



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:40 am GMT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

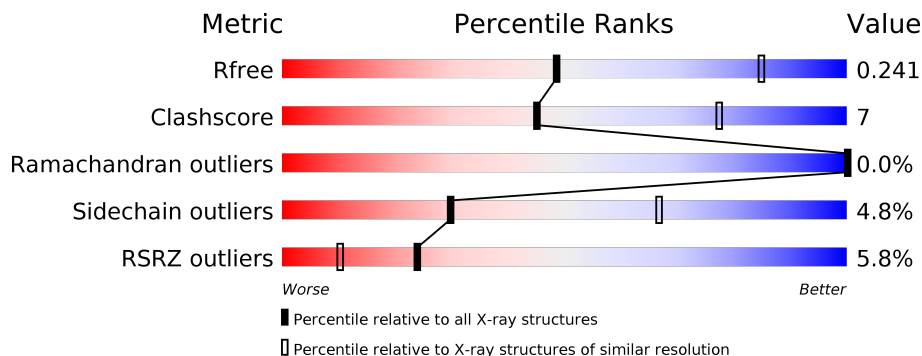
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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.



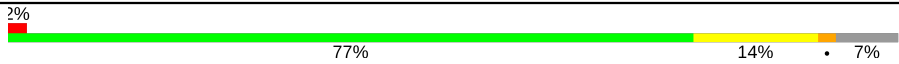

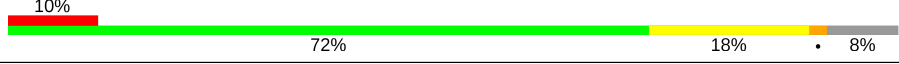
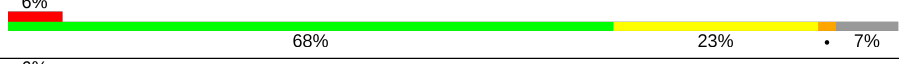

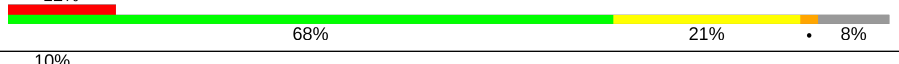
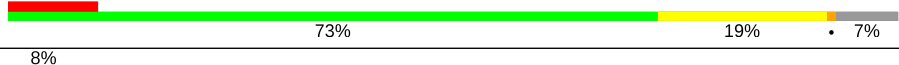

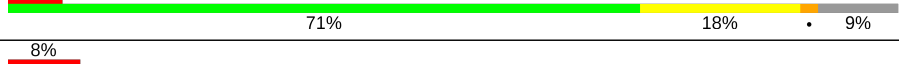

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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  $\geq 3$ , 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	<div> <div>2%</div> <div>76% 15% 8%</div> </div>
1	B	242	<div> <div>4%</div> <div>75% 16% 8%</div> </div>
1	C	242	<div> <div>2%</div> <div>71% 19% 7%</div> </div>
1	D	242	<div> <div>2%</div> <div>77% 15% 7%</div> </div>
1	E	242	<div> <div>2%</div> <div>74% 18% 8%</div> </div>
1	F	242	<div> <div>2%</div> <div>77% 14% 8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	242	
1	H	242	
1	I	242	
1	J	242	
1	K	242	
1	L	242	
1	M	242	
1	N	242	
1	O	242	
1	P	242	

## 2 Entry composition

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

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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

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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

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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

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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	P	3	Total Ba 3 3	0	0
2	G	4	Total Ba 4 4	0	0
2	J	2	Total Ba 2 2	0	0
2	D	5	Total Ba 5 5	0	0
2	K	4	Total Ba 4 4	0	0
2	E	6	Total Ba 6 6	0	0
2	H	2	Total Ba 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total 4	Ba 4	0	0
2	I	3	Total 3	Ba 3	0	0
2	C	3	Total 3	Ba 3	0	0
2	A	5	Total 5	Ba 5	0	0
2	N	3	Total 3	Ba 3	0	0
2	O	3	Total 3	Ba 3	0	0
2	L	2	Total 2	Ba 2	0	0
2	F	4	Total 4	Ba 4	0	0
2	M	4	Total 4	Ba 4	0	0

- Molecule 3 is water.

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

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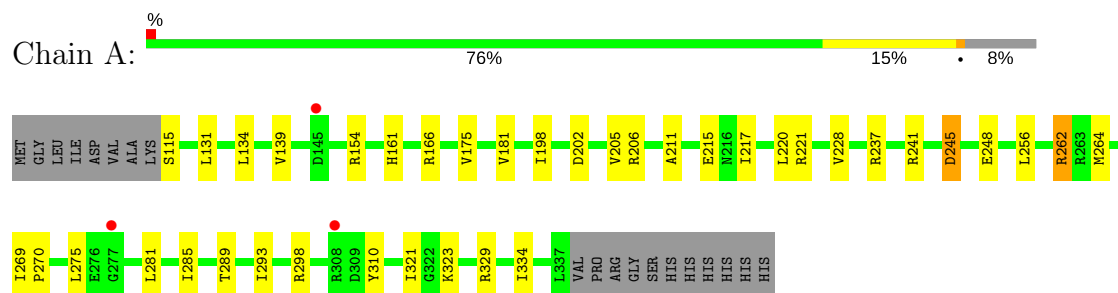
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	2	Total	O	0	0
			2	2		
3	P	1	Total	O	0	0
			1	1		

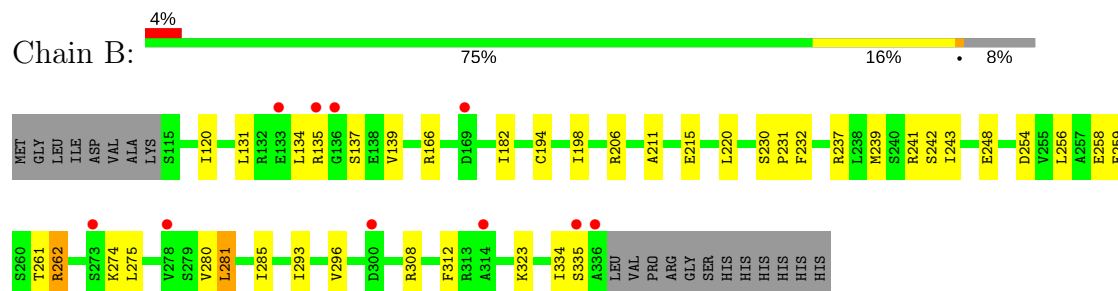
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

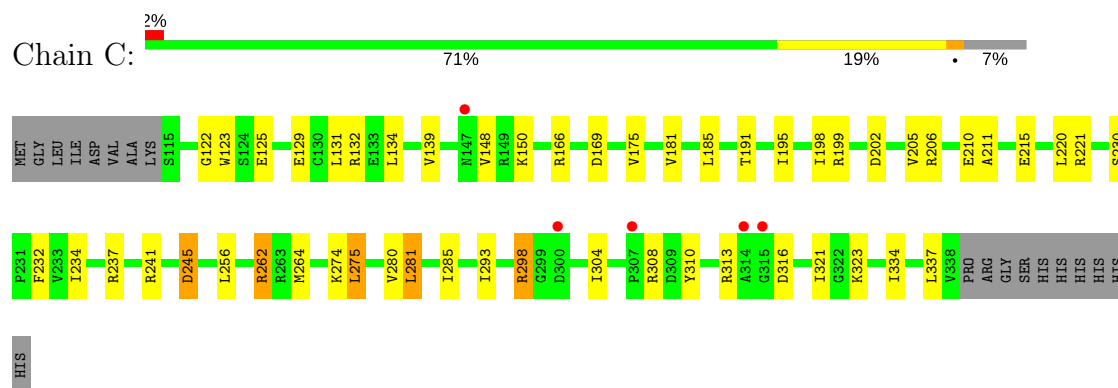
#### • Molecule 1: Calcium-gated potassium channel mthK



