wwPDB X-ray Structure Validation Summary Report (i)

Feb 18, 2024 – 09:08 AM EST

PDB ID	:	4EI2
Title	:	Crystal Structures of MthK RCK gating ring bound to Barium
Authors	:	Smith, F.J.; Cingolani, G.; Rothberg, B.S.
Deposited on	:	2012-04-04
Resolution	:	3.11 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:

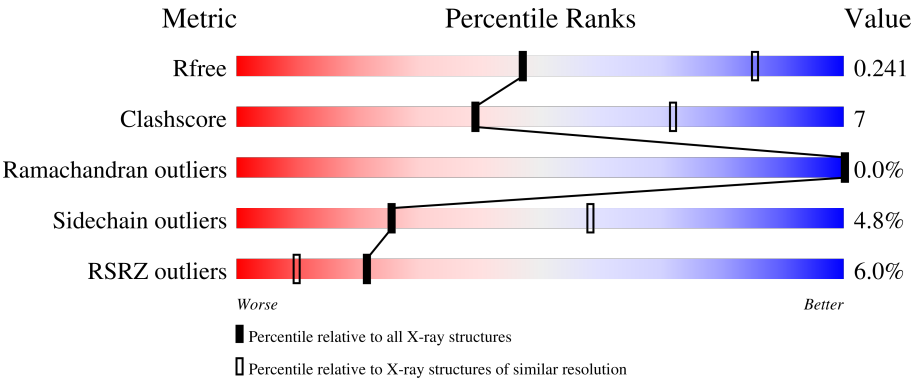
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.11 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	242	2% 76% 15% • 8%
1	B	242	4% 75% 16% • 8%
1	C	242	2% 71% 19% • 7%
1	D	242	2% 77% 15% • 7%
1	E	242	2% 74% 18% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	242	3% 77% 14% • 8%
1	G	242	2% 77% 14% • 7%
1	H	242	4% 67% 24% • 8%
1	I	242	11% 72% 18% • 8%
1	J	242	6% 68% 23% • 7%
1	K	242	6% 72% 19% • 7%
1	L	242	12% 68% 21% • 8%
1	M	242	10% 73% 19% • 7%
1	N	242	9% 69% 20% • 7%
1	O	242	7% 71% 18% • 9%
1	P	242	8% 71% 19% • 9%

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	BA	B	404	-	-	-	X
2	BA	O	403	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 27805 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	223	Total	C	N	O	S	0	0	0
			1732	1078	307	340	7			
1	B	222	Total	C	N	O	S	0	0	0
			1724	1072	306	339	7			
1	C	224	Total	C	N	O	S	0	0	0
			1739	1083	308	341	7			
1	D	225	Total	C	N	O	S	0	0	0
			1746	1088	309	342	7			
1	E	223	Total	C	N	O	S	0	0	0
			1732	1078	307	340	7			
1	F	223	Total	C	N	O	S	0	0	0
			1732	1078	307	340	7			
1	G	225	Total	C	N	O	S	0	0	0
			1746	1088	309	342	7			
1	H	223	Total	C	N	O	S	0	0	0
			1732	1078	307	340	7			
1	I	222	Total	C	N	O	S	0	0	0
			1721	1071	306	337	7			
1	J	224	Total	C	N	O	S	0	0	0
			1739	1083	308	341	7			
1	K	224	Total	C	N	O	S	0	0	0
			1739	1083	308	341	7			
1	L	222	Total	C	N	O	S	0	0	0
			1718	1069	303	339	7			
1	M	224	Total	C	N	O	S	0	0	0
			1739	1083	308	341	7			
1	N	224	Total	C	N	O	S	0	0	0
			1739	1083	308	341	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			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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	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	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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	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
G	337	LEU	-	expression tag	UNP O27564
G	338	VAL	-	expression tag	UNP O27564
G	339	PRO	-	expression tag	UNP O27564
G	340	ARG	-	expression tag	UNP O27564
G	341	GLY	-	expression tag	UNP O27564
G	342	SER	-	expression tag	UNP O27564
G	343	HIS	-	expression tag	UNP O27564
G	344	HIS	-	expression tag	UNP O27564
G	345	HIS	-	expression tag	UNP O27564
G	346	HIS	-	expression tag	UNP O27564
G	347	HIS	-	expression tag	UNP O27564
G	348	HIS	-	expression tag	UNP O27564

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	337	LEU	-	expression tag	UNP O27564
H	338	VAL	-	expression tag	UNP O27564
H	339	PRO	-	expression tag	UNP O27564
H	340	ARG	-	expression tag	UNP O27564
H	341	GLY	-	expression tag	UNP O27564
H	342	SER	-	expression tag	UNP O27564
H	343	HIS	-	expression tag	UNP O27564
H	344	HIS	-	expression tag	UNP O27564
H	345	HIS	-	expression tag	UNP O27564
H	346	HIS	-	expression tag	UNP O27564
H	347	HIS	-	expression tag	UNP O27564
H	348	HIS	-	expression tag	UNP O27564
I	337	LEU	-	expression tag	UNP O27564
I	338	VAL	-	expression tag	UNP O27564
I	339	PRO	-	expression tag	UNP O27564
I	340	ARG	-	expression tag	UNP O27564
I	341	GLY	-	expression tag	UNP O27564
I	342	SER	-	expression tag	UNP O27564
I	343	HIS	-	expression tag	UNP O27564
I	344	HIS	-	expression tag	UNP O27564
I	345	HIS	-	expression tag	UNP O27564
I	346	HIS	-	expression tag	UNP O27564
I	347	HIS	-	expression tag	UNP O27564
I	348	HIS	-	expression tag	UNP O27564
J	337	LEU	-	expression tag	UNP O27564
J	338	VAL	-	expression tag	UNP O27564
J	339	PRO	-	expression tag	UNP O27564
J	340	ARG	-	expression tag	UNP O27564
J	341	GLY	-	expression tag	UNP O27564
J	342	SER	-	expression tag	UNP O27564
J	343	HIS	-	expression tag	UNP O27564
J	344	HIS	-	expression tag	UNP O27564
J	345	HIS	-	expression tag	UNP O27564
J	346	HIS	-	expression tag	UNP O27564
J	347	HIS	-	expression tag	UNP O27564
J	348	HIS	-	expression tag	UNP O27564
K	337	LEU	-	expression tag	UNP O27564
K	338	VAL	-	expression tag	UNP O27564
K	339	PRO	-	expression tag	UNP O27564
K	340	ARG	-	expression tag	UNP O27564
K	341	GLY	-	expression tag	UNP O27564
K	342	SER	-	expression tag	UNP O27564

