Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 09:08 AM EST

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

This is a 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:

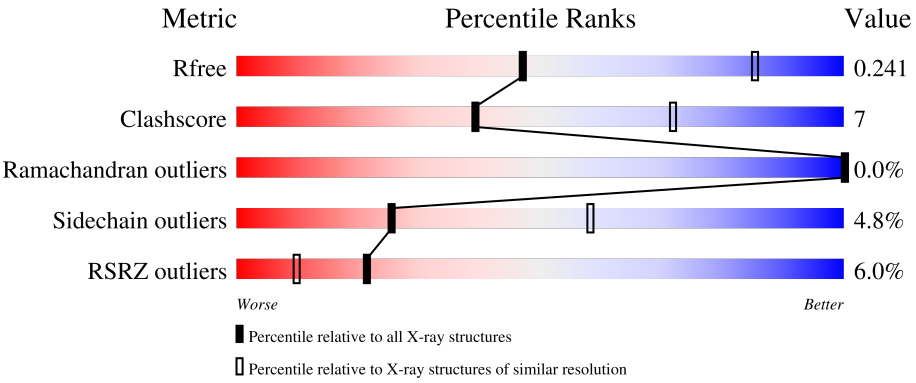
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	242	2% 76% 15% • 8%
1	B	242	4% 75% 16% • 8%
1	C	242	2% 71% 19% • 7%
1	D	242	2% 77% 15% • 7%
1	E	242	2% 74% 18% 8%

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BA	B	404	-	-	-	X
2	BA	O	403	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 27805 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Calcium-gated potassium channel mthK.

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

There are 192 discrepancies between the modelled and reference sequences:

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

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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	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 Ba 2 2	0	0
2	I	3	Total Ba 3 3	0	0
2	J	2	Total Ba 2 2	0	0
2	K	4	Total Ba 4 4	0	0
2	L	2	Total Ba 2 2	0	0
2	M	4	Total Ba 4 4	0	0
2	N	3	Total Ba 3 3	0	0
2	O	3	Total Ba 3 3	0	0
2	P	3	Total Ba 3 3	0	0

- Molecule 3 is water.

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

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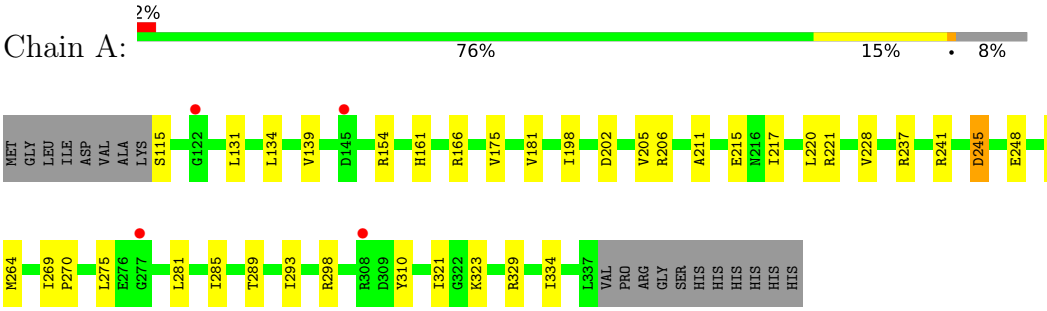
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	2	Total O 2 2	0	0
3	P	1	Total O 1 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

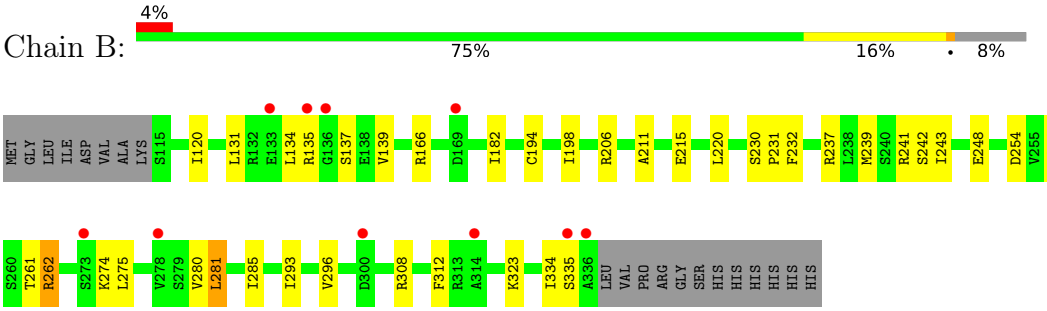
• Molecule 1: Calcium-gated potassium channel mthK