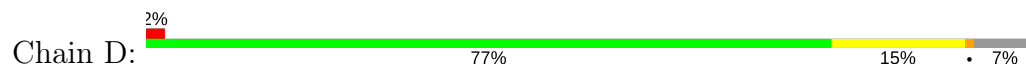
#### • Molecule 1: Calcium-gated potassium channel mthK



#### • Molecule 1: Calcium-gated potassium channel mthK



#### • Molecule 1: Calcium-gated potassium channel mthK





Chain I:

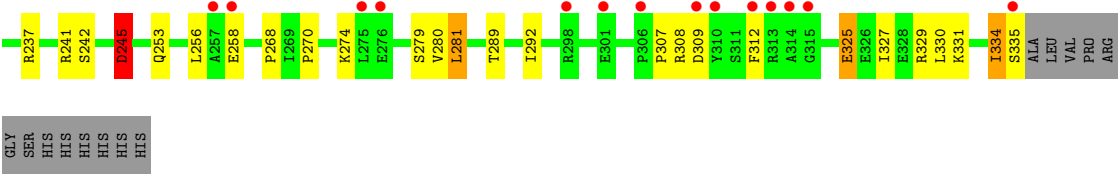
Amino Acid	Category
Met	Grey
Gly	Green
Leu	Green
Ile	Green
Asp	Grey
Val	Green
Ala	Green
Lys	Green
R115	Green
R116	Red
G122	Yellow
L131	Green
V139	Green
R150	Yellow
R154	Green
R166	Yellow
V175	Green
R176	Red
V181	Green
D184	Green
T191	Green
I195	Green
D202	Green
V205	Green
R206	Green
E215	Green
R221	Green
V228	Green
I229	Green
S230	Green
R237	Green
R241	Green
S242	Green
D245	Yellow
Q253	Green
D254	Green
V255	Green
L256	Green
K257	Green
F258	Green

[illegible][illegible]

Chain L: 







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 3.11Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.209 , 0.242 0.209 , 0.241	Depositor DCC
$R_{free}$ test set	3746 reflections (1.53%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.2	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 103.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	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 <sup>2</sup> )	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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(°)	Ideal(°)
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

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

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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.

