



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:29 AM UTC

PDB ID : 4EI2 / pdb_00004ei2
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

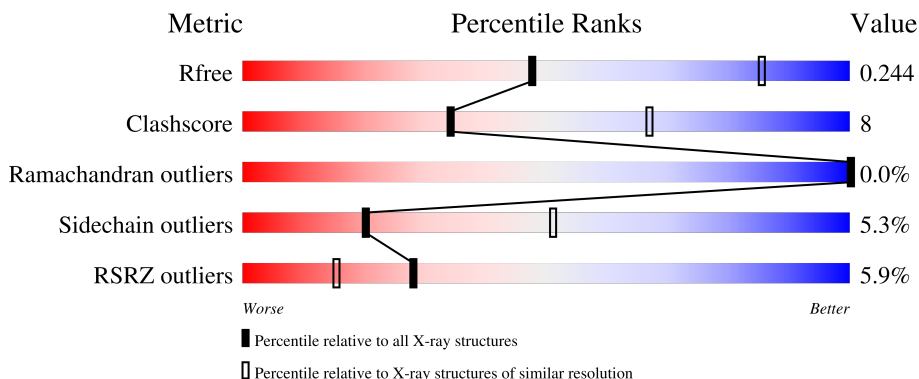
1 Overall quality at a glance

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	242	
1	B	242	
1	C	242	
1	D	242	
1	E	242	

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Mol	Chain	Length	Quality of chain
1	F	242	<p>3% 78% 12% • 8%</p>
1	G	242	<p>1% 76% 14% • 7%</p>
1	H	242	<p>3% 66% 23% • 8%</p>
1	I	242	<p>7% 71% 18% • 8%</p>
1	J	242	<p>3% 67% 24% • 7%</p>
1	K	242	<p>4% 70% 20% • 7%</p>
1	L	242	<p>7% 68% 21% • 8%</p>
1	M	242	<p>2% 73% 19% • 7%</p>
1	N	242	<p>2% 69% 19% 5% 7%</p>
1	O	242	<p>69% 19% • 9%</p>
1	P	242	<p>2% 70% 20% • 9%</p>

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
			Total	C	N	O	S			
1	A	223	Total 1732	C 1078	N 307	O 340	S 7	0	0	0
1	B	222	Total 1724	C 1072	N 306	O 339	S 7	0	0	0
1	C	224	Total 1739	C 1083	N 308	O 341	S 7	0	0	0
1	D	225	Total 1746	C 1088	N 309	O 342	S 7	0	0	0
1	E	223	Total 1732	C 1078	N 307	O 340	S 7	0	0	0
1	F	223	Total 1732	C 1078	N 307	O 340	S 7	0	0	0
1	G	225	Total 1746	C 1088	N 309	O 342	S 7	0	0	0
1	H	223	Total 1732	C 1078	N 307	O 340	S 7	0	0	0
1	I	222	Total 1721	C 1071	N 306	O 337	S 7	0	0	0
1	J	224	Total 1739	C 1083	N 308	O 341	S 7	0	0	0
1	K	224	Total 1739	C 1083	N 308	O 341	S 7	0	0	0
1	L	222	Total 1718	C 1069	N 303	O 339	S 7	0	0	0
1	M	224	Total 1739	C 1083	N 308	O 341	S 7	0	0	0
1	N	224	Total 1739	C 1083	N 308	O 341	S 7	0	0	0
1	O	221	Total 1719	C 1069	N 305	O 338	S 7	0	0	0
1	P	221	Total 1719	C 1069	N 305	O 338	S 7	0	0	0

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 (CCD ID: 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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	2	Total 2	Ba 2	0	0
2	I	3	Total 3	Ba 3	0	0
2	J	2	Total 2	Ba 2	0	0
2	K	4	Total 4	Ba 4	0	0
2	L	2	Total 2	Ba 2	0	0
2	M	4	Total 4	Ba 4	0	0
2	N	3	Total 3	Ba 3	0	0
2	O	3	Total 3	Ba 3	0	0
2	P	3	Total 3	Ba 3	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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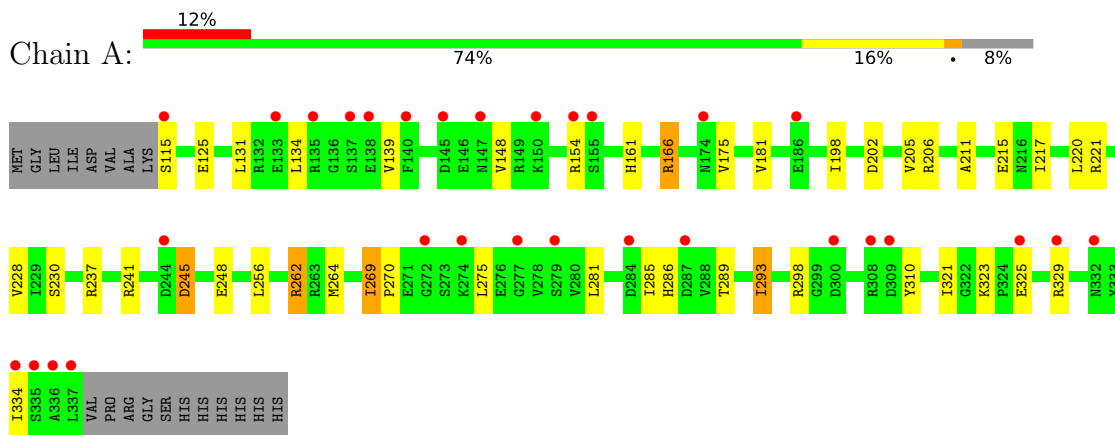
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	2	Total O 2 2	0	0
3	P	1	Total O 1 1	0	0