Chain A:



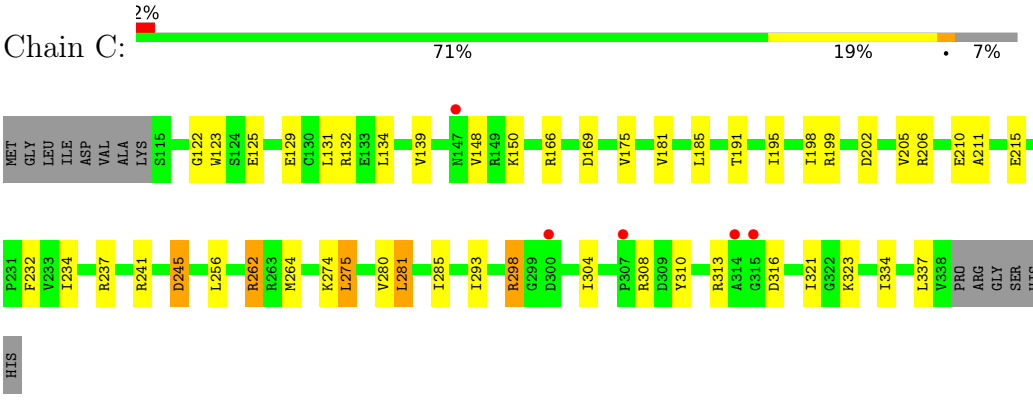
• Molecule 1: Calcium-gated potassium channel mthK

Chain B:



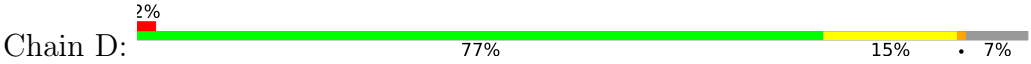
• Molecule 1: Calcium-gated potassium channel mthK

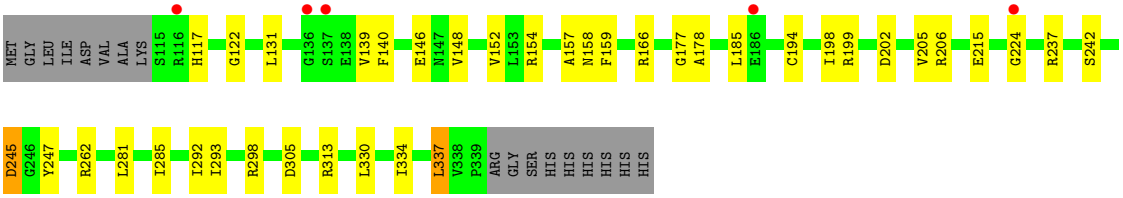
Chain C:



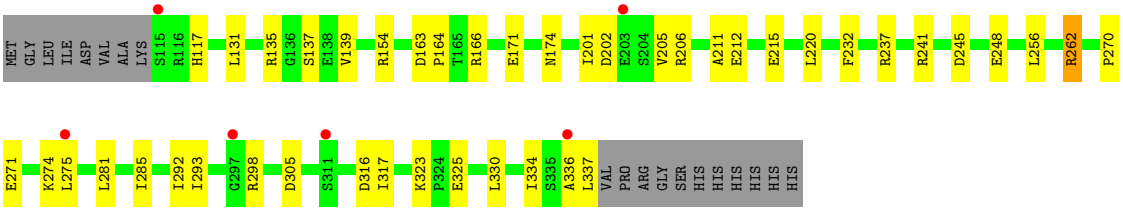
• Molecule 1: Calcium-gated potassium channel mthK

Chain D:

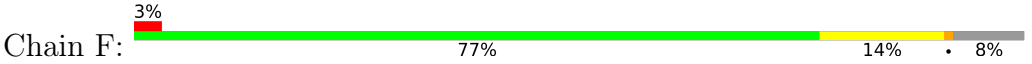


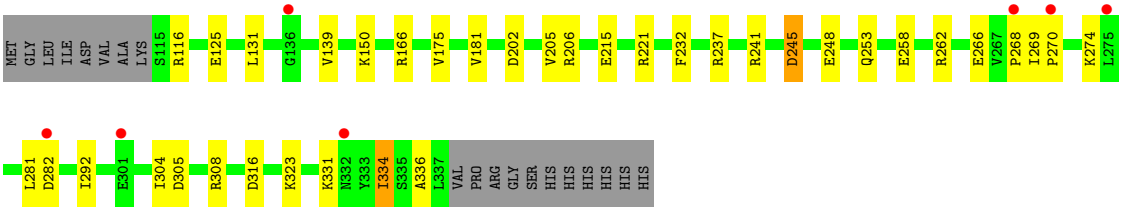


• Molecule 1: Calcium-gated potassium channel mthK

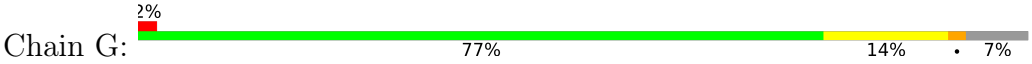


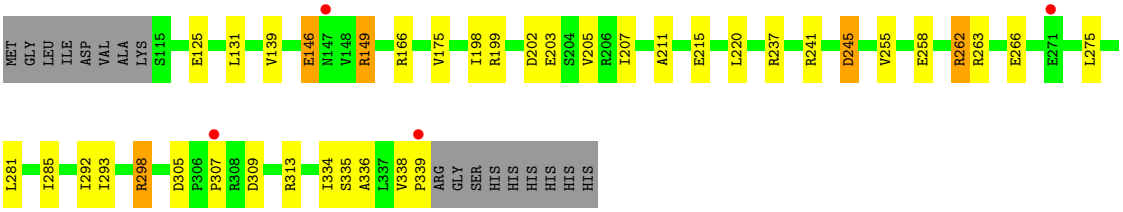
• Molecule 1: Calcium-gated potassium channel mthK