All (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
1:D:199:ARG:NH2	1:D:205:VAL:O	2.18	0.76
1:H:199:ARG:NH1	1:H:203:GLU:O	2.18	0.76
1:D:242:SER:O	1:E:206:ARG:NH2	2.20	0.74
1:A:211:ALA:HB2	1:A:220:LEU:HD22	1.68	0.74
1:J:232:PHE:HD1	1:K:125:GLU:HB3	1.53	0.73
1:G:146:GLU:HG2	1:G:149:ARG:HH21	1.51	0.73
1:C:274:LYS:HG3	1:C:275:LEU:HD23	1.72	0.70
1:C:169:ASP:OD1	1:E:154:ARG:NH2	2.24	0.70
1:G:211:ALA:HB2	1:G:220:LEU:HD22	1.74	0.69
1:F:305:ASP:HB2	1:G:292:ILE:HD11	1.75	0.69
1:N:211:ALA:HB2	1:N:220:LEU:HD22	1.76	0.68
1:K:202:ASP:OD1	1:K:205:VAL:N	2.27	0.68
1:A:206:ARG:NH2	1:H:242:SER:O	2.27	0.67
1:E:131:LEU:HD21	1:E:139:VAL:HG11	1.76	0.66
1:D:245:ASP:OD1	1:D:245:ASP:N	2.27	0.66
1:C:281:LEU:HD22	1:C:308:ARG:HD2	1.78	0.66
1:A:298:ARG:NH1	1:A:310:TYR:OH	2.28	0.66
1:J:232:PHE:HE2	1:K:232:PHE:HE2	1.43	0.65
1:D:131:LEU:HD21	1:D:139:VAL:HG11	1.77	0.65
1:N:237:ARG:NH1	1:N:248:GLU:OE2	2.28	0.65
1:B:131:LEU:HD21	1:B:139:VAL:HG11	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:131:LEU:HD21	1:P:139:VAL:HG11	1.79	0.64
1:E:211:ALA:HB2	1:E:220:LEU:HD22	1.80	0.64
1:L:305:ASP:HB3	1:M:262:ARG:HH12	1.63	0.64
1:K:117:HIS:NE2	1:K:174:ASN:O	2.29	0.64
1:I:237:ARG:NH1	1:P:256:LEU:O	2.31	0.64
1:C:245:ASP:N	1:C:245:ASP:OD1	2.30	0.64
1:B:242:SER:O	1:C:206:ARG:NH2	2.31	0.63
1:F:292:ILE:HD11	1:G:305:ASP:HB2	1.81	0.63
1:K:199:ARG:NH2	1:K:205:VAL:O	2.29	0.63
1:K:274:LYS:NZ	1:K:335:SER:O	2.26	0.63
1:N:245:ASP:OD2	1:N:245:ASP:N	2.32	0.63
1:L:281:LEU:HB2	1:L:308:ARG:HB3	1.79	0.62
1:M:211:ALA:HB2	1:M:220:LEU:HD22	1.81	0.62
1:J:135:ARG:NH1	1:J:137:SER:OG	2.32	0.62
1:J:245:ASP:N	1:J:245:ASP:OD2	2.31	0.62
1:I:305:ASP:HB2	1:P:292:ILE:HD11	1.80	0.62
1:P:174:ASN:ND2	3:P:501:HOH:O	2.33	0.62
1:N:292:ILE:HD11	1:O:305:ASP:HB2	1.81	0.61
1:B:211:ALA:HB2	1:B:220:LEU:HD22	1.82	0.61
1:N:131:LEU:HD21	1:N:139:VAL:HG11	1.82	0.60
1:A:289:THR:O	1:A:329:ARG:NH2	2.33	0.60
1:H:245:ASP:N	1:H:245:ASP:OD2	2.33	0.60
1:O:298:ARG:NH1	1:O:316:ASP:OD2	2.35	0.60
1:K:245:ASP:OD2	1:K:245:ASP:N	2.35	0.60
1:L:305:ASP:HB2	1:M:292:ILE:HD11	1.84	0.60
1:D:330:LEU:O	1:D:334:ILE:HG13	2.02	0.59
1:M:285:ILE:HG21	1:M:293:ILE:HD11	1.85	0.59
1:B:285:ILE:HG21	1:B:293:ILE:HD11	1.84	0.59
1:F:245:ASP:N	1:F:245:ASP:OD1	2.33	0.59
1:P:202:ASP:OD1	1:P:205:VAL:N	2.36	0.59
1:L:269:ILE:HD12	1:L:316:ASP:HB2	1.85	0.58
1:D:247:TYR:HE1	1:E:317:ILE:HD13	1.68	0.58
1:E:274:LYS:HE3	1:E:336:ALA:HB3	1.85	0.58
1:P:237:ARG:NE	1:P:241:ARG:HH22	2.02	0.58
1:D:285:ILE:HD12	1:D:293:ILE:HD11	1.85	0.58
1:K:285:ILE:HG21	1:K:293:ILE:HD11	1.86	0.58
1:L:182:ILE:HD13	1:M:239:MET:HB3	1.86	0.58
1:H:131:LEU:HD21	1:H:139:VAL:HG11	1.84	0.58
1:M:298:ARG:NH1	1:M:316:ASP:OD2	2.37	0.58
1:A:262:ARG:NH1	1:A:323:LYS:HG3	2.19	0.58
1:P:289:THR:O	1:P:329:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:ASP:OD1	1:F:205:VAL:N	2.37	0.58
1:J:237:ARG:NH2	1:K:256:LEU:O	2.37	0.58
1:N:298:ARG:NH1	1:N:310:TYR:OH	2.37	0.58
1:D:199:ARG:NH1	1:D:224:GLY:O	2.37	0.57
1:L:116:ARG:NH2	1:L:138:GLU:OE2	2.37	0.57
1:N:221:ARG:NH2	1:O:258:GLU:OE1	2.36	0.57
1:J:281:LEU:HD22	1:J:308:ARG:HD2	1.85	0.57
1:L:237:ARG:NH2	1:M:256:LEU:O	2.38	0.57
1:G:245:ASP:OD2	1:G:245:ASP:N	2.36	0.57
1:M:230:SER:O	1:M:234:ILE:HG13	2.04	0.57
1:K:269:ILE:HD12	1:K:316:ASP:HB2	1.87	0.57
1:I:206:ARG:NH2	1:P:242:SER:O	2.38	0.57
1:B:237:ARG:HH11	1:B:241:ARG:NH1	2.02	0.57
1:C:175:VAL:HG11	1:C:198:ILE:HG23	1.86	0.57
1:C:298:ARG:NH1	1:C:313:ARG:HD2	2.20	0.56
1:H:199:ARG:NH2	1:H:205:VAL:O	2.38	0.56
1:A:161:HIS:CE1	1:C:150:LYS:HD2	2.41	0.56
1:J:211:ALA:HB2	1:J:220:LEU:HD22	1.86	0.56
1:P:199:ARG:NH2	1:P:205:VAL:O	2.37	0.56
1:O:199:ARG:NH2	1:O:205:VAL:O	2.39	0.56
1:O:245:ASP:N	1:O:245:ASP:OD2	2.38	0.56
1:J:232:PHE:HE2	1:K:232:PHE:CE2	2.24	0.56
1:C:211:ALA:HB2	1:C:220:LEU:HD22	1.87	0.55
1:N:281:LEU:HD22	1:N:308:ARG:HD2	1.87	0.55
1:A:237:ARG:NH2	1:A:248:GLU:OE2	2.39	0.55
1:O:146:GLU:OE2	1:O:149:ARG:NH1	2.39	0.55
1:F:131:LEU:HD21	1:F:139:VAL:HG11	1.87	0.55
1:O:274:LYS:HG2	1:O:275:LEU:HD22	1.88	0.55
1:K:140:PHE:HD1	1:K:158:ASN:HB2	1.71	0.55
1:L:202:ASP:OD1	1:L:205:VAL:N	2.39	0.55
1:L:211:ALA:HB2	1:L:220:LEU:HD22	1.89	0.55
1:M:117:HIS:NE2	1:M:174:ASN:O	2.31	0.55
1:P:281:LEU:HD22	1:P:308:ARG:HD2	1.88	0.55
1:A:175:VAL:HG11	1:A:198:ILE:HG23	1.89	0.54
1:I:274:LYS:HE3	1:I:333:TYR:O	2.06	0.54
1:C:298:ARG:NH1	1:C:316:ASP:OD1	2.40	0.54
1:G:199:ARG:NH2	1:G:205:VAL:O	2.40	0.54
1:L:262:ARG:HB3	1:L:322:GLY:C	2.28	0.54
1:F:274:LYS:HE3	1:F:336:ALA:HB3	1.88	0.54
1:F:237:ARG:NH1	1:F:248:GLU:OE2	2.39	0.54
1:C:202:ASP:OD1	1:C:205:VAL:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:ASP:OD1	1:E:205:VAL:N	2.41	0.54
1:M:245:ASP:N	1:M:245:ASP:OD1	2.40	0.54
1:O:131:LEU:HD21	1:O:139:VAL:HG11	1.89	0.54
1:A:202:ASP:OD1	1:A:205:VAL:N	2.41	0.54
1:F:232:PHE:HD1	1:G:125:GLU:HB3	1.73	0.54
1:F:221:ARG:NH2	1:G:258:GLU:OE1	2.37	0.54
1:L:307:PRO:HB2	1:L:309:ASP:OD1	2.08	0.54
1:P:144:GLU:O	1:P:161:HIS:NE2	2.37	0.54
1:E:330:LEU:O	1:E:334:ILE:HG12	2.08	0.53
1:I:131:LEU:HD21	1:I:139:VAL:HG11	1.88	0.53
1:I:274:LYS:HG3	1:I:275:LEU:HD13	1.91	0.53
1:I:329:ARG:O	1:I:332:ASN:ND2	2.41	0.53
1:N:258:GLU:OE1	1:O:221:ARG:NH2	2.40	0.53
1:E:237:ARG:HH21	1:E:241:ARG:NH1	2.07	0.53
1:L:131:LEU:HD21	1:L:139:VAL:HG11	1.90	0.53
1:C:199:ARG:NH2	1:C:205:VAL:O	2.41	0.53
1:D:305:ASP:HB2	1:E:292:ILE:HD11	1.90	0.53
1:K:298:ARG:NH1	1:K:316:ASP:OD2	2.40	0.53
1:I:269:ILE:HD12	1:I:316:ASP:HB2	1.91	0.53
1:L:310:TYR:OH	1:L:313:ARG:NH1	2.41	0.53
1:E:237:ARG:NH2	1:E:248:GLU:OE2	2.32	0.52
1:J:150:LYS:HD2	1:L:161:HIS:ND1	2.23	0.52
1:C:131:LEU:HD21	1:C:139:VAL:HG11	1.91	0.52
1:N:202:ASP:OD1	1:N:205:VAL:N	2.42	0.52
1:L:194:CYS:O	1:L:198:ILE:HG13	2.09	0.52
1:A:175:VAL:HG13	1:A:181:VAL:HG21	1.91	0.52
1:H:264:MET:HG2	1:H:321:ILE:HG12	1.90	0.52
1:A:285:ILE:HG21	1:A:293:ILE:HD11	1.91	0.52
1:D:202:ASP:OD1	1:D:205:VAL:N	2.43	0.52
1:B:280:VAL:HG22	1:B:308:ARG:HA	1.92	0.52
1:L:237:ARG:NH1	1:L:248:GLU:OE2	2.43	0.52
1:A:245:ASP:HB2	1:H:266:GLU:OE1	2.10	0.51
1:P:199:ARG:NH1	1:P:224:GLY:O	2.43	0.51