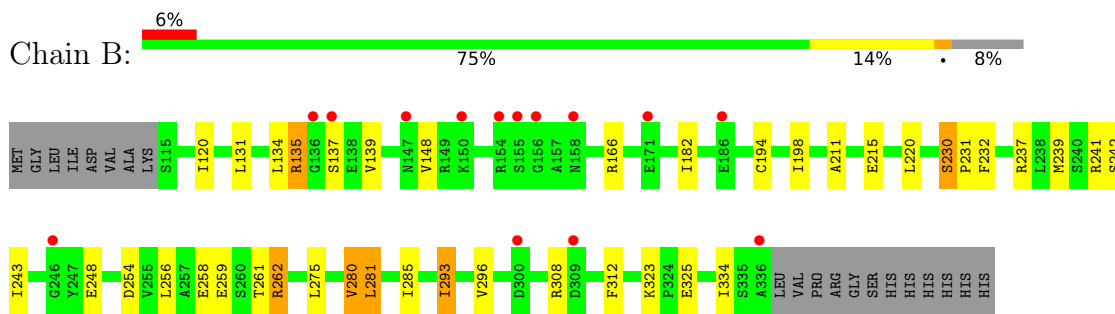
3 Residue-property plots [i](#)

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.

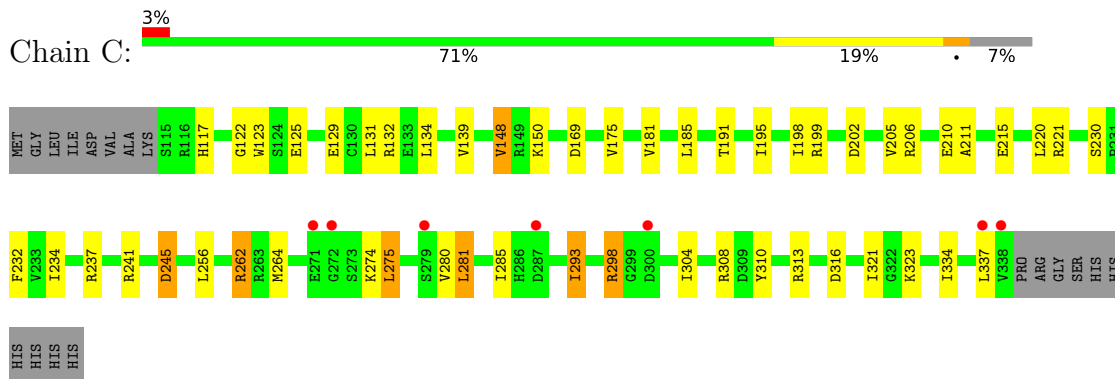
- Molecule 1: Calcium-gated potassium channel mthK



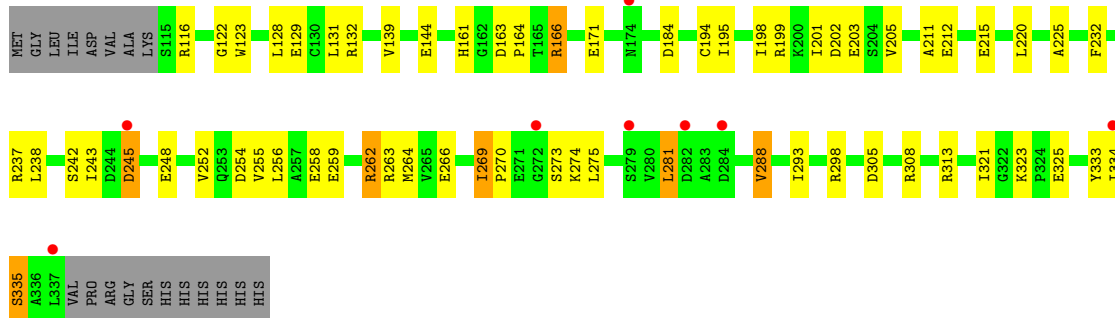
- Molecule 1: Calcium-gated potassium channel mthK