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	343	HIS	-	expression tag	UNP O27564
K	344	HIS	-	expression tag	UNP O27564
K	345	HIS	-	expression tag	UNP O27564
K	346	HIS	-	expression tag	UNP O27564
K	347	HIS	-	expression tag	UNP O27564
K	348	HIS	-	expression tag	UNP O27564
L	337	LEU	-	expression tag	UNP O27564
L	338	VAL	-	expression tag	UNP O27564
L	339	PRO	-	expression tag	UNP O27564
L	340	ARG	-	expression tag	UNP O27564
L	341	GLY	-	expression tag	UNP O27564
L	342	SER	-	expression tag	UNP O27564
L	343	HIS	-	expression tag	UNP O27564
L	344	HIS	-	expression tag	UNP O27564
L	345	HIS	-	expression tag	UNP O27564
L	346	HIS	-	expression tag	UNP O27564
L	347	HIS	-	expression tag	UNP O27564
L	348	HIS	-	expression tag	UNP O27564
M	337	LEU	-	expression tag	UNP O27564
M	338	VAL	-	expression tag	UNP O27564
M	339	PRO	-	expression tag	UNP O27564
M	340	ARG	-	expression tag	UNP O27564
M	341	GLY	-	expression tag	UNP O27564
M	342	SER	-	expression tag	UNP O27564
M	343	HIS	-	expression tag	UNP O27564
M	344	HIS	-	expression tag	UNP O27564
M	345	HIS	-	expression tag	UNP O27564
M	346	HIS	-	expression tag	UNP O27564
M	347	HIS	-	expression tag	UNP O27564
M	348	HIS	-	expression tag	UNP O27564
N	337	LEU	-	expression tag	UNP O27564
N	338	VAL	-	expression tag	UNP O27564
N	339	PRO	-	expression tag	UNP O27564
N	340	ARG	-	expression tag	UNP O27564
N	341	GLY	-	expression tag	UNP O27564
N	342	SER	-	expression tag	UNP O27564
N	343	HIS	-	expression tag	UNP O27564
N	344	HIS	-	expression tag	UNP O27564
N	345	HIS	-	expression tag	UNP O27564
N	346	HIS	-	expression tag	UNP O27564
N	347	HIS	-	expression tag	UNP O27564
N	348	HIS	-	expression tag	UNP O27564

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
O	337	LEU	-	expression tag	UNP O27564
O	338	VAL	-	expression tag	UNP O27564
O	339	PRO	-	expression tag	UNP O27564
O	340	ARG	-	expression tag	UNP O27564
O	341	GLY	-	expression tag	UNP O27564
O	342	SER	-	expression tag	UNP O27564
O	343	HIS	-	expression tag	UNP O27564
O	344	HIS	-	expression tag	UNP O27564
O	345	HIS	-	expression tag	UNP O27564
O	346	HIS	-	expression tag	UNP O27564
O	347	HIS	-	expression tag	UNP O27564
O	348	HIS	-	expression tag	UNP O27564
P	337	LEU	-	expression tag	UNP O27564
P	338	VAL	-	expression tag	UNP O27564
P	339	PRO	-	expression tag	UNP O27564
P	340	ARG	-	expression tag	UNP O27564
P	341	GLY	-	expression tag	UNP O27564
P	342	SER	-	expression tag	UNP O27564
P	343	HIS	-	expression tag	UNP O27564
P	344	HIS	-	expression tag	UNP O27564
P	345	HIS	-	expression tag	UNP O27564
P	346	HIS	-	expression tag	UNP O27564
P	347	HIS	-	expression tag	UNP O27564
P	348	HIS	-	expression tag	UNP O27564

- Molecule 2 is BARIUM ION (three-letter code: BA) (formula: Ba).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total Ba 5 5	0	0
2	B	4	Total Ba 4 4	0	0
2	C	3	Total Ba 3 3	0	0
2	D	5	Total Ba 5 5	0	0
2	E	6	Total Ba 6 6	0	0
2	F	4	Total Ba 4 4	0	0
2	G	4	Total Ba 4 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	2	Total Ba 2 2	0	0
2	I	3	Total Ba 3 3	0	0
2	J	2	Total Ba 2 2	0	0
2	K	4	Total Ba 4 4	0	0
2	L	2	Total Ba 2 2	0	0
2	M	4	Total Ba 4 4	0	0
2	N	3	Total Ba 3 3	0	0
2	O	3	Total Ba 3 3	0	0
2	P	3	Total Ba 3 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total O 6 6	0	0
3	B	6	Total O 6 6	0	0
3	C	2	Total O 2 2	0	0
3	D	3	Total O 3 3	0	0
3	E	3	Total O 3 3	0	0
3	F	1	Total O 1 1	0	0
3	G	2	Total O 2 2	0	0
3	H	4	Total O 4 4	0	0
3	J	1	Total O 1 1	0	0
3	M	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