1:F:245:ASP:HB2	1:G:266:GLU:OE1	2.11	0.51
1:G:298:ARG:NH1	1:G:313:ARG:HD2	2.26	0.51
1:J:266:GLU:OE1	1:K:245:ASP:HB2	2.09	0.51
1:J:296:VAL:HG21	1:J:312:PHE:HE2	1.75	0.51
1:M:273:SER:HA	1:M:335:SER:O	2.11	0.51
1:D:140:PHE:HD1	1:D:158:ASN:HB2	1.75	0.51
1:J:262:ARG:NH2	1:J:323:LYS:HG3	2.25	0.51
1:I:237:ARG:HH21	1:I:241:ARG:NH1	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:211:ALA:HB2	1:K:220:LEU:HD22	1.91	0.51
1:M:202:ASP:OD1	1:M:205:VAL:N	2.44	0.51
1:B:262:ARG:HE	1:C:304:ILE:HB	1.75	0.51
1:D:237:ARG:NH2	1:E:256:LEU:O	2.43	0.51
1:E:135:ARG:NH1	1:E:137:SER:OG	2.44	0.51
1:H:288:VAL:HG11	1:H:333:TYR:CE1	2.46	0.51
1:K:199:ARG:NH1	1:K:224:GLY:O	2.44	0.51
1:J:285:ILE:HG21	1:J:293:ILE:HD11	1.92	0.51
1:K:171:GLU:HG3	1:K:201:ILE:HD13	1.92	0.51
1:O:298:ARG:CZ	1:O:313:ARG:HD3	2.41	0.51
1:A:131:LEU:HD21	1:A:139:VAL:HG11	1.92	0.50
1:N:237:ARG:NH2	1:O:256:LEU:O	2.44	0.50
1:J:269:ILE:HD12	1:J:316:ASP:HB2	1.93	0.50
1:L:144:GLU:O	1:L:161:HIS:NE2	2.39	0.50
1:P:274:LYS:NZ	1:P:335:SER:OG	2.44	0.50
1:H:129:GLU:OE2	1:H:132:ARG:NH1	2.44	0.50
1:C:237:ARG:O	1:C:241:ARG:HG3	2.11	0.50
1:E:285:ILE:HG21	1:E:293:ILE:HD11	1.92	0.50
1:A:237:ARG:NH1	1:H:256:LEU:O	2.45	0.50
1:F:237:ARG:HH11	1:F:241:ARG:NH1	2.10	0.50
1:L:241:ARG:NH1	1:M:259:GLU:OE2	2.44	0.50
1:I:256:LEU:O	1:P:237:ARG:NH2	2.45	0.50
1:G:237:ARG:HH11	1:G:241:ARG:NH1	2.11	0.49
1:N:266:GLU:OE1	1:O:245:ASP:HB2	2.12	0.49
1:A:256:LEU:O	1:H:237:ARG:NH2	2.45	0.49
1:B:237:ARG:NH2	1:C:256:LEU:O	2.46	0.49
1:K:237:ARG:HH11	1:K:241:ARG:NH1	2.09	0.49
1:K:262:ARG:NH1	1:K:323:LYS:HG3	2.28	0.49
1:G:131:LEU:HD21	1:G:139:VAL:HG11	1.94	0.49
1:N:237:ARG:HH11	1:N:241:ARG:NH1	2.11	0.49
1:E:270:PRO:HD2	1:E:334:ILE:HG22	1.94	0.49
1:J:166:ARG:NH2	1:P:125:GLU:OE2	2.44	0.49
1:L:270:PRO:HD2	1:L:334:ILE:HG22	1.95	0.49
1:K:136:GLY:O	1:K:157:ALA:HA	2.13	0.49
1:N:296:VAL:HG21	1:N:312:PHE:HE2	1.78	0.49
1:C:175:VAL:HG13	1:C:181:VAL:HG21	1.95	0.48
1:E:117:HIS:NE2	1:E:174:ASN:O	2.42	0.48
1:H:194:CYS:O	1:H:198:ILE:HG13	2.13	0.48
1:O:175:VAL:HG13	1:O:181:VAL:HG21	1.95	0.48
1:M:264:MET:HE1	1:M:319:LEU:HD21	1.95	0.48
1:O:289:THR:HG21	1:O:330:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:CYS:O	1:B:198:ILE:HG13	2.13	0.48
1:J:125:GLU:CD	1:L:166:ARG:HH22	2.16	0.48
1:I:191:THR:O	1:I:195:ILE:HG13	2.14	0.48
1:M:131:LEU:HD21	1:M:139:VAL:HG11	1.95	0.48
1:P:325:GLU:O	1:P:329:ARG:HG3	2.12	0.48
1:B:243:ILE:HD12	1:C:134:LEU:HD21	1.96	0.48
1:J:307:PRO:HB2	1:J:309:ASP:OD1	2.14	0.48
1:H:123:TRP:CZ2	1:H:128:LEU:HD13	2.49	0.48
1:N:285:ILE:HG21	1:N:293:ILE:HD11	1.95	0.48
1:B:256:LEU:O	1:C:237:ARG:NH2	2.47	0.47
1:M:161:HIS:HE1	1:O:150:LYS:HD2	1.79	0.47
1:P:212:GLU:HG3	1:P:232:PHE:CD1	2.49	0.47
1:F:268:PRO:O	1:F:270:PRO:HD3	2.14	0.47
1:N:150:LYS:HD2	1:P:161:HIS:ND1	2.29	0.47
1:N:154:ARG:HH22	1:P:162:GLY:HA2	1.79	0.47
1:K:214:TYR:HD1	1:K:214:TYR:O	1.96	0.47
1:N:262:ARG:HE	1:O:304:ILE:HB	1.79	0.47
1:J:296:VAL:HG21	1:J:312:PHE:CE2	2.50	0.47
1:E:298:ARG:NH1	1:E:316:ASP:OD2	2.47	0.47
1:O:285:ILE:HG21	1:O:293:ILE:HD11	1.95	0.47
1:C:191:THR:O	1:C:195:ILE:HG13	2.14	0.47
1:F:266:GLU:OE1	1:G:245:ASP:HB2	2.15	0.47
1:J:125:GLU:OE2	1:L:166:ARG:NH2	2.46	0.47
1:J:252:VAL:HA	1:J:256:LEU:HD23	1.97	0.47
1:L:237:ARG:HH11	1:L:241:ARG:NH2	2.11	0.47
1:H:122:GLY:HA3	1:H:184:ASP:O	2.15	0.47
1:O:120:ILE:HG12	1:O:182:ILE:HB	1.96	0.47
1:A:237:ARG:HH21	1:A:241:ARG:NH1	2.13	0.47
1:E:262:ARG:NH1	1:E:323:LYS:HG3	2.30	0.47
1:D:122:GLY:HA3	1:D:185:LEU:HD23	1.97	0.47
1:I:258:GLU:OE1	1:P:221:ARG:NH2	2.43	0.47
1:I:329:ARG:HA	1:I:332:ASN:HD22	1.79	0.47
1:B:134:LEU:HB3	1:B:137:SER:OG	2.16	0.47
1:I:298:ARG:CD	1:I:313:ARG:HH11	2.28	0.47
1:J:122:GLY:HA3	1:J:184:ASP:O	2.15	0.47
1:M:296:VAL:HG21	1:M:312:PHE:HE2	1.79	0.47
1:G:202:ASP:OD1	1:G:205:VAL:N	2.49	0.46
1:G:335:SER:OG	1:G:336:ALA:N	2.49	0.46
1:N:256:LEU:O	1:O:237:ARG:NH2	2.48	0.46
1:A:245:ASP:OD2	1:A:245:ASP:N	2.49	0.46
1:I:122:GLY:HA3	1:I:184:ASP:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:PHE:HD1	1:C:125:GLU:HB3	1.78	0.46
1:H:211:ALA:HB2	1:H:220:LEU:HD22	1.96	0.46
1:L:150:LYS:O	1:L:154:ARG:HB2	2.16	0.46
1:N:199:ARG:NH2	1:N:202:ASP:O	2.48	0.46
1:H:273:SER:HA	1:H:335:SER:HA	1.98	0.46
1:F:253:GLN:NE2	1:F:258:GLU:OE1	2.47	0.46
1:J:195:ILE:HD13	1:J:225:ALA:HB2	1.97	0.46
1:K:122:GLY:HA3	1:K:185:LEU:HD23	1.98	0.46
1:F:304:ILE:HB	1:G:262:ARG:HE	1.81	0.46
1:I:166:ARG:NH2	1:K:125:GLU:OE2	2.49	0.46
1:B:239:MET:CE	1:C:210:GLU:HB2	2.46	0.46
1:C:129:GLU:OE2	1:C:132:ARG:NH1	2.49	0.46
1:F:175:VAL:HG13	1:F:181:VAL:HG21	1.98	0.46
1:H:212:GLU:HG3	1:H:232:PHE:HD1	1.81	0.46
1:H:195:ILE:HD13	1:H:225:ALA:HB2	1.97	0.46
1:I:298:ARG:HD2	1:I:313:ARG:HH11	1.81	0.46
1:L:272:GLY:O	1:L:336:ALA:HA	2.16	0.46
1:P:307:PRO:HB2	1:P:309:ASP:OD1	2.16	0.46
1:I:245:ASP:HA	1:P:206:ARG:CZ	2.46	0.45
1:K:298:ARG:NH1	1:K:310:TYR:OH	2.49	0.45
1:N:304:ILE:HB	1:O:262:ARG:HE	1.82	0.45
1:B:259:GLU:OE2	1:C:237:ARG:NH1	2.49	0.45
1:D:292:ILE:HD11	1:E:305:ASP:HB2	1.97	0.45
1:M:289:THR:O	1:M:329:ARG:HD2	2.16	0.45
1:B:296:VAL:HG21	1:B:312:PHE:HE2	1.82	0.45
1:C:285:ILE:HG21	1:C:293:ILE:HD11	1.98	0.45
1:H:288:VAL:HG11	1:H:333:TYR:CD1	2.51	0.45
1:K:148:VAL:HG12	1:K:159:PHE:CE1	2.51	0.45
1:I:253:GLN:NE2	1:I:258:GLU:OE1	2.48	0.45
1:J:131:LEU:HD21	1:J:139:VAL:HG11	1.97	0.45
1:N:240:SER:O	1:N:243:ILE:HG22	2.16	0.45
1:H:171:GLU:HG3	1:H:201:ILE:HD13	1.97	0.45
1:G:307:PRO:HB2	1:G:309:ASP:OD1	2.17	0.45
1:O:191:THR:O	1:O:195:ILE:HG13	2.17	0.45
1:N:221:ARG:HH22	1:O:258:GLU:CD	2.19	0.45
1:G:255:VAL:HG13	1:G:263:ARG:HA	1.98	0.45
1:L:122:GLY:HA3	1:L:184:ASP:O	2.17	0.45
1:B:281:LEU:HB2	1:B:308:ARG:HB3	1.98	0.45
1:D:177:GLY:HA2	3:D:502:HOH:O	2.17	0.45
1:L:285:ILE:HD12	1:L:293:ILE:HD11	1.98	0.45
1:N:254:ASP:OD2	1:N:261:THR:OG1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:305:ASP:HB2	1:O:292:ILE:HD11	1.99	0.45
1:P:129:GLU:OE2	1:P:132:ARG:NH1	2.50	0.45
1:J:254:ASP:O	1:J:259:GLU:N	2.49	0.45
1:H:262:ARG:NH1	1:H:323:LYS:HE3	2.32	0.44
1:H:270:PRO:HD2	1:H:334:ILE:HG21	1.97	0.44