- Molecule 1: Calcium-gated potassium channel mthK

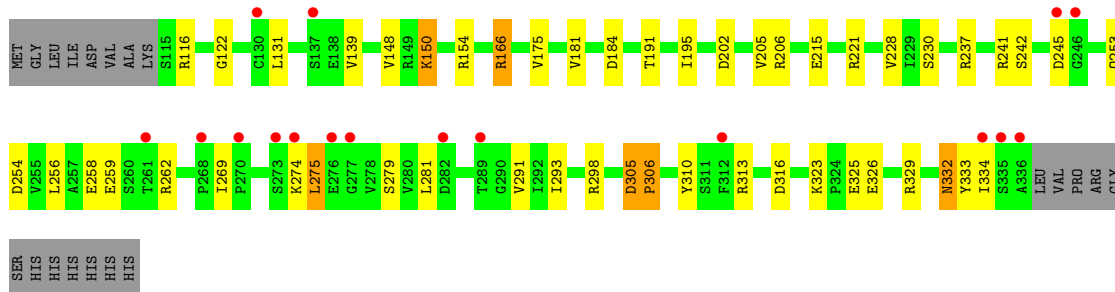


Chain H:  3% 66% 23% 8%



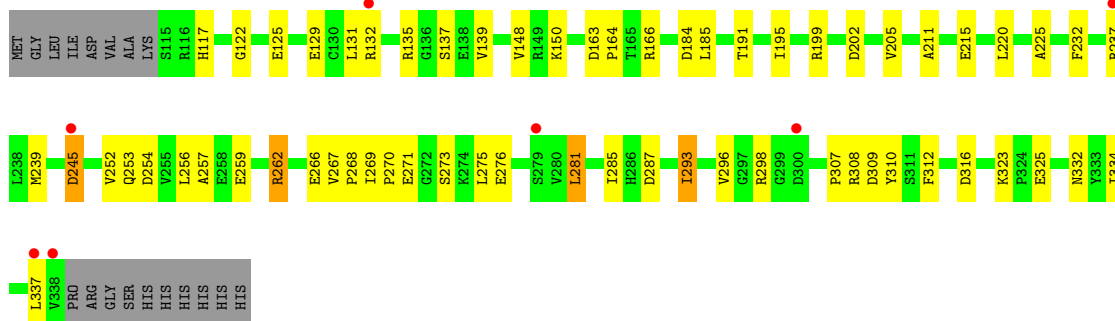
• Molecule 1: Calcium-gated potassium channel mthK

Chain I:  7% 71% 18% 8%



• Molecule 1: Calcium-gated potassium channel mthK

Chain J:  3% 67% 24% 7%



• Molecule 1: Calcium-gated potassium channel mthK

Chain K:  4% 70% 20% 7%





• Molecule 1: Calcium-gated potassium channel mthK



4 Data and refinement statistics

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 30.00 – 3.11	Depositor EDS
% Data completeness (in resolution range)	93.9 (30.00-3.11) 90.7 (30.00-3.11)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 3.11Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.209 , 0.242 0.210 , 0.244	Depositor DCC
R_{free} test set	2000 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å ²)	69.9	Xtrriage
Anisotropy	0.182	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 119.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.48	0/1753	0.92	4/2366 (0.2%)
1	B	0.42	0/1745	0.89	2/2355 (0.1%)
1	C	0.41	0/1760	0.86	0/2376
1	D	0.47	0/1768	0.89	2/2388 (0.1%)
1	E	0.47	0/1753	0.95	6/2366 (0.3%)
1	F	0.39	0/1753	0.89	2/2366 (0.1%)
1	G	0.41	0/1768	0.86	1/2388 (0.0%)
1	H	0.43	0/1753	0.92	5/2366 (0.2%)
1	I	0.44	0/1742	0.94	5/2351 (0.2%)
1	J	0.39	0/1760	0.85	2/2376 (0.1%)
1	K	0.42	0/1760	0.88	1/2376 (0.0%)
1	L	0.45	0/1739	0.88	4/2348 (0.2%)
1	M	0.43	0/1760	0.89	1/2376 (0.0%)
1	N	0.41	0/1760	0.89	4/2376 (0.2%)
1	O	0.40	0/1740	0.85	2/2348 (0.1%)
1	P	0.43	0/1740	0.88	0/2348
All	All	0.43	0/28054	0.89	41/37870 (0.1%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	269	ILE	CA-C-N	7.68	127.58	120.21
1	F	269	ILE	C-N-CA	7.68	127.58	120.21
1	H	269	ILE	CA-C-N	6.84	128.38	119.84
1	H	269	ILE	C-N-CA	6.84	128.38	119.84
1	N	269	ILE	CA-C-N	6.45	126.41	120.21
1	N	269	ILE	C-N-CA	6.45	126.41	120.21
1	D	269	ILE	CA-C-N	6.29	127.70	119.84
1	D	269	ILE	C-N-CA	6.29	127.70	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	269	ILE	CA-C-N	6.03	126.00	120.21
1	L	269	ILE	C-N-CA	6.03	126.00	120.21
1	A	230	SER	CA-C-N	5.98	125.60	119.56
1	A	230	SER	C-N-CA	5.98	125.60	119.56
1	A	269	ILE	CA-C-N	5.97	125.94	120.21
1	A	269	ILE	C-N-CA	5.97	125.94	120.21
1	M	285	ILE	N-CA-C	5.93	116.67	110.62
1	H	288	VAL	CB-CA-C	-5.90	104.15	111.94
1	E	335	SER	N-CA-C	5.72	119.97	112.13
1	E	230	SER	CA-C-N	5.61	125.22	119.56
1	E	230	SER	C-N-CA	5.61	125.22	119.56
1	N	163	ASP	CA-C-N	5.55	125.22	119.56
1	N	163	ASP	C-N-CA	5.55	125.22	119.56
1	E	269	ILE	CA-C-N	5.51	126.28	120.11
1	E	269	ILE	C-N-CA	5.51	126.28	120.11
1	O	230	SER	CA-C-N	5.47	125.14	119.56
1	O	230	SER	C-N-CA	5.47	125.14	119.56
1	J	267	VAL	CA-C-N	5.35	125.56	120.31
1	J	267	VAL	C-N-CA	5.35	125.56	120.31
1	I	306	PRO	O-C-N	5.33	123.76	121.31
1	H	335	SER	CB-CA-C	-5.32	108.87	115.89
1	L	290	GLY	N-CA-C	-5.22	107.34	114.64
1	I	305	ASP	CA-C-N	5.21	123.47	119.66
1	I	305	ASP	C-N-CA	5.21	123.47	119.66
1	K	290	GLY	N-CA-C	-5.21	108.14	114.92
1	L	306	PRO	O-C-N	5.19	123.70	121.31
1	G	281	LEU	N-CA-C	-5.17	105.56	111.14
1	B	230	SER	CA-C-N	5.14	124.64	119.19
1	B	230	SER	C-N-CA	5.14	124.64	119.19
1	H	335	SER	N-CA-C	5.13	117.64	109.02
1	I	323	LYS	CA-C-N	5.10	125.13	119.32
1	I	323	LYS	C-N-CA	5.10	125.13	119.32
1	E	243	ILE	N-CA-C	-5.01	105.82	110.53