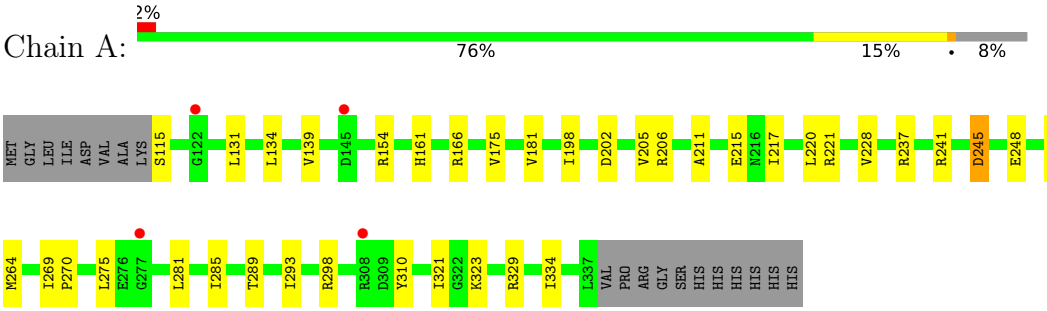
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	2	Total O 2 2	0	0
3	P	1	Total O 1 1	0	0

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.

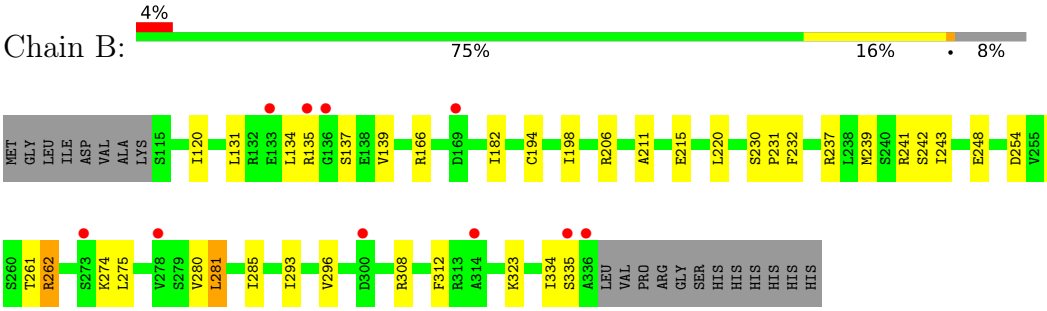
• Molecule 1: Calcium-gated potassium channel mthK

Chain A:



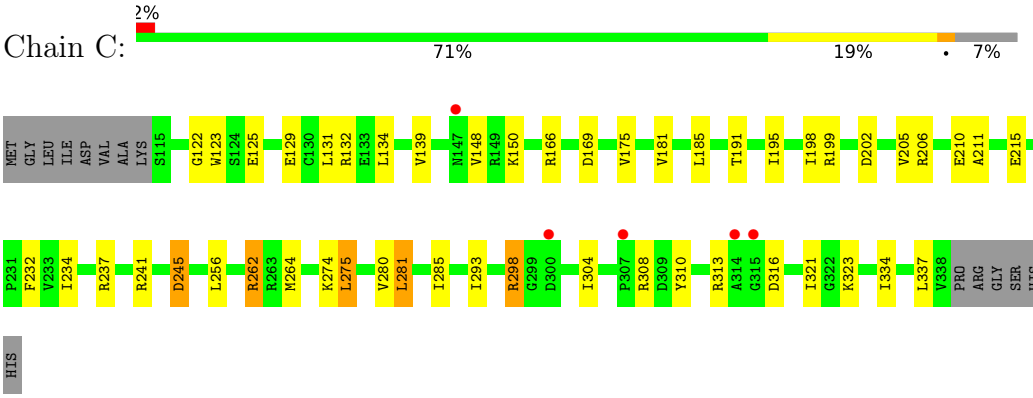
• Molecule 1: Calcium-gated potassium channel mthK

Chain B:



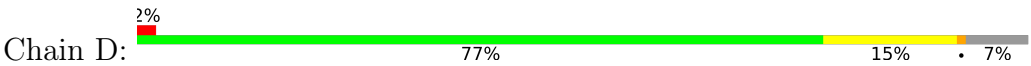
• Molecule 1: Calcium-gated potassium channel mthK

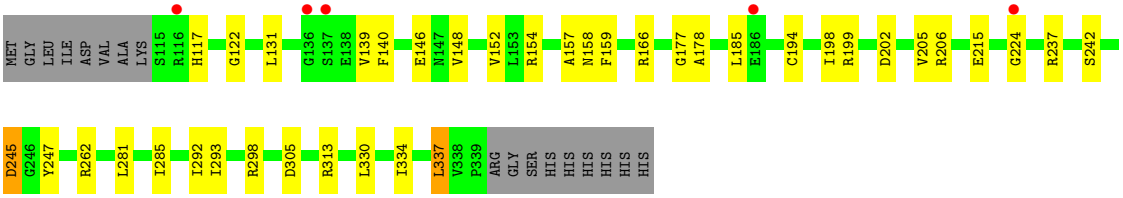
Chain C:



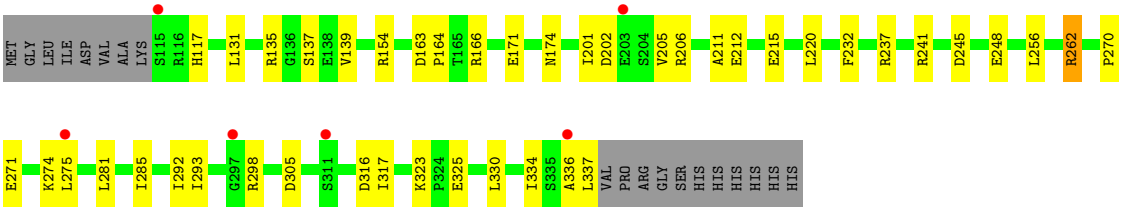
• Molecule 1: Calcium-gated potassium channel mthK

Chain D:

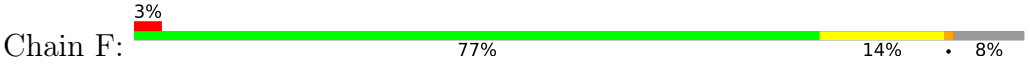


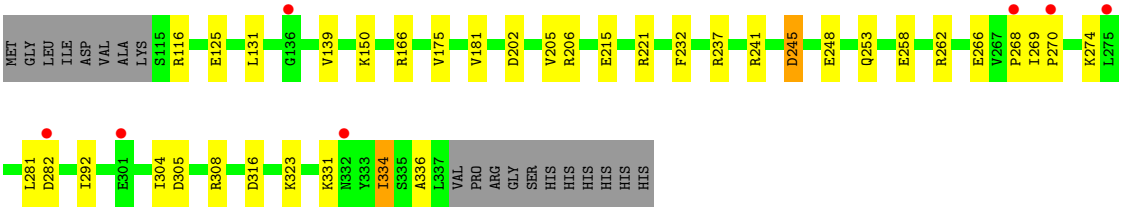


• Molecule 1: Calcium-gated potassium channel mthK

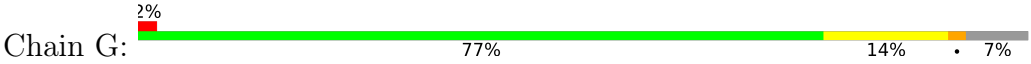


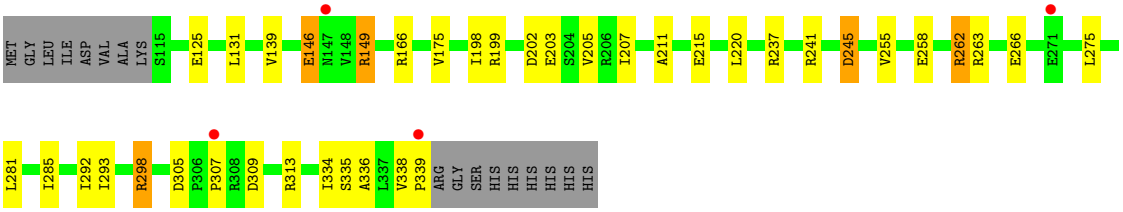
• Molecule 1: Calcium-gated potassium channel mthK



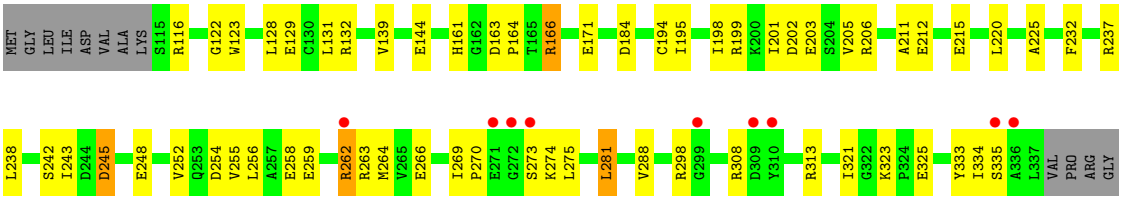


• Molecule 1: Calcium-gated potassium channel mthK



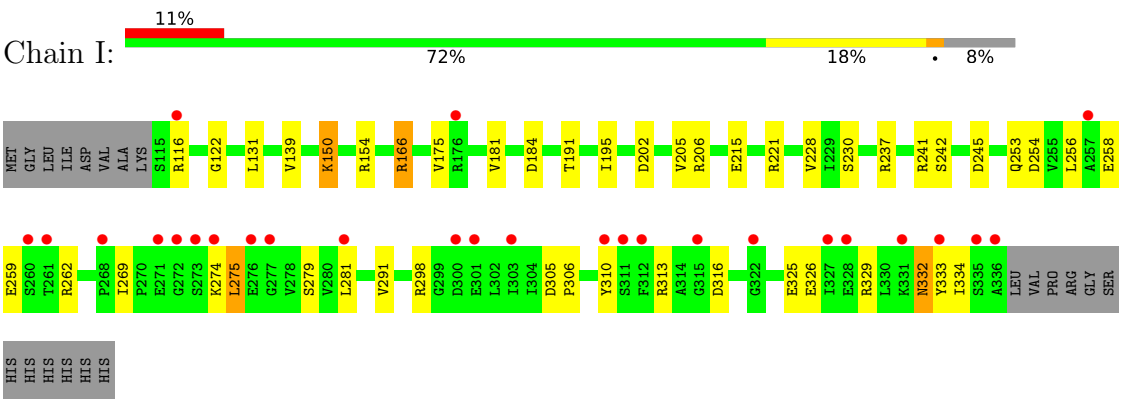


• Molecule 1: Calcium-gated potassium channel mthK



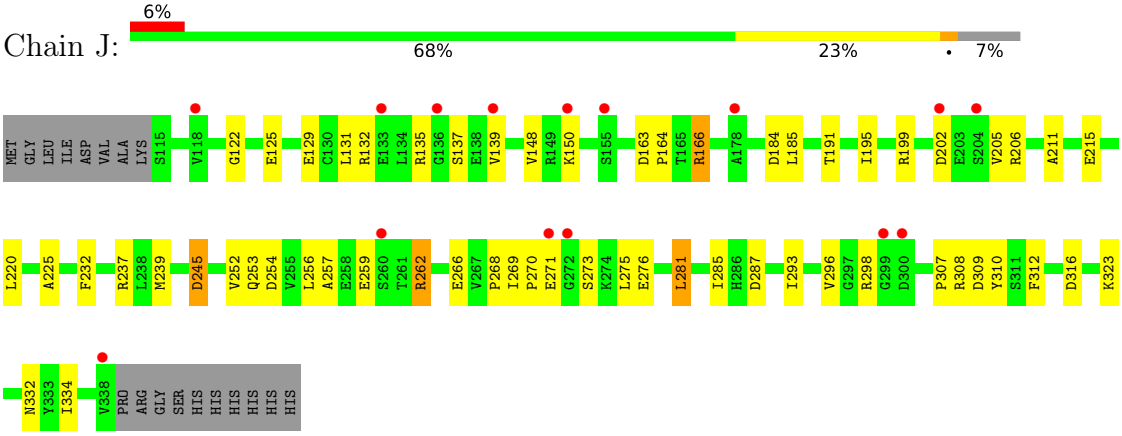
• Molecule 1: Calcium-gated potassium channel mthK