1:I:279:SER:HA	1:I:310:TYR:O	2.17	0.44
1:H:123:TRP:HZ2	1:H:128:LEU:HD13	1.81	0.44
1:P:199:ARG:HD3	1:P:203:GLU:HA	1.99	0.44
1:A:217:ILE:HG23	1:A:228:VAL:HG11	1.99	0.44
1:F:308:ARG:NH1	1:N:288:VAL:HA	2.32	0.44
1:O:150:LYS:HG2	1:O:150:LYS:H	1.49	0.44
1:I:202:ASP:OD1	1:I:205:VAL:N	2.51	0.44
1:I:254:ASP:O	1:I:259:GLU:N	2.45	0.44
1:L:140:PHE:HD1	1:L:158:ASN:HB2	1.82	0.44
1:O:171:GLU:HG3	1:O:201:ILE:HD13	1.98	0.44
1:A:264:MET:HG2	1:A:321:ILE:HG12	1.99	0.44
1:B:254:ASP:OD2	1:B:261:THR:OG1	2.35	0.44
1:E:171:GLU:HG3	1:E:201:ILE:HD13	1.99	0.44
1:I:306:PRO:HB3	1:I:310:TYR:CD2	2.53	0.44
1:N:213:ARG:HB2	1:N:216:ASN:ND2	2.32	0.44
1:O:202:ASP:OD1	1:O:205:VAL:N	2.51	0.44
1:H:254:ASP:O	1:H:259:GLU:N	2.50	0.44
1:J:202:ASP:OD1	1:J:205:VAL:N	2.50	0.44
1:O:211:ALA:HB2	1:O:220:LEU:HD22	2.00	0.44
1:E:163:ASP:HA	1:E:164:PRO:HD2	1.87	0.44
1:L:262:ARG:HB3	1:L:322:GLY:O	2.18	0.44
1:L:266:GLU:OE1	1:M:245:ASP:HB2	2.18	0.44
1:K:169:ASP:OD2	1:M:154:ARG:NH2	2.51	0.44
1:B:262:ARG:NH2	1:B:323:LYS:HG3	2.33	0.43
1:E:212:GLU:HG3	1:E:232:PHE:HD1	1.83	0.43
1:L:117:HIS:NE2	1:L:174:ASN:O	2.45	0.43
1:L:195:ILE:HG23	1:L:207:ILE:HD13	2.00	0.43
1:M:298:ARG:HD3	1:M:316:ASP:OD1	2.18	0.43
1:H:274:LYS:NZ	1:H:335:SER:O	2.44	0.43
1:A:269:ILE:HA	1:A:270:PRO:HD3	1.86	0.43
1:J:129:GLU:OE2	1:J:132:ARG:NH2	2.51	0.43
1:B:232:PHE:HE2	1:C:232:PHE:CE2	2.36	0.43
1:C:230:SER:O	1:C:234:ILE:HG13	2.19	0.43
1:C:337:LEU:HD23	1:C:337:LEU:HA	1.85	0.43
1:K:166:ARG:NH2	1:M:125:GLU:OE2	2.51	0.43
1:O:255:VAL:HG13	1:O:263:ARG:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:269:ILE:HA	1:H:270:PRO:HD3	1.81	0.43
1:H:281:LEU:HD22	1:H:308:ARG:HD2	2.00	0.43
1:J:273:SER:HB3	1:J:276:GLU:HB2	2.00	0.43
1:O:176:ARG:NH2	1:O:202:ASP:OD2	2.47	0.43
1:I:228:VAL:O	1:P:253:GLN:HG3	2.19	0.43
1:O:122:GLY:HA3	1:O:184:ASP:O	2.18	0.43
1:P:330:LEU:O	1:P:334:ILE:HG13	2.19	0.43
1:F:269:ILE:HD12	1:F:316:ASP:HB2	2.00	0.43
1:I:175:VAL:HG13	1:I:181:VAL:HG21	2.00	0.43
1:K:298:ARG:CZ	1:K:313:ARG:HD2	2.49	0.43
1:L:233:VAL:HA	1:M:129:GLU:HG3	2.01	0.43
1:N:149:ARG:O	1:N:153:LEU:HG	2.18	0.43
1:I:221:ARG:NH2	1:P:258:GLU:OE1	2.48	0.43
1:F:282:ASP:OD1	1:N:323:LYS:NZ	2.52	0.43
1:I:291:VAL:HG23	1:I:326:GLU:HB3	2.01	0.43
1:N:148:VAL:HG12	1:N:159:PHE:CE1	2.54	0.43
1:B:232:PHE:CE2	1:C:232:PHE:HE2	2.36	0.42
1:C:122:GLY:HA3	1:C:185:LEU:HD23	1.99	0.42
1:J:239:MET:HB3	1:K:182:ILE:HD13	2.01	0.42
1:K:294:ILE:HD13	1:K:294:ILE:HA	1.91	0.42
1:J:287:ASP:OD1	1:K:308:ARG:NH1	2.52	0.42
1:L:245:ASP:HB2	1:M:266:GLU:OE1	2.18	0.42
1:F:262:ARG:HH22	1:F:323:LYS:HE3	1.83	0.42
1:L:163:ASP:HA	1:L:164:PRO:HD2	1.95	0.42
1:N:163:ASP:HA	1:N:164:PRO:HD2	1.87	0.42
1:D:298:ARG:NH2	1:D:313:ARG:HH21	2.18	0.42
1:C:298:ARG:HH12	1:C:313:ARG:HB2	1.84	0.42
1:F:331:LYS:O	1:F:334:ILE:HG22	2.19	0.42
1:G:285:ILE:HD12	1:G:293:ILE:HD11	2.01	0.42
1:H:144:GLU:O	1:H:161:HIS:NE2	2.49	0.42
1:J:191:THR:O	1:J:195:ILE:HG13	2.20	0.42
1:I:230:SER:N	1:P:253:GLN:OE1	2.49	0.42
1:H:163:ASP:HA	1:H:164:PRO:HD2	1.91	0.42
1:F:125:GLU:CD	1:H:166:ARG:HH22	2.22	0.42
1:J:298:ARG:NH1	1:J:310:TYR:OH	2.52	0.42
1:N:116:ARG:HE	1:N:116:ARG:HB3	1.53	0.42
1:G:338:VAL:HA	1:G:339:PRO:HD3	1.83	0.42
1:I:116:ARG:HA	1:I:116:ARG:NE	2.34	0.42
1:J:253:GLN:O	1:J:257:ALA:HB3	2.20	0.42
1:K:122:GLY:HA3	1:K:184:ASP:O	2.19	0.42
1:L:287:ASP:OD1	1:L:287:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:237:ARG:O	1:M:241:ARG:HG3	2.20	0.42
1:P:122:GLY:HA3	1:P:185:LEU:HD23	2.02	0.42
1:J:166:ARG:HH22	1:P:125:GLU:CD	2.23	0.42
1:B:274:LYS:NZ	1:B:335:SER:O	2.40	0.42
1:B:232:PHE:CE2	1:C:232:PHE:CE2	3.07	0.42
1:D:117:HIS:CE1	1:D:178:ALA:HA	2.55	0.42
1:I:150:LYS:H	1:I:150:LYS:HG2	1.38	0.42
1:O:274:LYS:NZ	1:O:333:TYR:O	2.43	0.42
1:P:327:ILE:HG22	1:P:331:LYS:HE3	2.02	0.42
1:H:298:ARG:CZ	1:H:313:ARG:HD2	2.50	0.42
1:P:268:PRO:O	1:P:270:PRO:HD3	2.20	0.42
1:M:242:SER:HA	1:M:245:ASP:O	2.19	0.41
1:O:200:LYS:HE3	1:O:200:LYS:HB3	1.88	0.41
1:P:176:ARG:NH2	1:P:202:ASP:OD2	2.53	0.41
1:P:280:VAL:HG12	1:P:312:PHE:CZ	2.55	0.41
1:B:230:SER:HA	1:B:231:PRO:HD2	1.91	0.41
1:J:163:ASP:HA	1:J:164:PRO:HD2	1.95	0.41
1:C:264:MET:HG2	1:C:321:ILE:HG12	2.00	0.41
1:G:199:ARG:HE	1:G:207:ILE:HD12	1.84	0.41
1:L:281:LEU:HD13	1:L:308:ARG:HD2	2.01	0.41
1:N:125:GLU:CD	1:P:166:ARG:HH22	2.23	0.41
1:L:268:PRO:O	1:L:270:PRO:HD3	2.19	0.41
1:L:123:TRP:CD1	1:L:148:VAL:HG22	2.56	0.41
1:M:269:ILE:HA	1:M:270:PRO:HD3	1.90	0.41
1:P:245:ASP:OD1	1:P:245:ASP:N	2.53	0.41
1:D:152:VAL:HG13	1:D:157:ALA:HB3	2.03	0.41
1:H:248:GLU:O	1:H:252:VAL:HG23	2.21	0.41
1:H:255:VAL:HG13	1:H:263:ARG:HA	2.02	0.41
1:A:134:LEU:HD21	1:H:243:ILE:HD12	2.02	0.41
1:B:120:ILE:HG12	1:B:182:ILE:HB	2.01	0.41
1:D:148:VAL:HG12	1:D:159:PHE:CE1	2.56	0.41
1:F:150:LYS:HD2	1:H:161:HIS:CE1	2.56	0.41
1:H:202:ASP:OD1	1:H:205:VAL:N	2.53	0.41
1:J:122:GLY:HA3	1:J:185:LEU:HD23	2.03	0.41
1:J:268:PRO:O	1:J:270:PRO:HD3	2.21	0.41
1:J:256:LEU:O	1:K:237:ARG:NH2	2.54	0.41
1:H:116:ARG:HA	1:H:116:ARG:HD2	1.78	0.41
1:C:123:TRP:CD1	1:C:148:VAL:HG22	2.55	0.41
1:J:199:ARG:HH22	1:J:205:VAL:HG12	1.86	0.41
1:N:242:SER:O	1:O:206:ARG:NH2	2.53	0.41
1:E:271:GLU:OE1	1:E:271:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:175:VAL:HG11	1:G:198:ILE:HG23	2.03	0.41
1:K:270:PRO:HD2	1:K:334:ILE:HG22	2.03	0.41
1:L:330:LEU:O	1:L:334:ILE:HG13	2.21	0.41
1:D:194:CYS:O	1:D:198:ILE:HG13	2.20	0.41
1:A:221:ARG:NH2	1:H:258:GLU:OE1	2.36	0.41
1:I:166:ARG:HH22	1:K:125:GLU:CD	2.24	0.41
1:B:280:VAL:CG2	1:B:308:ARG:HA	2.50	0.40
1:H:238:LEU:HA	1:H:238:LEU:HD23	1.92	0.40
1:K:212:GLU:HG3	1:K:232:PHE:HD1	1.86	0.40
1:B:258:GLU:OE1	1:C:221:ARG:NH2	2.50	0.40
1:B:237:ARG:NH1	1:B:248:GLU:OE2	2.55	0.40
1:C:280:VAL:HG13	1:C:310:TYR:O	2.22	0.40
1:C:262:ARG:NH1	1:C:323:LYS:HG3	2.36	0.40
1:J:271:GLU:N	1:J:271:GLU:OE1	2.53	0.40
1:N:268:PRO:O	1:N:270:PRO:HD3	2.21	0.40
1:N:330:LEU:O	1:N:334:ILE:HG13	2.22	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	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	32	71
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 ⓘ

