
1	A	265	VAL	CB-CA-C	-5.17	101.59	111.40

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	85	0
All	All	1719	0	1726	85	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 25.

All (85) 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:A:202:ASP:HB3	1:A:205:VAL:HG23	1.41	1.02
1:A:294:ILE:O	1:A:294:ILE:HG12	1.63	0.95
1:A:330:LEU:HD22	1:A:334:ILE:HD11	1.50	0.92
1:A:202:ASP:HB3	1:A:205:VAL:CG2	2.09	0.83
1:A:281:LEU:HB2	1:A:308:ARG:HB2	1.62	0.80
1:A:252:VAL:HA	1:A:256:LEU:HD13	1.64	0.79
1:A:307:PRO:HB2	1:A:309:ASP:OD1	1.82	0.79
1:A:285:ILE:O	1:A:289:THR:HG22	1.85	0.77
1:A:119:VAL:HG22	1:A:140:PHE:HB2	1.68	0.74
1:A:255:VAL:HB	1:A:256:LEU:HD12	1.71	0.72
1:A:261:THR:HG23	1:A:323:LYS:NZ	2.07	0.69
1:A:294:ILE:HD12	1:A:321:ILE:CG2	2.23	0.68
1:A:202:ASP:CB	1:A:205:VAL:HG23	2.23	0.67
1:A:153:LEU:C	1:A:155:SER:H	1.99	0.66
1:A:261:THR:HG23	1:A:323:LYS:HZ2	1.62	0.65
1:A:248:GLU:O	1:A:252:VAL:HG23	1.97	0.65
1:A:298:ARG:HH12	1:A:313:ARG:HG3	1.61	0.65
1:A:228:VAL:O	1:A:229:ILE:HD12	1.97	0.65
1:A:202:ASP:C	1:A:204:SER:H	2.01	0.64
1:A:275:LEU:HD12	1:A:334:ILE:HG23	1.78	0.64
1:A:202:ASP:CB	1:A:205:VAL:CG2	2.77	0.62
1:A:252:VAL:O	1:A:256:LEU:HB2	1.99	0.61
1:A:208:ILE:HG23	1:A:227:GLN:HB3	1.83	0.61
1:A:253:GLN:O	1:A:257:ALA:HB3	2.01	0.60
1:A:217:ILE:HG23	1:A:228:VAL:HG21	1.84	0.59
1:A:294:ILE:HD12	1:A:321:ILE:HG23	1.85	0.58
1:A:294:ILE:O	1:A:294:ILE:CG1	2.43	0.57
1:A:196:LEU:HD23	1:A:199:ARG:HH21	1.70	0.56
1:A:302:LEU:HG	1:A:304:ILE:HG13	1.86	0.56
1:A:283:ALA:HB1	1:A:285:ILE:CD1	2.35	0.56
1:A:283:ALA:HB1	1:A:285:ILE:HD12	1.87	0.56
1:A:269:ILE:HG12	1:A:334:ILE:HG21	1.88	0.56
1:A:294:ILE:HD11	1:A:319:LEU:CD2	2.37	0.55
1:A:119:VAL:HB	1:A:181:VAL:HG22	1.89	0.55
1:A:298:ARG:HH22	1:A:313:ARG:CG	2.19	0.55
1:A:153:LEU:O	1:A:155:SER:N	2.41	0.54
1:A:140:PHE:CD2	1:A:158:ASN:HB2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ASN:HB3	1:A:220:LEU:HD12	1.91	0.53
1:A:187:SER:HB3	1:A:190:GLU:HG3	1.91	0.53
1:A:289:THR:HG23	1:A:291:VAL:H	1.74	0.52
1:A:330:LEU:O	1:A:334:ILE:HG13	2.10	0.52
1:A:280:VAL:HB	1:A:308:ARG:HA	1.89	0.52
1:A:253:GLN:HA	1:A:257:ALA:HB3	1.92	0.52
1:A:126:SER:O	1:A:130:CYS:HB2	2.10	0.52
1:A:316:ASP:C	1:A:317:ILE:HD12	2.30	0.51
1:A:323:LYS:O	1:A:326:GLU:HB2	2.09	0.51
1:A:269:ILE:HG22	1:A:314:ALA:HA	1.92	0.51
1:A:298:ARG:HH22	1:A:313:ARG:HG2	1.75	0.50
1:A:150:LYS:HG3	1:A:151:LYS:N	2.25	0.50
1:A:207:ILE:HD13	1:A:224:GLY:O	2.11	0.50
1:A:293:ILE:HD13	1:A:318:ILE:HG23	1.95	0.49
1:A:238:LEU:O	1:A:242:SER:N	2.46	0.49
1:A:153:LEU:C	1:A:155:SER:N	2.66	0.48
1:A:221:ARG:HA	1:A:225:ALA:HB3	1.96	0.48
1:A:229:ILE:CG2	1:A:231:PRO:HD3	2.45	0.47
1:A:237:ARG:O	1:A:238:LEU:C	2.53	0.47
1:A:131:LEU:HD11	1:A:157:ALA:CB	2.44	0.47
1:A:255:VAL:HA	1:A:262:ARG:O	2.15	0.46
1:A:321:ILE:O	1:A:321:ILE:HG13	2.13	0.46
1:A:202:ASP:C	1:A:204:SER:N	2.68	0.46
1:A:130:CYS:O	1:A:134:LEU:HB2	2.16	0.46
1:A:170:LEU:HB3	1:A:175:VAL:HG21	1.99	0.46
1:A:123:TRP:CE3	1:A:148:VAL:HG11	2.52	0.45
1:A:229:ILE:HG23	1:A:231:PRO:HD3	1.99	0.45
1:A:116:ARG:HB3	1:A:179:ARG:CZ	2.47	0.45
1:A:230:SER:HB2	1:A:233:VAL:HG23	1.98	0.45
1:A:195:ILE:O	1:A:198:ILE:HG22	2.17	0.44
1:A:119:VAL:O	1:A:181:VAL:HA	2.18	0.44
1:A:148:VAL:O	1:A:149:ARG:C	2.57	0.44
1:A:117:HIS:N	1:A:179:ARG:HB2	2.33	0.43
1:A:275:LEU:HB2	1:A:334:ILE:HG23	1.99	0.43
1:A:261:THR:CG2	1:A:323:LYS:HZ2	2.29	0.43
1:A:131:LEU:HD11	1:A:157:ALA:HB3	2.02	0.42
1:A:217:ILE:CG2	1:A:228:VAL:HG21	2.47	0.42
1:A:281:LEU:HB2	1:A:308:ARG:CB	2.40	0.42
1:A:269:ILE:HA	1:A:270:PRO:HD3	1.76	0.42
1:A:216:ASN:O	1:A:217:ILE:C	2.57	0.42
1:A:120:ILE:HG12	1:A:182:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ILE:HD12	1:A:321:ILE:HG22	2.00	0.42
1:A:281:LEU:HD13	1:A:308:ARG:HG3	2.02	0.42
1:A:265:VAL:HG21	1:A:327:ILE:HG12	2.02	0.42
1:A:261:THR:CG2	1:A:323:LYS:NZ	2.82	0.41
1:A:217:ILE:O	1:A:220:LEU:HB2	2.21	0.41
1:A:267:VAL:HA	1:A:268:PRO:HD2	1.75	0.40
1:A:198:ILE:CG2	1:A:199:ARG:N	2.85	0.40