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	26	0
1	B	1724	0	1731	29	0
1	C	1739	0	1751	39	0
1	D	1746	0	1758	20	0
1	E	1732	0	1742	25	0
1	F	1732	0	1742	25	0
1	G	1746	0	1758	26	0
1	H	1732	0	1742	40	0
1	I	1721	0	1729	32	0
1	J	1739	0	1751	39	0
1	K	1739	0	1751	39	0
1	L	1718	0	1720	39	0
1	M	1739	0	1751	29	0
1	N	1739	0	1751	38	0
1	O	1719	0	1726	36	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	424	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 8.

All (424) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD2	1:J:245:ASP:N	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:OD2	1:H:245:ASP:N	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:OD1	1:F:245:ASP:N	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:L:262:ARG:HB3	1:L:322:GLY:C	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:G:245:ASP:OD2	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:OD2	1:O:245:ASP:N	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:221:ARG:NH2	1:G:258:GLU:OE1	2.37	0.54
1:F:232:PHE:HD1	1:G:125:GLU:HB3	1.73	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:J:125:GLU:CD	1:L:166:ARG:HH22	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:256:LEU:O	1:P:237:ARG:NH2	2.45	0.50
1:L:241:ARG:NH1	1:M:259:GLU:OE2	2.44	0.50
1:N:221:ARG:HH22	1:O:258:GLU:CD	2.19	0.49
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:O:289:THR:HG21	1:O:330:LEU:HD13	1.95	0.48
1:B:194:CYS:O	1:B:198:ILE:HG13	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:264:MET:HE2	1:M:319:LEU:HD11	1.96	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:O	1:K:214:TYR:HD1	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:H:122:GLY:HA3	1:H:184:ASP:O	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:O:120:ILE:HG12	1:O:182:ILE:HB	1.96	0.47
1:O:274:LYS:NZ	1:O:333:TYR:O	2.43	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:F:125:GLU:CD	1:H:166:ARG:HH22	2.22	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:J:166:ARG:HH22	1:P:125:GLU:CD	2.23	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:N:125:GLU:CD	1:P:166:ARG:HH22	2.23	0.46
1:N:258:GLU:CD	1:O:221:ARG:HH22	2.24	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:I:166:ARG:HH22	1:K:125:GLU:CD	2.24	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H	1:O:150:LYS:HG2	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:K:169:ASP:OD2	1:M:154:ARG:NH2	2.51	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: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:K:264:MET:HE3	1:K:294:ILE:HG13	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:221:ARG:HH22	1:G:258:GLU:CD	2.24	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:I:221:ARG:NH2	1:P:258:GLU:OE1	2.48	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: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:J:287:ASP:OD1	1:K:308:ARG:NH1	2.52	0.42
1:K:294:ILE:HD13	1:K:294:ILE:HA	1.91	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:166:ARG:HH22	1:M:125:GLU:CD	2.27	0.42
1:N:247:TYR:HB2	1:O:266:GLU:CD	2.45	0.42
1:L:287:ASP:OD1	1:L:287:ASP:N	2.52	0.42
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: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:E:166:ARG:HH22	1:G:125:GLU:CD	2.28	0.42
1:I:150:LYS:H	1:I:150:LYS:HG2	1.38	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:M:262:ARG:HB3	1:M:322:GLY:C	2.45	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:B:135:ARG:C	1:B:137:SER:H	2.28	0.41
1:L:268:PRO:O	1:L:270:PRO:HD3	2.19	0.41
1:A:286:HIS:HE2	1:H:305:ASP:CG	2.28	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:256:LEU:O	1:K:237:ARG:NH2	2.54	0.41
1:J:268:PRO:O	1:J:270:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:116:ARG:HD2	1:H:116:ARG:HA	1.78	0.41
1:C:123:TRP:CD1	1:C:148:VAL:HG22	2.55	0.41
1:E:271:GLU:OE1	1:E:271:GLU:N	2.54	0.41
1:G:175:VAL:HG11	1:G:198:ILE:HG23	2.03	0.41
1:J:199:ARG:HH22	1:J:205:VAL:HG12	1.86	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:N:242:SER:O	1:O:206:ARG:NH2	2.53	0.41
1:A:125:GLU:CD	1:G:166:ARG:HH22	2.28	0.41
1:A:221:ARG:NH2	1:H:258:GLU:OE1	2.36	0.41
1:D:194:CYS:O	1:D:198:ILE:HG13	2.20	0.41
1:B:280:VAL:CG2	1:B:308:ARG:HA	2.50	0.40
1:H:238:LEU:HD23	1:H:238:LEU:HA	1.92	0.40
1:K:212:GLU:HG3	1:K:232:PHE:HD1	1.86	0.40
1:K:235:SER:OG	1:K:239:MET:HE3	2.22	0.40
1:A:166:ARG:HH22	1:C:125:GLU:CD	2.29	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:262:ARG:NH1	1:C:323:LYS:HG3	2.36	0.40
1:C:280:VAL:HG13	1:C:310:TYR:O	2.22	0.40
1:J:271:GLU:OE1	1:J:271:GLU:N	2.53	0.40
1:N:268:PRO:O	1:N:270:PRO:HD3	2.21	0.40
1:B:258:GLU:CD	1:C:221:ARG:HH22	2.29	0.40
1:N:330:LEU:O	1:N:334:ILE:HG13	2.22	0.40
1:O:139:VAL:C	1:O:140:PHE:HD1	2.30	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	24	57
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%)	180 (94%)	11 (6%)	18	48
1	B	190/207 (92%)	179 (94%)	11 (6%)	18	48
1	C	192/207 (93%)	182 (95%)	10 (5%)	21	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	193/207 (93%)	185 (96%)	8 (4%)	27	59
1	E	191/207 (92%)	182 (95%)	9 (5%)	23	55
1	F	191/207 (92%)	184 (96%)	7 (4%)	30	61
1	G	193/207 (93%)	182 (94%)	11 (6%)	18	49
1	H	191/207 (92%)	183 (96%)	8 (4%)	26	58
1	I	189/207 (91%)	177 (94%)	12 (6%)	16	45
1	J	192/207 (93%)	180 (94%)	12 (6%)	16	45
1	K	192/207 (93%)	182 (95%)	10 (5%)	21	51
1	L	189/207 (91%)	181 (96%)	8 (4%)	26	58
1	M	192/207 (93%)	181 (94%)	11 (6%)	18	49
1	N	192/207 (93%)	178 (93%)	14 (7%)	13	40
1	O	190/207 (92%)	178 (94%)	12 (6%)	16	45
1	P	190/207 (92%)	181 (95%)	9 (5%)	23	55
All	All	3058/3312 (92%)	2895 (95%)	163 (5%)	20	51

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	VAL
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	293	ILE
1	A	325	GLU
1	A	334	ILE
1	B	135	ARG
1	B	148	VAL
1	B	166	ARG
1	B	215	GLU
1	B	262	ARG
1	B	275	LEU
1	B	280	VAL
1	B	281	LEU

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Mol	Chain	Res	Type
1	B	293	ILE
1	B	325	GLU
1	B	334	ILE
1	C	117	HIS
1	C	148	VAL
1	C	215	GLU
1	C	245	ASP
1	C	262	ARG
1	C	275	LEU
1	C	281	LEU
1	C	293	ILE
1	C	298	ARG
1	C	334	ILE
1	D	146	GLU
1	D	148	VAL
1	D	154	ARG
1	D	215	GLU
1	D	245	ASP
1	D	262	ARG
1	D	281	LEU
1	D	337	LEU
1	E	148	VAL
1	E	166	ARG
1	E	215	GLU
1	E	262	ARG
1	E	275	LEU
1	E	280	VAL
1	E	281	LEU
1	E	293	ILE
1	E	325	GLU
1	F	215	GLU
1	F	245	ASP
1	F	262	ARG
1	F	274	LYS
1	F	281	LEU
1	F	293	ILE
1	F	334	ILE
1	G	146	GLU
1	G	148	VAL
1	G	149	ARG
1	G	215	GLU
1	G	245	ASP