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%)	34	71
1	B	190/207 (92%)	182 (96%)	8 (4%)	34	71
1	C	192/207 (93%)	184 (96%)	8 (4%)	34	71
1	D	193/207 (93%)	184 (95%)	9 (5%)	30	67
1	E	191/207 (92%)	184 (96%)	7 (4%)	39	75
1	F	191/207 (92%)	184 (96%)	7 (4%)	39	75
1	G	193/207 (93%)	183 (95%)	10 (5%)	27	63
1	H	191/207 (92%)	183 (96%)	8 (4%)	34	71
1	I	189/207 (91%)	179 (95%)	10 (5%)	26	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	192/207 (93%)	182 (95%)	10 (5%)	27	63
1	K	192/207 (93%)	182 (95%)	10 (5%)	27	63
1	L	189/207 (91%)	181 (96%)	8 (4%)	34	71
1	M	192/207 (93%)	181 (94%)	11 (6%)	24	60
1	N	192/207 (93%)	177 (92%)	15 (8%)	15	48
1	O	190/207 (92%)	180 (95%)	10 (5%)	26	63
1	P	190/207 (92%)	182 (96%)	8 (4%)	34	71
All	All	3058/3312 (92%)	2911 (95%)	147 (5%)	30	67

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	ARG
1	A	166	ARG
1	A	215	GLU
1	A	245	ASP
1	A	262	ARG
1	A	275	LEU
1	A	281	LEU
1	A	334	ILE
1	B	135	ARG
1	B	166	ARG
1	B	206	ARG
1	B	215	GLU
1	B	262	ARG
1	B	275	LEU
1	B	281	LEU
1	B	334	ILE
1	C	166	ARG
1	C	215	GLU
1	C	245	ASP
1	C	262	ARG
1	C	275	LEU
1	C	281	LEU
1	C	298	ARG
1	C	334	ILE
1	D	146	GLU
1	D	154	ARG
1	D	166	ARG
1	D	206	ARG