Chain I:



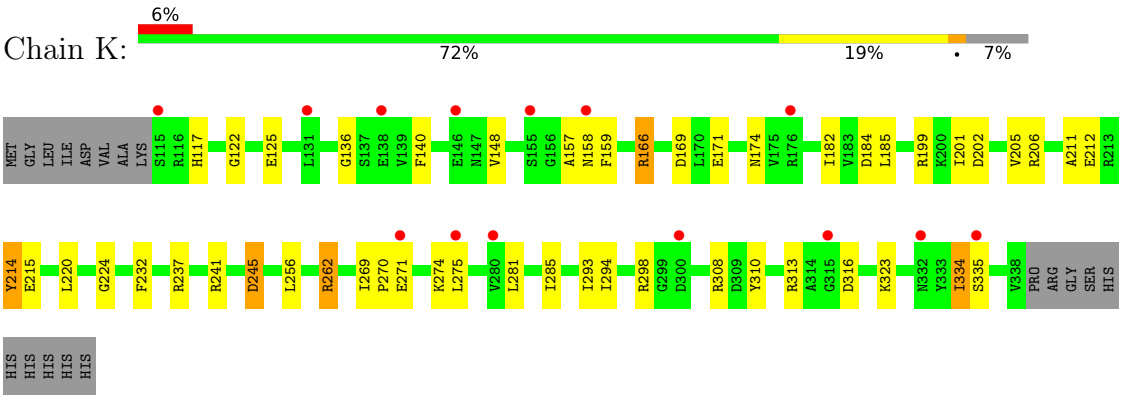
• Molecule 1: Calcium-gated potassium channel mthK

Chain J:



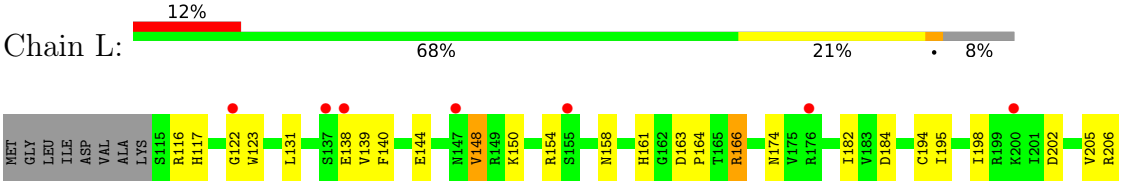
• Molecule 1: Calcium-gated potassium channel mthK

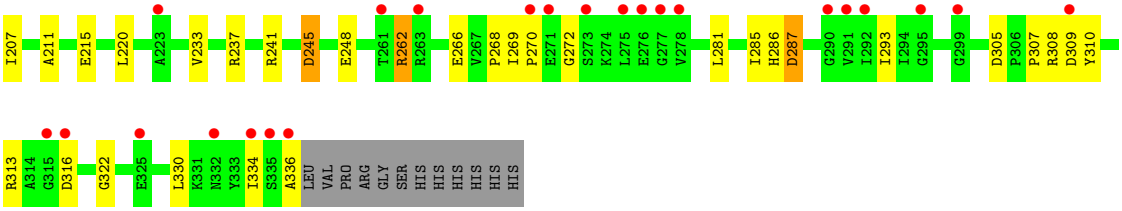
Chain K:



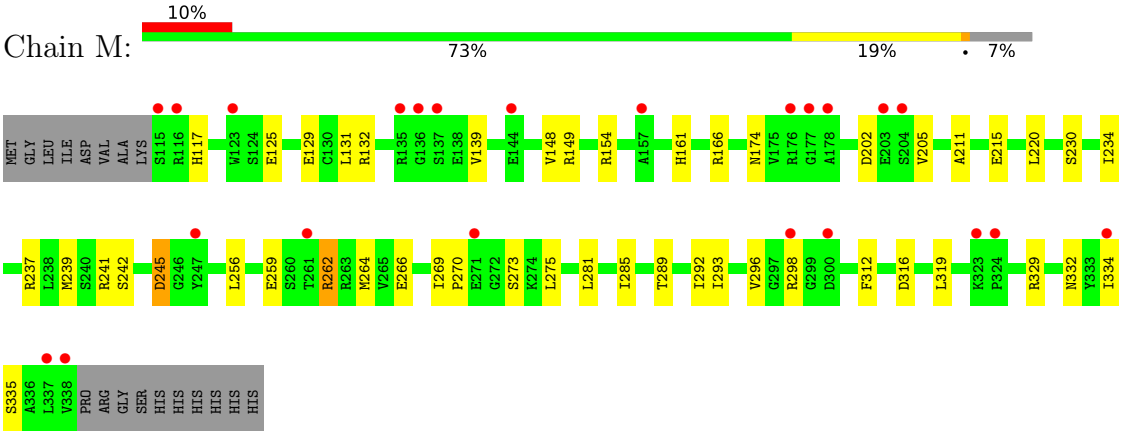
• Molecule 1: Calcium-gated potassium channel mthK

Chain L:

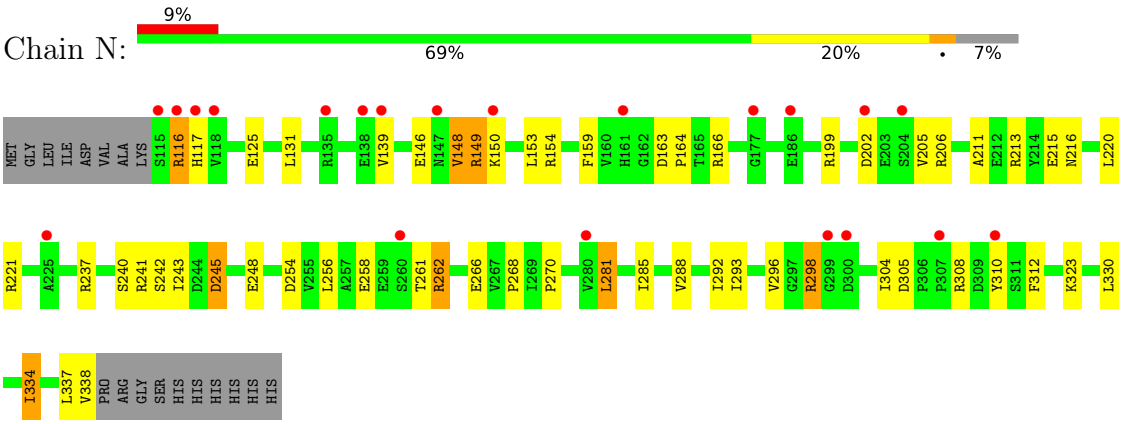




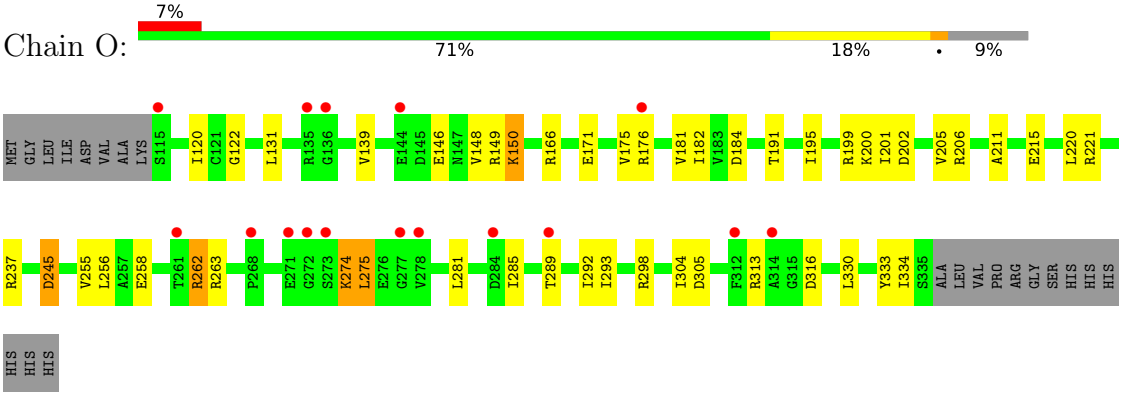
• Molecule 1: Calcium-gated potassium channel mthK



• Molecule 1: Calcium-gated potassium channel mthK

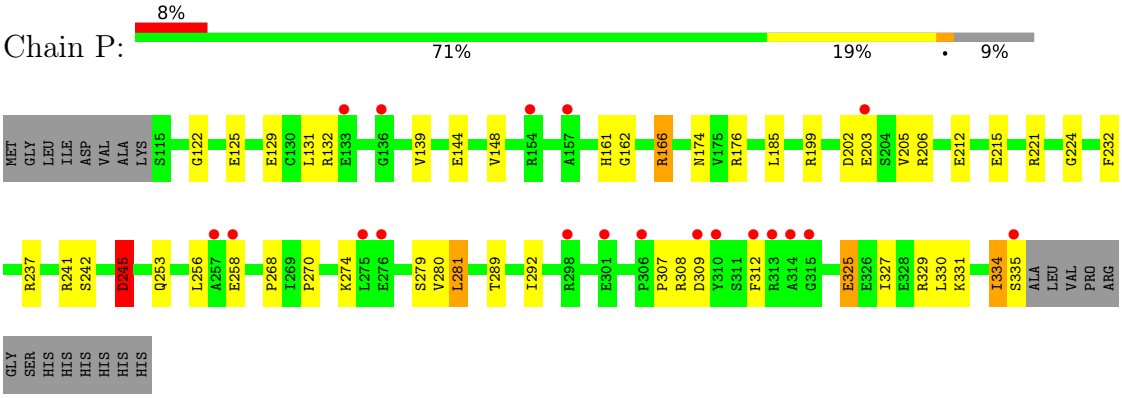


• Molecule 1: Calcium-gated potassium channel mthK



• Molecule 1: Calcium-gated potassium channel mthK

Chain P:


8%
71%
19%
9%
MET GLY LEU ILE ASP VAL ALA LYS S115 G122 E125 E129 C130 L131 R132 E133 G136 V139 E144 V148 R154 A157 H161 G162 R166 N174 V175 R176 L185 R199 D202 E203 S204 V205 R206 E212 E215 R221 G224 F232
R237 R241 S242 D245 Q253 L256 A257 E258 P268 I269 P270 K274 L275 E276 S279 V280 L281 T289 I292 R298 E301 P306 P307 R308 D309 Y310 S311 F312 R313 A314 G315 E325 E326 I327 E328 R329 L330 K331 I334 S335 ALA LEU VAL PRO ARG
GLY SER HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	110.05Å 136.42Å 498.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.11 30.11 – 3.11	Depositor EDS
% Data completeness (in resolution range)	93.9 (30.00-3.11) 90.9 (30.11-3.11)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 3.11Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.209 , 0.242 0.210 , 0.241	Depositor DCC
R_{free} test set	1966 reflections (1.53%)	wwPDB-VP
Wilson B-factor (Å^2)	69.9	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 103.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	27805	wwPDB-VP
Average B, all atoms (Å^2)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: BA