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Mol	Chain	Res	Type
1	G	262	ARG
1	G	275	LEU
1	G	281	LEU
1	G	293	ILE
1	G	298	ARG
1	G	334	ILE
1	H	166	ARG
1	H	215	GLU
1	H	245	ASP
1	H	262	ARG
1	H	275	LEU
1	H	281	LEU
1	H	293	ILE
1	H	325	GLU
1	I	148	VAL
1	I	150	LYS
1	I	154	ARG
1	I	166	ARG
1	I	215	GLU
1	I	262	ARG
1	I	275	LEU
1	I	281	LEU
1	I	293	ILE
1	I	325	GLU
1	I	332	ASN
1	I	334	ILE
1	J	117	HIS
1	J	148	VAL
1	J	215	GLU
1	J	245	ASP
1	J	262	ARG
1	J	275	LEU
1	J	281	LEU
1	J	293	ILE
1	J	325	GLU
1	J	332	ASN
1	J	334	ILE
1	J	337	LEU
1	K	148	VAL
1	K	215	GLU
1	K	245	ASP
1	K	262	ARG

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Mol	Chain	Res	Type
1	K	271	GLU
1	K	275	LEU
1	K	281	LEU
1	K	293	ILE
1	K	325	GLU
1	K	334	ILE
1	L	148	VAL
1	L	166	ARG
1	L	215	GLU
1	L	245	ASP
1	L	262	ARG
1	L	287	ASP
1	L	293	ILE
1	L	325	GLU
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
1	M	325	GLU
1	M	332	ASN
1	M	334	ILE
1	N	116	ARG
1	N	146	GLU
1	N	148	VAL
1	N	149	ARG
1	N	154	ARG
1	N	215	GLU
1	N	245	ASP
1	N	262	ARG
1	N	281	LEU
1	N	293	ILE
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

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Mol	Chain	Res	Type
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	293	ILE
1	O	325	GLU
1	O	334	ILE
1	P	148	VAL
1	P	215	GLU
1	P	245	ASP
1	P	262	ARG
1	P	279	SER
1	P	281	LEU
1	P	293	ILE
1	P	325	GLU
1	P	334	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	GLN
1	B	158	ASN
1	B	227	GLN
1	C	117	HIS
1	C	227	GLN
1	D	227	GLN
1	G	227	GLN
1	H	227	GLN
1	I	227	GLN
1	I	332	ASN
1	L	219	GLN
1	L	227	GLN
1	O	158	ASN
1	O	227	GLN