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Mol	Chain	Res	Type
1	D	215	GLU
1	D	245	ASP
1	D	262	ARG
1	D	281	LEU
1	D	337	LEU
1	E	166	ARG
1	E	215	GLU
1	E	245	ASP
1	E	262	ARG
1	E	275	LEU
1	E	281	LEU
1	E	325	GLU
1	F	116	ARG
1	F	166	ARG
1	F	206	ARG
1	F	215	GLU
1	F	245	ASP
1	F	281	LEU
1	F	334	ILE
1	G	146	GLU
1	G	149	ARG
1	G	166	ARG
1	G	215	GLU
1	G	245	ASP
1	G	262	ARG
1	G	275	LEU
1	G	281	LEU
1	G	298	ARG
1	G	334	ILE
1	H	166	ARG
1	H	206	ARG
1	H	215	GLU
1	H	245	ASP
1	H	262	ARG
1	H	275	LEU
1	H	281	LEU
1	H	325	GLU
1	I	150	LYS
1	I	154	ARG
1	I	166	ARG
1	I	215	GLU
1	I	262	ARG

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Mol	Chain	Res	Type
1	I	275	LEU
1	I	281	LEU
1	I	325	GLU
1	I	332	ASN
1	I	334	ILE
1	J	148	VAL
1	J	166	ARG
1	J	206	ARG
1	J	215	GLU
1	J	245	ASP
1	J	262	ARG
1	J	275	LEU
1	J	281	LEU
1	J	332	ASN
1	J	334	ILE
1	K	166	ARG
1	K	206	ARG
1	K	214	TYR
1	K	215	GLU
1	K	245	ASP
1	K	262	ARG
1	K	271	GLU
1	K	275	LEU
1	K	281	LEU
1	K	334	ILE
1	L	148	VAL
1	L	166	ARG
1	L	206	ARG
1	L	215	GLU
1	L	245	ASP
1	L	262	ARG
1	L	286	HIS
1	L	287	ASP
1	M	132	ARG
1	M	148	VAL
1	M	149	ARG
1	M	166	ARG
1	M	215	GLU
1	M	245	ASP
1	M	262	ARG
1	M	275	LEU
1	M	281	LEU

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Mol	Chain	Res	Type
1	M	332	ASN
1	M	334	ILE
1	N	116	ARG
1	N	117	HIS
1	N	146	GLU
1	N	148	VAL
1	N	149	ARG
1	N	166	ARG
1	N	206	ARG
1	N	215	GLU
1	N	245	ASP
1	N	262	ARG
1	N	281	LEU
1	N	298	ARG
1	N	334	ILE
1	N	337	LEU
1	N	338	VAL
1	O	148	VAL
1	O	150	LYS
1	O	166	ARG
1	O	215	GLU
1	O	245	ASP
1	O	262	ARG
1	O	274	LYS
1	O	275	LEU
1	O	281	LEU
1	O	334	ILE
1	P	148	VAL
1	P	166	ARG
1	P	215	GLU
1	P	245	ASP
1	P	279	SER
1	P	281	LEU
1	P	325	GLU
1	P	334	ILE

Some 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 carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	223/242 (92%)	0.18	3 (1%) 77 59	85, 127, 182, 198	0
1	B	222/242 (91%)	0.37	10 (4%) 34 16	93, 133, 182, 200	0
1	C	224/242 (92%)	0.30	5 (2%) 62 41	94, 136, 183, 201	0
1	D	225/242 (92%)	0.29	6 (2%) 55 30	94, 129, 186, 204	0
1	E	223/242 (92%)	0.21	6 (2%) 55 30	88, 128, 184, 200	0
1	F	223/242 (92%)	0.27	6 (2%) 55 30	91, 135, 182, 218	0
1	G	225/242 (92%)	0.32	4 (1%) 69 47	93, 134, 186, 265	0
1	H	223/242 (92%)	0.27	8 (3%) 43 21	89, 132, 184, 204	0
1	I	222/242 (91%)	0.62	24 (10%) 6 2	109, 142, 193, 223	0
1	J	224/242 (92%)	0.37	15 (6%) 19 7	110, 142, 184, 205	0
1	K	224/242 (92%)	0.37	14 (6%) 21 8	115, 148, 186, 232	0
1	L	222/242 (91%)	0.78	30 (13%) 3 1	112, 150, 199, 229	0
1	M	224/242 (92%)	0.57	23 (10%) 7 2	108, 142, 186, 214	0
1	N	224/242 (92%)	0.42	19 (8%) 11 4	107, 145, 186, 209	0
1	O	221/242 (91%)	0.38	15 (6%) 18 7	106, 139, 184, 209	0
1	P	221/242 (91%)	0.50	19 (8%) 11 4	106, 139, 187, 207	0
All	All	3570/3872 (92%)	0.39	207 (5%) 24 10	85, 139, 188, 265	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	273	SER	9.2
1	L	137	SER	8.3
1	L	336	ALA	7.8
1	O	136	GLY	7.2
1	L	335	SER	7.1

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Mol	Chain	Res	Type	RSRZ
1	N	115	SER	5.3
1	M	177	GLY	5.2
1	B	336	ALA	5.0
1	I	310	TYR	4.9
1	N	147	ASN	4.8
1	B	300	ASP	4.7
1	B	135	ARG	4.6
1	P	335	SER	4.6
1	I	311	SER	4.5
1	L	290	GLY	4.4
1	L	277	GLY	4.3
1	J	300	ASP	4.2
1	P	157	ALA	4.1
1	D	137	SER	3.9
1	C	300	ASP	3.9
1	O	277	GLY	3.9
1	M	157	ALA	3.9
1	M	338	VAL	3.8
1	L	334	ILE	3.8
1	N	300	ASP	3.8
1	I	260	SER	3.8
1	G	271	GLU	3.8
1	K	158	ASN	3.7
1	H	335	SER	3.7
1	G	307	PRO	3.6
1	N	150	LYS	3.6
1	O	271	GLU	3.6
1	L	270	PRO	3.6
1	L	278	VAL	3.6
1	I	322	GLY	3.5
1	F	282	ASP	3.5
1	L	316	ASP	3.5
1	N	177	GLY	3.5
1	G	339	PRO	3.5
1	L	273	SER	3.5
1	L	332	ASN	3.4
1	L	315	GLY	3.3
1	L	122	GLY	3.3
1	J	260	SER	3.3
1	E	115	SER	3.3
1	M	135	ARG	3.2
1	L	200	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	M	136	GLY	3.1
1	N	117	HIS	3.1
1	F	268	PRO	3.1
1	C	314	ALA	3.1
1	M	271	GLU	3.0
1	M	115	SER	3.0
1	M	323	LYS	3.0
1	N	161	HIS	3.0
1	M	176	ARG	3.0
1	P	275	LEU	3.0
1	H	336	ALA	2.9
1	L	291	VAL	2.9
1	C	307	PRO	2.9
1	K	275	LEU	2.9
1	P	312	PHE	2.9
1	L	276	GLU	2.9
1	J	271	GLU	2.9
1	J	338	VAL	2.9
1	P	310	TYR	2.9
1	O	115	SER	2.8
1	B	169	ASP	2.8
1	P	258	GLU	2.8
1	A	277	GLY	2.8
1	B	335	SER	2.8
1	M	203	GLU	2.8
1	L	299	GLY	2.8
1	D	116	ARG	2.8
1	F	275	LEU	2.8
1	O	272	GLY	2.8
1	K	115	SER	2.8
1	L	292	ILE	2.8
1	L	275	LEU	2.7
1	P	203	GLU	2.7
1	H	310	TYR	2.7
1	I	301	GLU	2.7
1	N	138	GLU	2.7
1	N	139	VAL	2.7
1	N	280	VAL	2.7
1	H	271	GLU	2.7
1	J	150	LYS	2.7
1	I	276	GLU	2.7
1	B	314	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	272	GLY	2.6
1	J	155	SER	2.6
1	L	325	GLU	2.6
1	O	268	PRO	2.6
1	I	331	LYS	2.6
1	F	301	GLU	2.6
1	C	315	GLY	2.6
1	L	176	ARG	2.6
1	P	309	ASP	2.6
1	O	261	THR	2.6
1	I	268	PRO	2.6
1	P	133	GLU	2.6
1	K	335	SER	2.6
1	P	276	GLU	2.5
1	L	138	GLU	2.5
1	O	135	ARG	2.5
1	N	202	ASP	2.5
1	E	203	GLU	2.5
1	E	336	ALA	2.5
1	E	311	SER	2.5
1	L	147	ASN	2.5
1	K	176	ARG	2.5
1	I	312	PHE	2.5
1	O	314	ALA	2.5
1	I	274	LYS	2.5
1	M	298	ARG	2.5
1	N	307	PRO	2.5
1	O	284	ASP	2.5
1	P	306	PRO	2.5
1	P	314	ALA	2.5
1	H	273	SER	2.5
1	L	271	GLU	2.5
1	J	202	ASP	2.5
1	O	273	SER	2.5
1	K	300	ASP	2.4
1	M	204	SER	2.4
1	P	315	GLY	2.4
1	M	144	GLU	2.4
1	M	300	ASP	2.4
1	M	116	ARG	2.4
1	M	337	LEU	2.4
1	D	136	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	P	136	GLY	2.4
1	P	313	ARG	2.4
1	I	261	THR	2.4
1	K	138	GLU	2.4
1	L	155	SER	2.4
1	I	277	GLY	2.4
1	I	327	ILE	2.4
1	K	155	SER	2.4
1	P	298	ARG	2.4
1	M	247	TYR	2.4
1	K	315	GLY	2.4
1	O	278	VAL	2.4
1	I	272	GLY	2.3
1	F	136	GLY	2.3
1	O	176	ARG	2.3
1	L	261	THR	2.3
1	J	133	GLU	2.3
1	H	262	ARG	2.3
1	A	145	ASP	2.3
1	L	309	ASP	2.3
1	P	154	ARG	2.3
1	I	333	TYR	2.3
1	M	299	GLY	2.3
1	K	280	VAL	2.3
1	N	116	ARG	2.3
1	I	328	GLU	2.3
1	I	300	ASP	2.3
1	K	332	ASN	2.2
1	M	261	THR	2.2
1	I	271	GLU	2.2
1	M	336	ALA	2.2
1	O	289	THR	2.2
1	H	299	GLY	2.2
1	B	273	SER	2.2
1	L	295	GLY	2.2
1	I	176	ARG	2.2
1	P	257	ALA	2.2
1	J	299	GLY	2.2
1	C	147	ASN	2.2
1	F	270	PRO	2.2
1	J	204	SER	2.2
1	N	225	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	335	SER	2.1
1	B	136	GLY	2.1
1	J	178	ALA	2.1
1	K	146	GLU	2.1
1	N	204	SER	2.1
1	I	303	ILE	2.1
1	M	178	ALA	2.1
1	H	272	GLY	2.1
1	N	299	GLY	2.1
1	M	324	PRO	2.1
1	I	116	ARG	2.1
1	E	297	GLY	2.1
1	N	135	ARG	2.1
1	N	310	TYR	2.1
1	K	271	GLU	2.1
1	A	308	ARG	2.1
1	L	263	ARG	2.1
1	B	133	GLU	2.1
1	I	336	ALA	2.1
1	J	139	VAL	2.1
1	L	223	ALA	2.1
1	M	137	SER	2.1
1	E	275	LEU	2.0
1	B	278	VAL	2.0
1	O	144	GLU	2.0
1	D	273	SER	2.0
1	J	118	VAL	2.0
1	J	136	GLY	2.0
1	G	147	ASN	2.0
1	P	301	GLU	2.0
1	K	131	LEU	2.0
1	D	339	PRO	2.0
1	D	186	GLU	2.0
1	N	154	ARG	2.0