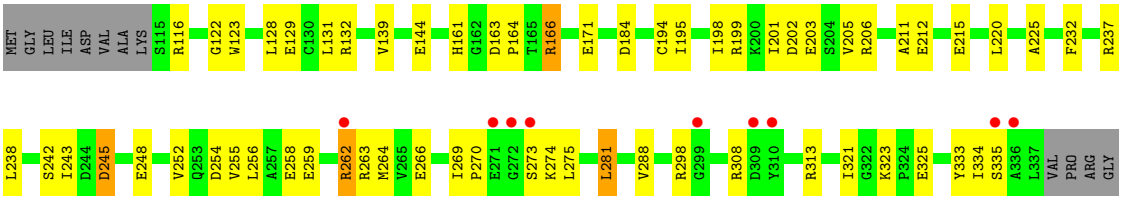


• Molecule 1: Calcium-gated potassium channel mthK

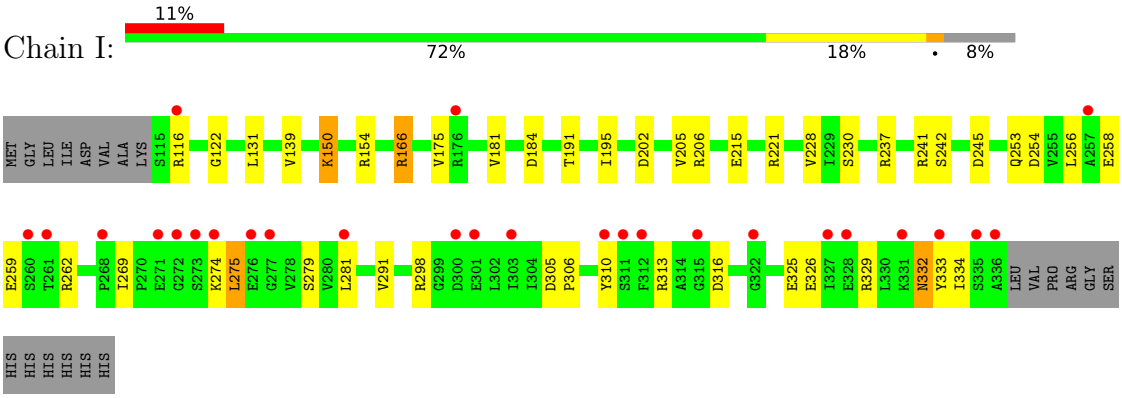




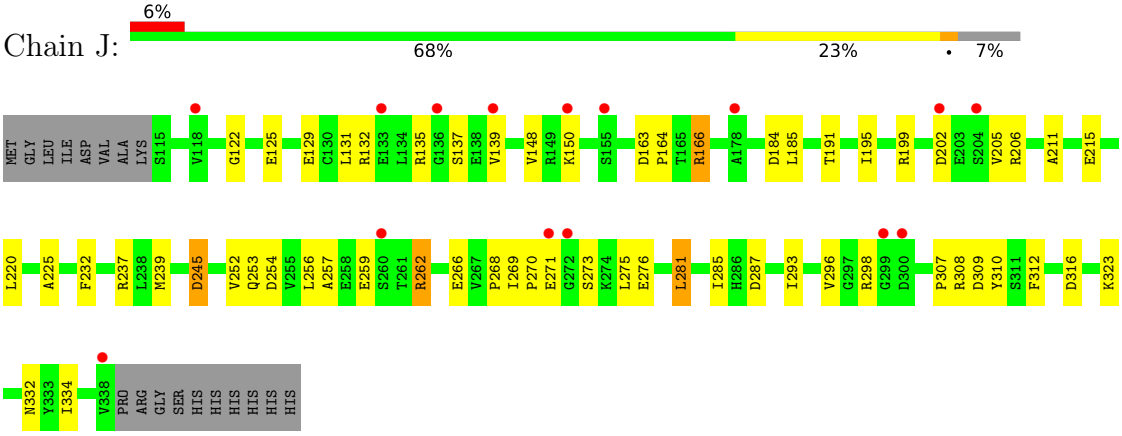
• Molecule 1: Calcium-gated potassium channel mthK



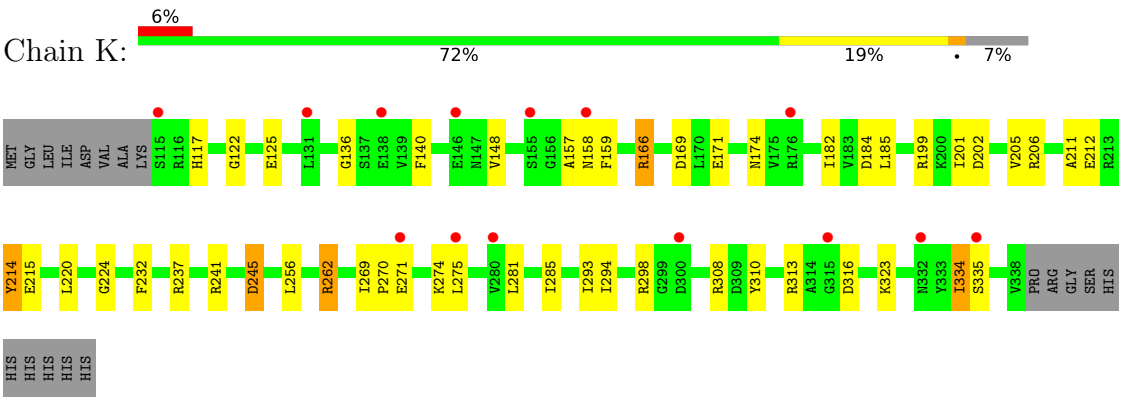
• Molecule 1: Calcium-gated potassium channel mthK