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	0/1753	0.58	0/2366
1	B	0.33	0/1745	0.55	0/2355
1	C	0.32	0/1760	0.54	0/2376
1	D	0.36	0/1768	0.56	1/2388 (0.0%)
1	E	0.35	0/1753	0.59	0/2366
1	F	0.31	0/1753	0.52	0/2366
1	G	0.33	0/1768	0.53	0/2388
1	H	0.33	0/1753	0.57	0/2366
1	I	0.36	0/1742	0.55	0/2351
1	J	0.34	0/1760	0.51	0/2376
1	K	0.35	0/1760	0.52	0/2376
1	L	0.37	0/1739	0.53	0/2348
1	M	0.36	0/1760	0.53	0/2376
1	N	0.34	0/1760	0.52	0/2376
1	O	0.33	0/1740	0.51	0/2348
1	P	0.35	0/1740	0.54	0/2348
All	All	0.34	0/28054	0.54	1/37870 (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	D	337	LEU	CA-CB-CG	5.00	126.80	115.30

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	1732	0	1742	23	0
1	B	1724	0	1731	28	0
1	C	1739	0	1751	37	0
1	D	1746	0	1758	20	0
1	E	1732	0	1742	24	0
1	F	1732	0	1742	24	0
1	G	1746	0	1758	23	0
1	H	1732	0	1742	39	0
1	I	1721	0	1729	32	0
1	J	1739	0	1751	39	0
1	K	1739	0	1751	36	0
1	L	1718	0	1720	39	0
1	M	1739	0	1751	27	0
1	N	1739	0	1751	36	0
1	O	1719	0	1726	33	0
1	P	1719	0	1726	37	0
2	A	5	0	0	0	0
2	B	4	0	0	0	0
2	C	3	0	0	0	0
2	D	5	0	0	0	0
2	E	6	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	2	0	0	0	0
2	I	3	0	0	0	0
2	J	2	0	0	0	0
2	K	4	0	0	0	0
2	L	2	0	0	0	0
2	M	4	0	0	0	0
2	N	3	0	0	0	0
2	O	3	0	0	0	0
2	P	3	0	0	0	0
3	A	6	0	0	1	0
3	B	6	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	1	0
3	E	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1	0	0	0	0
3	G	2	0	0	0	0
3	H	4	0	0	0	0
3	J	1	0	0	0	0
3	M	1	0	0	0	0
3	O	2	0	0	0	0
3	P	1	0	0	1	0
All	All	27805	0	27871	411	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 7.

The worst 5 of 411 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:F:269:ILE:HG12	1:F:334:ILE:HD11	1.52	0.89
1:I:242:SER:O	1:P:206:ARG:NH2	2.10	0.84
1:G:199:ARG:NH1	1:G:203:GLU:O	2.11	0.83
1:E:336:ALA:HB1	1:E:337:LEU:HA	1.62	0.80
1:A:115:SER:OG	3:A:505:HOH:O	2.02	0.77

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	221/242 (91%)	215 (97%)	6 (3%)	0	100	100
1	B	220/242 (91%)	213 (97%)	7 (3%)	0	100	100
1	C	222/242 (92%)	215 (97%)	7 (3%)	0	100	100
1	D	223/242 (92%)	217 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	221/242 (91%)	210 (95%)	11 (5%)	0	100	100
1	F	221/242 (91%)	213 (96%)	8 (4%)	0	100	100
1	G	223/242 (92%)	215 (96%)	8 (4%)	0	100	100
1	H	221/242 (91%)	214 (97%)	7 (3%)	0	100	100
1	I	220/242 (91%)	210 (96%)	10 (4%)	0	100	100
1	J	222/242 (92%)	216 (97%)	6 (3%)	0	100	100
1	K	222/242 (92%)	217 (98%)	5 (2%)	0	100	100
1	L	220/242 (91%)	215 (98%)	5 (2%)	0	100	100
1	M	222/242 (92%)	216 (97%)	6 (3%)	0	100	100
1	N	222/242 (92%)	215 (97%)	7 (3%)	0	100	100
1	O	219/242 (90%)	215 (98%)	4 (2%)	0	100	100
1	P	219/242 (90%)	211 (96%)	7 (3%)	1 (0%)	29	64
All	All	3538/3872 (91%)	3427 (97%)	110 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	245	ASP

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	191/207 (92%)	183 (96%)	8 (4%)	30	62
1	B	190/207 (92%)	182 (96%)	8 (4%)	30	62
1	C	192/207 (93%)	184 (96%)	8 (4%)	30	62
1	D	193/207 (93%)	184 (95%)	9 (5%)	26	59
1	E	191/207 (92%)	184 (96%)	7 (4%)	34	66
1	F	191/207 (92%)	184 (96%)	7 (4%)	34	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	193/207 (93%)	183 (95%)	10 (5%)	23	55
1	H	191/207 (92%)	183 (96%)	8 (4%)	30	62
1	I	189/207 (91%)	179 (95%)	10 (5%)	22	54
1	J	192/207 (93%)	182 (95%)	10 (5%)	23	55
1	K	192/207 (93%)	182 (95%)	10 (5%)	23	55
1	L	189/207 (91%)	181 (96%)	8 (4%)	30	62
1	M	192/207 (93%)	181 (94%)	11 (6%)	20	52
1	N	192/207 (93%)	177 (92%)	15 (8%)	12	40
1	O	190/207 (92%)	180 (95%)	10 (5%)	22	54
1	P	190/207 (92%)	182 (96%)	8 (4%)	30	62
All	All	3058/3312 (92%)	2911 (95%)	147 (5%)	25	58

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	117	HIS
1	P	279	SER
1	N	166	ARG
1	O	150	LYS
1	G	149	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 57 ligands modelled in this entry, 57 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