5.3.3 RNA

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 oligosaccharides 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 [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	223/242 (92%)	0.82	30 (13%) 7 4	85, 127, 182, 198	0
1	B	222/242 (91%)	0.48	14 (6%) 26 14	93, 133, 182, 200	0
1	C	224/242 (92%)	0.41	7 (3%) 51 30	94, 136, 183, 201	0
1	D	225/242 (92%)	0.88	41 (18%) 3 1	94, 129, 186, 204	0
1	E	223/242 (92%)	0.79	29 (13%) 7 4	88, 128, 184, 200	0
1	F	223/242 (92%)	0.30	8 (3%) 46 26	91, 135, 182, 218	0
1	G	225/242 (92%)	0.31	2 (0%) 81 63	93, 134, 186, 265	0
1	H	223/242 (92%)	0.49	8 (3%) 46 26	89, 132, 184, 204	0
1	I	222/242 (91%)	0.67	17 (7%) 19 10	109, 142, 193, 223	0
1	J	224/242 (92%)	0.41	7 (3%) 51 30	110, 142, 184, 205	0
1	K	224/242 (92%)	0.50	10 (4%) 38 20	115, 148, 186, 232	0
1	L	222/242 (91%)	0.82	18 (8%) 18 10	112, 150, 199, 229	0
1	M	224/242 (92%)	0.55	6 (2%) 56 35	108, 142, 186, 214	0
1	N	224/242 (92%)	0.39	6 (2%) 56 35	107, 145, 186, 209	0
1	O	221/242 (91%)	0.23	1 (0%) 87 73	106, 139, 184, 209	0
1	P	221/242 (91%)	0.47	6 (2%) 56 35	106, 139, 187, 207	0
All	All	3570/3872 (92%)	0.53	210 (5%) 28 15	85, 139, 188, 265	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	271	GLU	5.2
1	I	245	ASP	4.9
1	D	279	SER	4.6
1	D	287	ASP	4.4
1	D	308	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	287	ASP	4.2
1	A	335	SER	4.1
1	C	338	VAL	4.1
1	D	311	SER	4.0
1	D	282	ASP	4.0
1	F	336	ALA	3.9
1	A	274	LYS	3.8
1	D	272	GLY	3.8
1	L	314	ALA	3.7
1	I	270	PRO	3.7
1	H	279	SER	3.6
1	C	300	ASP	3.6
1	A	137	SER	3.5
1	H	334	ILE	3.5
1	F	308	ARG	3.4
1	I	277	GLY	3.4
1	E	277	GLY	3.4
1	D	309	ASP	3.3
1	D	310	TYR	3.3
1	A	147	ASN	3.3
1	D	278	VAL	3.3
1	D	337	LEU	3.3
1	D	137	SER	3.3
1	F	279	SER	3.3
1	M	237	ARG	3.2
1	E	115	SER	3.2
1	D	284	ASP	3.2
1	L	137	SER	3.2
1	B	147	ASN	3.2
1	D	115	SER	3.1
1	E	336	ALA	3.1
1	D	275	LEU	3.1
1	H	337	LEU	3.1
1	E	315	GLY	3.1
1	E	284	ASP	3.1
1	A	337	LEU	3.0
1	I	246	GLY	3.0
1	A	115	SER	3.0
1	E	309	ASP	3.0
1	D	245	ASP	3.0
1	K	338	VAL	3.0
1	J	338	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	332	ASN	2.9
1	N	338	VAL	2.9
1	A	145	ASP	2.9
1	E	287	ASP	2.9
1	A	325	GLU	2.9
1	D	339	PRO	2.9
1	E	307	PRO	2.9
1	O	270	PRO	2.9
1	K	337	LEU	2.9
1	D	186	GLU	2.8
1	A	336	ALA	2.8
1	H	174	ASN	2.8
1	E	299	GLY	2.8
1	C	271	GLU	2.8
1	A	300	ASP	2.8
1	B	246	GLY	2.8
1	B	336	ALA	2.8
1	E	281	LEU	2.8
1	E	279	SER	2.7
1	H	284	ASP	2.7
1	D	312	PHE	2.7
1	A	244	ASP	2.7
1	A	174	ASN	2.7
1	D	270	PRO	2.7
1	B	150	LYS	2.7
1	E	282	ASP	2.7