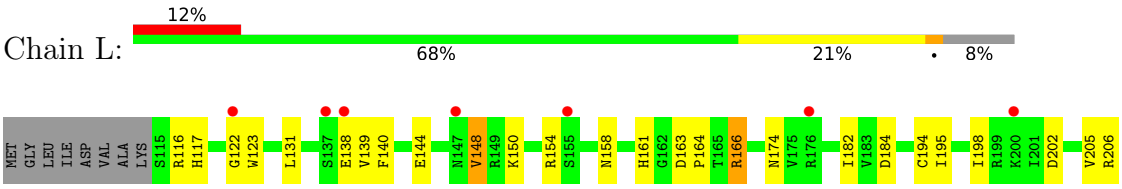
• Molecule 1: Calcium-gated potassium channel mthK

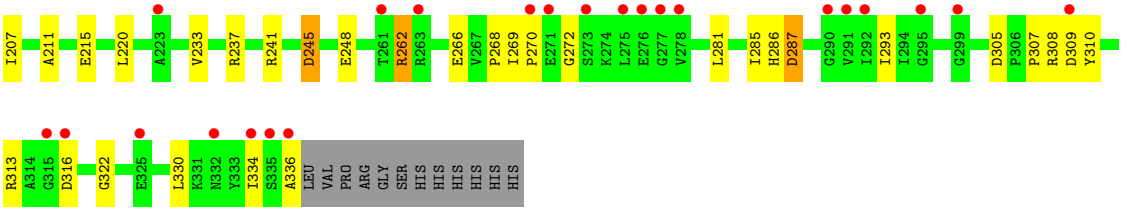


• Molecule 1: Calcium-gated potassium channel mthK



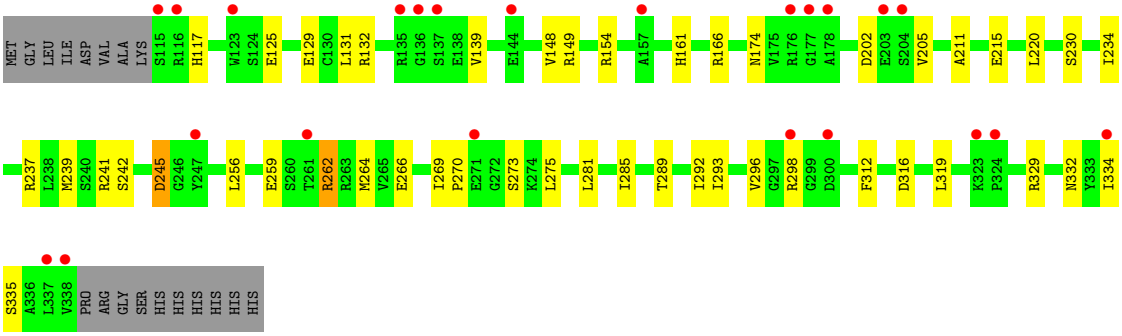
• Molecule 1: Calcium-gated potassium channel mthK





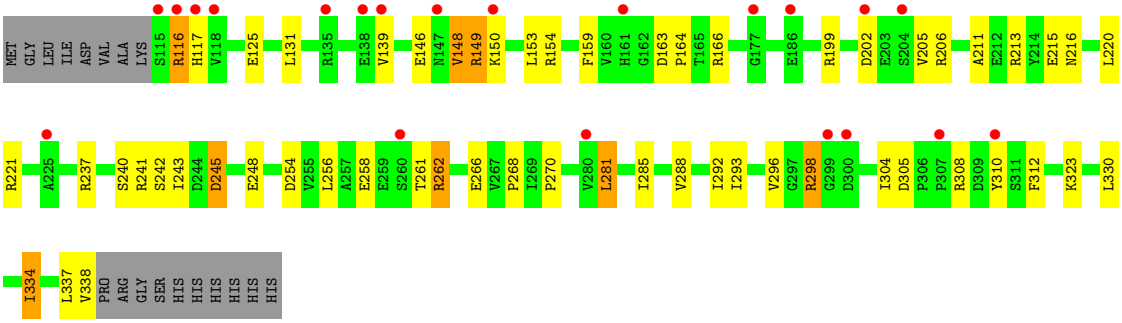
• Molecule 1: Calcium-gated potassium channel mthK