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	223/242 (92%)	0.20	4 (1%) 68 47	85, 127, 182, 198	0
1	B	222/242 (91%)	0.40	10 (4%) 33 16	93, 133, 182, 200	0
1	C	224/242 (92%)	0.32	5 (2%) 62 41	94, 136, 183, 201	0
1	D	225/242 (92%)	0.31	5 (2%) 62 41	94, 129, 186, 204	0
1	E	223/242 (92%)	0.23	6 (2%) 54 31	88, 128, 184, 200	0
1	F	223/242 (92%)	0.28	7 (3%) 49 26	91, 135, 182, 218	0
1	G	225/242 (92%)	0.34	4 (1%) 68 47	93, 134, 186, 265	0
1	H	223/242 (92%)	0.29	9 (4%) 38 19	89, 132, 184, 204	0
1	I	222/242 (91%)	0.65	27 (12%) 4 1	109, 142, 193, 223	0
1	J	224/242 (92%)	0.40	15 (6%) 17 7	110, 142, 184, 205	0
1	K	224/242 (92%)	0.39	14 (6%) 20 8	115, 148, 186, 232	0
1	L	222/242 (91%)	0.79	30 (13%) 3 1	112, 150, 199, 229	0
1	M	224/242 (92%)	0.58	23 (10%) 6 2	108, 142, 186, 214	0
1	N	224/242 (92%)	0.44	21 (9%) 8 3	107, 145, 186, 209	0
1	O	221/242 (91%)	0.40	16 (7%) 15 6	106, 139, 184, 209	0
1	P	221/242 (91%)	0.52	19 (8%) 10 4	106, 139, 187, 207	0
All	All	3570/3872 (92%)	0.41	215 (6%) 21 10	85, 139, 188, 265	0

The worst 5 of 215 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	273	SER	9.5
1	L	137	SER	8.0
1	L	336	ALA	7.6
1	O	136	GLY	7.2
1	L	335	SER	6.9

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, 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	BA	I	403	1/1	-0.07	0.32	297,297,297,297	0
2	BA	D	404	1/1	0.02	0.20	251,251,251,251	0
2	BA	K	404	1/1	0.18	0.36	276,276,276,276	0
2	BA	B	404	1/1	0.23	0.56	355,355,355,355	0
2	BA	D	405	1/1	0.26	0.29	254,254,254,254	0
2	BA	L	402	1/1	0.27	0.13	320,320,320,320	0
2	BA	M	401	1/1	0.33	0.15	290,290,290,290	0
2	BA	F	403	1/1	0.37	0.12	262,262,262,262	0
2	BA	J	401	1/1	0.48	0.22	269,269,269,269	0
2	BA	M	404	1/1	0.50	0.20	306,306,306,306	0
2	BA	M	402	1/1	0.51	0.10	237,237,237,237	0
2	BA	A	404	1/1	0.53	0.11	265,265,265,265	0
2	BA	C	403	1/1	0.53	0.09	256,256,256,256	0
2	BA	B	403	1/1	0.54	0.29	245,245,245,245	0
2	BA	F	401	1/1	0.54	0.13	222,222,222,222	0
2	BA	K	402	1/1	0.57	0.18	271,271,271,271	0
2	BA	G	404	1/1	0.57	0.15	259,259,259,259	0
2	BA	P	403	1/1	0.58	0.12	276,276,276,276	0
2	BA	O	403	1/1	0.59	0.42	313,313,313,313	0
2	BA	A	405	1/1	0.61	0.15	241,241,241,241	0
2	BA	E	404	1/1	0.62	0.09	256,256,256,256	0
2	BA	O	402	1/1	0.64	0.10	248,248,248,248	0
2	BA	D	402	1/1	0.64	0.07	250,250,250,250	0
2	BA	J	402	1/1	0.64	0.13	282,282,282,282	0
2	BA	A	403	1/1	0.65	0.12	230,230,230,230	0
2	BA	D	403	1/1	0.66	0.10	229,229,229,229	0
2	BA	F	402	1/1	0.67	0.17	253,253,253,253	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BA	E	405	1/1	0.67	0.08	259,259,259,259	0
2	BA	D	401	1/1	0.67	0.14	235,235,235,235	0
2	BA	G	403	1/1	0.69	0.09	229,229,229,229	0
2	BA	B	401	1/1	0.71	0.16	206,206,206,206	0
2	BA	I	401	1/1	0.71	0.14	273,273,273,273	0
2	BA	E	402	1/1	0.73	0.07	233,233,233,233	0
2	BA	H	401	1/1	0.73	0.15	226,226,226,226	0
2	BA	E	403	1/1	0.73	0.18	230,230,230,230	0
2	BA	N	403	1/1	0.74	0.23	257,257,257,257	0
2	BA	B	402	1/1	0.74	0.19	272,272,272,272	0
2	BA	A	402	1/1	0.74	0.10	245,245,245,245	0
2	BA	I	402	1/1	0.74	0.09	267,267,267,267	0
2	BA	H	402	1/1	0.76	0.11	231,231,231,231	0
2	BA	G	402	1/1	0.77	0.13	236,236,236,236	0
2	BA	P	401	1/1	0.78	0.10	244,244,244,244	0
2	BA	F	404	1/1	0.79	0.15	252,252,252,252	0
2	BA	A	401	1/1	0.79	0.13	228,228,228,228	0
2	BA	P	402	1/1	0.81	0.19	309,309,309,309	0
2	BA	K	401	1/1	0.81	0.21	259,259,259,259	0
2	BA	M	403	1/1	0.83	0.14	263,263,263,263	0
2	BA	N	402	1/1	0.83	0.07	289,289,289,289	0
2	BA	E	401	1/1	0.84	0.08	200,200,200,200	0
2	BA	L	401	1/1	0.84	0.07	256,256,256,256	0
2	BA	K	403	1/1	0.85	0.05	250,250,250,250	0
2	BA	E	406	1/1	0.86	0.14	263,263,263,263	0
2	BA	C	402	1/1	0.87	0.08	232,232,232,232	0
2	BA	O	401	1/1	0.88	0.10	256,256,256,256	0
2	BA	C	401	1/1	0.89	0.13	232,232,232,232	0
2	BA	N	401	1/1	0.90	0.20	270,270,270,270	0
2	BA	G	401	1/1	0.93	0.15	230,230,230,230	0

6.5 Other polymers (i)

There are no such residues in this entry.