1	L	277	GLY	2.6
1	E	310	TYR	2.6
1	P	246	GLY	2.6
1	A	133	GLU	2.6
1	I	130	CYS	2.6
1	D	273	SER	2.6
1	L	312	PHE	2.6
1	P	312	PHE	2.6
1	L	336	ALA	2.6
1	E	308	ARG	2.6
1	I	274	LYS	2.6
1	H	282	ASP	2.6
1	E	147	ASN	2.6
1	D	281	LEU	2.6
1	E	280	VAL	2.6
1	A	334	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	329	ARG	2.6
1	D	329	ARG	2.6
1	K	161	HIS	2.5
1	F	300	ASP	2.5
1	D	276	GLU	2.5
1	A	308	ARG	2.5
1	A	284	ASP	2.5
1	E	332	ASN	2.5
1	I	276	GLU	2.5
1	A	140	PHE	2.5
1	L	315	GLY	2.5
1	E	137	SER	2.5
1	A	277	GLY	2.5
1	B	156	GLY	2.5
1	E	311	SER	2.5
1	A	186	GLU	2.5
1	B	309	ASP	2.5
1	B	137	SER	2.4
1	I	137	SER	2.4
1	D	277	GLY	2.4
1	B	171	GLU	2.4
1	F	146	GLU	2.4
1	L	155	SER	2.4
1	A	150	LYS	2.4
1	G	147	ASN	2.4
1	L	270	PRO	2.4
1	D	300	ASP	2.4
1	L	288	VAL	2.4
1	N	303	ILE	2.4
1	E	328	GLU	2.4
1	L	115	SER	2.4
1	C	272	GLY	2.4
1	B	154	ARG	2.4
1	I	273	SER	2.4
1	A	135	ARG	2.3
1	I	334	ILE	2.3
1	D	288	VAL	2.3
1	D	307	PRO	2.3
1	D	335	SER	2.3
1	P	115	SER	2.3
1	I	261	THR	2.3
1	I	289	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	337	LEU	2.3
1	E	312	PHE	2.3
1	M	337	LEU	2.3
1	N	161	HIS	2.3
1	B	186	GLU	2.3
1	E	288	VAL	2.3
1	A	154	ARG	2.3
1	A	272	GLY	2.3
1	D	334	ILE	2.3
1	L	268	PRO	2.3
1	F	137	SER	2.3
1	E	275	LEU	2.3
1	F	337	LEU	2.3
1	F	284	ASP	2.3
1	P	282	ASP	2.3
1	A	138	GLU	2.3
1	B	155	SER	2.3
1	E	335	SER	2.3
1	I	335	SER	2.3
1	E	154	ARG	2.3
1	G	338	VAL	2.3
1	B	136	GLY	2.2
1	I	336	ALA	2.2
1	L	154	ARG	2.2
1	E	145	ASP	2.2
1	L	276	GLU	2.2
1	D	313	ARG	2.2
1	A	279	SER	2.2
1	D	274	LYS	2.2
1	M	271	GLU	2.2
1	N	337	LEU	2.2
1	L	306	PRO	2.2
1	B	300	ASP	2.2
1	J	300	ASP	2.2
1	D	338	VAL	2.2
1	J	337	LEU	2.2
1	K	153	LEU	2.2
1	M	276	GLU	2.2
1	D	224	GLY	2.2
1	H	245	ASP	2.2
1	I	282	ASP	2.2
1	L	334	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	155	SER	2.1
1	C	279	SER	2.1
1	D	246	GLY	2.1
1	I	312	PHE	2.1
1	E	254	ASP	2.1
1	J	245	ASP	2.1
1	D	314	ALA	2.1
1	J	132	ARG	2.1
1	E	271	GLU	2.1
1	I	268	PRO	2.1
1	K	270	PRO	2.1
1	D	332	ASN	2.1
1	C	287	ASP	2.1
1	M	287	ASP	2.1
1	D	325	GLU	2.1
1	L	146	GLU	2.1
1	J	279	SER	2.1
1	L	316	ASP	2.1
1	D	289	THR	2.1
1	K	261	THR	2.1
1	K	268	PRO	2.1
1	B	158	ASN	2.1
1	M	281	LEU	2.1
1	A	309	ASP	2.1
1	H	272	GLY	2.1
1	N	140	PHE	2.1
1	P	271	GLU	2.1
1	K	172	LYS	2.0
1	K	308	ARG	2.0
1	K	317	ILE	2.0
1	N	117	HIS	2.0
1	D	315	GLY	2.0
1	D	133	GLU	2.0
1	E	133	GLU	2.0
1	J	237	ARG	2.0
1	P	281	LEU	2.0
1	L	303	ILE	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BA	O	403	1/1	0.58	0.19	313,313,313,313	0
2	BA	B	404	1/1	0.62	0.22	355,355,355,355	0