Chain M:



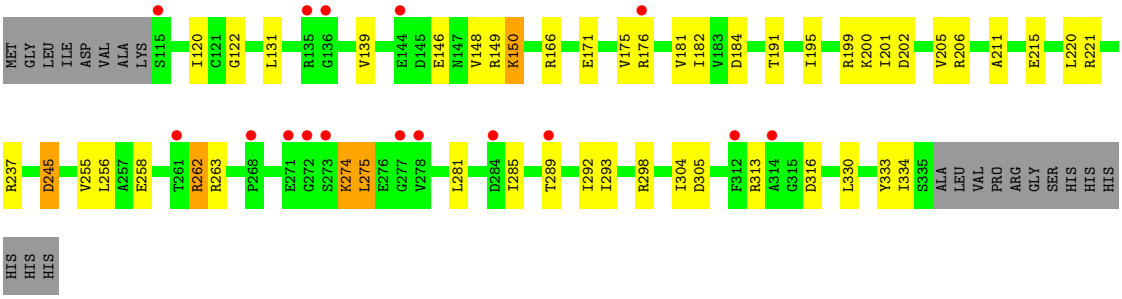
• Molecule 1: Calcium-gated potassium channel mthK

Chain N:



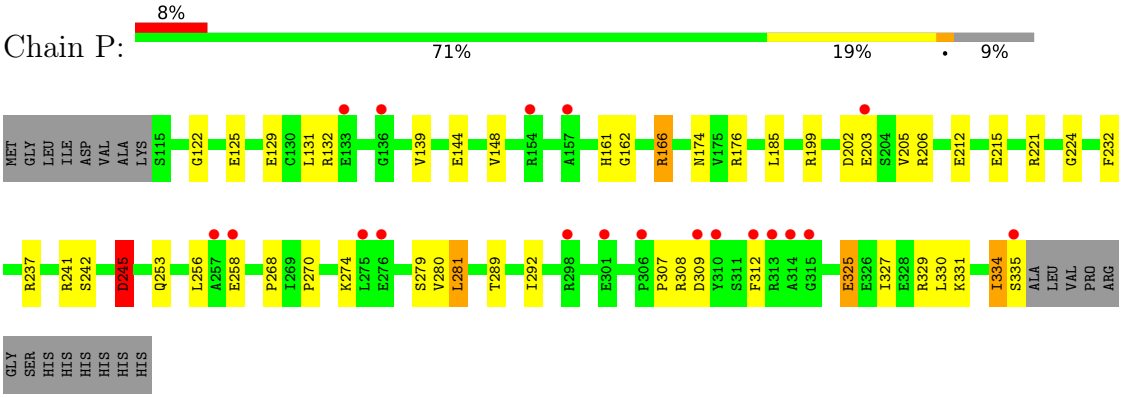
• Molecule 1: Calcium-gated potassium channel mthK

Chain O:



• Molecule 1: Calcium-gated potassium channel mthK

Chain P:


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

4 Data and refinement statistics (i)

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

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

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.36	0/1753	0.58	0/2366
1	B	0.33	0/1745	0.55	0/2355
1	C	0.32	0/1760	0.54	0/2376
1	D	0.36	0/1768	0.56	1/2388 (0.0%)
1	E	0.35	0/1753	0.59	0/2366
1	F	0.31	0/1753	0.52	0/2366
1	G	0.33	0/1768	0.53	0/2388
1	H	0.33	0/1753	0.57	0/2366
1	I	0.36	0/1742	0.55	0/2351
1	J	0.34	0/1760	0.51	0/2376
1	K	0.35	0/1760	0.52	0/2376
1	L	0.37	0/1739	0.53	0/2348
1	M	0.36	0/1760	0.53	0/2376
1	N	0.34	0/1760	0.52	0/2376
1	O	0.33	0/1740	0.51	0/2348
1	P	0.35	0/1740	0.54	0/2348
All	All	0.34	0/28054	0.54	1/37870 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	337	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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