## 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	BA	N	401	1/1	0.91	0.20	-0.73	270,270,270,270	0
2	BA	K	401	1/1	0.83	0.20	-1.52	259,259,259,259	0
2	BA	M	401	1/1	0.45	0.13	-1.54	290,290,290,290	0
2	BA	D	401	1/1	0.67	0.14	-1.74	235,235,235,235	0
2	BA	D	402	1/1	0.64	0.07	-1.93	250,250,250,250	0
2	BA	O	401	1/1	0.90	0.10	-3.08	256,256,256,256	0
2	BA	E	401	1/1	0.85	0.08	-4.03	200,200,200,200	0
2	BA	C	401	1/1	0.91	0.12	-5.09	232,232,232,232	0
2	BA	B	402	1/1	0.74	0.18	-	272,272,272,272	0
2	BA	I	403	1/1	-0.14	0.30	-	297,297,297,297	0
2	BA	F	404	1/1	0.79	0.13	-	252,252,252,252	0
2	BA	N	403	1/1	0.79	0.21	-	257,257,257,257	0
2	BA	N	402	1/1	0.83	0.07	-	289,289,289,289	0
2	BA	M	404	1/1	0.50	0.19	-	306,306,306,306	0
2	BA	A	403	1/1	0.66	0.12	-	230,230,230,230	0
2	BA	E	403	1/1	0.73	0.18	-	230,230,230,230	0
2	BA	H	401	1/1	0.72	0.16	-	226,226,226,226	0
2	BA	J	402	1/1	0.66	0.14	-	282,282,282,282	0
2	BA	I	402	1/1	0.74	0.08	-	267,267,267,267	0
2	BA	M	402	1/1	0.53	0.10	-	237,237,237,237	0
2	BA	O	402	1/1	0.63	0.10	-	248,248,248,248	0
2	BA	E	406	1/1	0.85	0.15	-	263,263,263,263	0
2	BA	O	403	1/1	0.65	0.46	-	313,313,313,313	0
2	BA	C	402	1/1	0.87	0.08	-	232,232,232,232	0
2	BA	E	402	1/1	0.76	0.07	-	233,233,233,233	0
2	BA	E	405	1/1	0.65	0.09	-	259,259,259,259	0
2	BA	B	404	1/1	0.16	0.57	-	355,355,355,355	0
2	BA	K	403	1/1	0.83	0.06	-	250,250,250,250	0
2	BA	E	404	1/1	0.66	0.08	-	256,256,256,256	0
2	BA	F	403	1/1	0.40	0.13	-	262,262,262,262	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BA	B	401	1/1	0.70	0.17	-	206,206,206,206	0
2	BA	G	404	1/1	0.58	0.15	-	259,259,259,259	0
2	BA	K	402	1/1	0.56	0.17	-	271,271,271,271	0
2	BA	F	401	1/1	0.56	0.12	-	222,222,222,222	0
2	BA	A	402	1/1	0.75	0.10	-	245,245,245,245	0
2	BA	P	402	1/1	0.79	0.17	-	309,309,309,309	0
2	BA	A	401	1/1	0.79	0.12	-	228,228,228,228	0
2	BA	G	402	1/1	0.78	0.12	-	236,236,236,236	0
2	BA	G	403	1/1	0.64	0.10	-	229,229,229,229	0
2	BA	B	403	1/1	0.54	0.28	-	245,245,245,245	0
2	BA	H	402	1/1	0.76	0.11	-	231,231,231,231	0
2	BA	K	404	1/1	0.15	0.35	-	276,276,276,276	0
2	BA	D	404	1/1	0.10	0.20	-	251,251,251,251	0
2	BA	L	402	1/1	0.35	0.13	-	320,320,320,320	0
2	BA	J	401	1/1	0.49	0.23	-	269,269,269,269	0
2	BA	F	402	1/1	0.67	0.15	-	253,253,253,253	0
2	BA	P	401	1/1	0.78	0.10	-	244,244,244,244	0
2	BA	C	403	1/1	0.56	0.08	-	256,256,256,256	0
2	BA	A	404	1/1	0.57	0.11	-	265,265,265,265	0
2	BA	P	403	1/1	0.54	0.13	-	276,276,276,276	0
2	BA	A	405	1/1	0.60	0.15	-	241,241,241,241	0
2	BA	D	405	1/1	0.25	0.29	-	254,254,254,254	0
2	BA	L	401	1/1	0.82	0.07	-	256,256,256,256	0
2	BA	I	401	1/1	0.71	0.14	-	273,273,273,273	0
2	BA	D	403	1/1	0.67	0.10	-	229,229,229,229	0
2	BA	G	401	1/1	0.93	0.15	-	230,230,230,230	0
2	BA	M	403	1/1	0.81	0.15	-	263,263,263,263	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.