2	BA	M	404	1/1	0.76	0.13	306,306,306,306	0
2	BA	A	402	1/1	0.77	0.10	245,245,245,245	0
2	BA	D	405	1/1	0.77	0.17	254,254,254,254	0
2	BA	D	402	1/1	0.78	0.13	250,250,250,250	0
2	BA	P	402	1/1	0.78	0.16	309,309,309,309	0
2	BA	N	402	1/1	0.79	0.10	289,289,289,289	0
2	BA	I	402	1/1	0.82	0.09	267,267,267,267	0
2	BA	I	403	1/1	0.82	0.14	297,297,297,297	0
2	BA	K	404	1/1	0.82	0.17	276,276,276,276	0
2	BA	L	402	1/1	0.82	0.09	320,320,320,320	0
2	BA	G	404	1/1	0.83	0.13	259,259,259,259	0
2	BA	E	404	1/1	0.83	0.10	256,256,256,256	0
2	BA	E	405	1/1	0.83	0.18	259,259,259,259	0
2	BA	A	404	1/1	0.84	0.13	265,265,265,265	0
2	BA	B	402	1/1	0.85	0.17	272,272,272,272	0
2	BA	J	402	1/1	0.85	0.09	282,282,282,282	0
2	BA	F	404	1/1	0.86	0.10	252,252,252,252	0
2	BA	G	403	1/1	0.86	0.10	229,229,229,229	0
2	BA	D	403	1/1	0.87	0.09	229,229,229,229	0
2	BA	C	403	1/1	0.87	0.09	256,256,256,256	0
2	BA	H	402	1/1	0.87	0.10	231,231,231,231	0
2	BA	E	402	1/1	0.87	0.08	233,233,233,233	0
2	BA	P	403	1/1	0.87	0.11	276,276,276,276	0
2	BA	F	402	1/1	0.88	0.10	253,253,253,253	0
2	BA	F	403	1/1	0.88	0.08	262,262,262,262	0
2	BA	M	402	1/1	0.88	0.11	237,237,237,237	0
2	BA	I	401	1/1	0.88	0.13	273,273,273,273	0
2	BA	C	402	1/1	0.89	0.09	232,232,232,232	0
2	BA	N	403	1/1	0.89	0.11	257,257,257,257	0
2	BA	F	401	1/1	0.89	0.11	222,222,222,222	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BA	A	405	1/1	0.89	0.08	241,241,241,241	0
2	BA	D	404	1/1	0.89	0.11	251,251,251,251	0
2	BA	N	401	1/1	0.90	0.16	270,270,270,270	0
2	BA	G	402	1/1	0.90	0.08	236,236,236,236	0
2	BA	E	406	1/1	0.90	0.20	263,263,263,263	0
2	BA	H	401	1/1	0.91	0.13	226,226,226,226	0
2	BA	P	401	1/1	0.91	0.14	244,244,244,244	0
2	BA	M	403	1/1	0.91	0.14	263,263,263,263	0
2	BA	O	402	1/1	0.91	0.07	248,248,248,248	0
2	BA	M	401	1/1	0.92	0.14	290,290,290,290	0
2	BA	K	402	1/1	0.92	0.07	271,271,271,271	0
2	BA	D	401	1/1	0.92	0.11	235,235,235,235	0
2	BA	A	403	1/1	0.92	0.08	230,230,230,230	0
2	BA	B	403	1/1	0.93	0.12	245,245,245,245	0
2	BA	K	403	1/1	0.93	0.07	250,250,250,250	0
2	BA	J	401	1/1	0.93	0.14	269,269,269,269	0
2	BA	E	403	1/1	0.93	0.12	230,230,230,230	0
2	BA	O	401	1/1	0.95	0.08	256,256,256,256	0
2	BA	K	401	1/1	0.95	0.13	259,259,259,259	0
2	BA	G	401	1/1	0.95	0.14	230,230,230,230	0
2	BA	B	401	1/1	0.96	0.10	206,206,206,206	0
2	BA	L	401	1/1	0.96	0.11	256,256,256,256	0
2	BA	A	401	1/1	0.96	0.11	228,228,228,228	0
2	BA	C	401	1/1	0.96	0.11	232,232,232,232	0
2	BA	E	401	1/1	0.98	0.08	200,200,200,200	0

6.5 Other polymers [i](#)

There are no such residues in this entry.