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	219/233 (94%)	180 (82%)	32 (15%)	7 (3%)	5 31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	ASP
1	A	154	ARG
1	A	149	ARG
1	A	232	PHE
1	A	132	ARG
1	A	217	ILE
1	A	229	ILE

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	189/197 (96%)	149 (79%)	40 (21%)	1	6

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ARG
1	A	124	SER
1	A	125	GLU
1	A	128	LEU
1	A	131	LEU
1	A	134	LEU
1	A	135	ARG
1	A	145	ASP
1	A	147	ASN
1	A	166	ARG
1	A	167	VAL
1	A	188	ASP
1	A	191	THR
1	A	198	ILE
1	A	199	ARG
1	A	205	VAL
1	A	220	LEU
1	A	222	MET
1	A	229	ILE
1	A	232	PHE
1	A	250	MET
1	A	258	GLU
1	A	261	THR
1	A	265	VAL
1	A	271	GLU
1	A	273	SER
1	A	276	GLU
1	A	285	ILE
1	A	287	ASP
1	A	291	VAL
1	A	293	ILE
1	A	294	ILE
1	A	306	PRO
1	A	308	ARG
1	A	311	SER

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Mol	Chain	Res	Type
1	A	321	ILE
1	A	328	GLU
1	A	330	LEU
1	A	333	TYR
1	A	334	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
1	A	286	HIS
1	A	332	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 [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	221/233 (94%)	-0.23	1 (0%) 91 88	93, 127, 141, 157	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	SER	3.6

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.