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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: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: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: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: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: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: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: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: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: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: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:N:221:ARG:HH22	1:O:258:GLU:CD	2.19	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
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: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: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: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:F:125:GLU:CD	1:H:166:ARG:HH22	2.22	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
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:J:166:ARG:HH22	1:P:125:GLU:CD	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:274:LYS:NZ	1:B:335:SER:O	2.40	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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: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%)	29	64
All	All	3538/3872 (91%)	3427 (97%)	110 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	245	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	191/207 (92%)	183 (96%)	8 (4%)	30	62
1	B	190/207 (92%)	182 (96%)	8 (4%)	30	62
1	C	192/207 (93%)	184 (96%)	8 (4%)	30	62
1	D	193/207 (93%)	184 (95%)	9 (5%)	26	59
1	E	191/207 (92%)	184 (96%)	7 (4%)	34	66
1	F	191/207 (92%)	184 (96%)	7 (4%)	34	66
1	G	193/207 (93%)	183 (95%)	10 (5%)	23	55
1	H	191/207 (92%)	183 (96%)	8 (4%)	30	62
1	I	189/207 (91%)	179 (95%)	10 (5%)	22	54

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

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

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

Mol	Chain	Res	Type
1	I	332	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	223/242 (92%)	0.20	4 (1%) 68 47	85, 127, 182, 198	0
1	B	222/242 (91%)	0.40	10 (4%) 33 16	93, 133, 182, 200	0
1	C	224/242 (92%)	0.32	5 (2%) 62 41	94, 136, 183, 201	0
1	D	225/242 (92%)	0.31	5 (2%) 62 41	94, 129, 186, 204	0
1	E	223/242 (92%)	0.23	6 (2%) 54 31	88, 128, 184, 200	0
1	F	223/242 (92%)	0.28	7 (3%) 49 26	91, 135, 182, 218	0
1	G	225/242 (92%)	0.34	4 (1%) 68 47	93, 134, 186, 265	0
1	H	223/242 (92%)	0.29	9 (4%) 38 19	89, 132, 184, 204	0
1	I	222/242 (91%)	0.65	27 (12%) 4 1	109, 142, 193, 223	0
1	J	224/242 (92%)	0.40	15 (6%) 17 7	110, 142, 184, 205	0
1	K	224/242 (92%)	0.39	14 (6%) 20 8	115, 148, 186, 232	0
1	L	222/242 (91%)	0.79	30 (13%) 3 1	112, 150, 199, 229	0
1	M	224/242 (92%)	0.58	23 (10%) 6 2	108, 142, 186, 214	0
1	N	224/242 (92%)	0.44	21 (9%) 8 3	107, 145, 186, 209	0
1	O	221/242 (91%)	0.40	16 (7%) 15 6	106, 139, 184, 209	0
1	P	221/242 (91%)	0.52	19 (8%) 10 4	106, 139, 187, 207	0
All	All	3570/3872 (92%)	0.41	215 (6%) 21 10	85, 139, 188, 265	0

All (215) RSRZ outliers are listed below:

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

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Mol	Chain	Res	Type	RSRZ
1	N	115	SER	5.4
1	M	177	GLY	5.2
1	I	310	TYR	5.0
1	B	135	ARG	4.9
1	N	147	ASN	4.8
1	L	290	GLY	4.7
1	P	335	SER	4.7
1	B	336	ALA	4.5
1	L	277	GLY	4.3
1	B	300	ASP	4.3
1	I	311	SER	4.2
1	J	300	ASP	4.2
1	P	157	ALA	4.2
1	M	157	ALA	4.1
1	G	271	GLU	4.1
1	O	277	GLY	4.1
1	M	338	VAL	4.0
1	D	137	SER	3.9
1	N	300	ASP	3.9
1	G	307	PRO	3.9
1	L	270	PRO	3.9
1	C	300	ASP	3.9
1	O	271	GLU	3.9
1	L	273	SER	3.8
1	L	334	ILE	3.8
1	N	150	LYS	3.8
1	I	260	SER	3.7
1	I	322	GLY	3.7
1	H	335	SER	3.6
1	G	339	PRO	3.6
1	N	177	GLY	3.6
1	K	158	ASN	3.5
1	N	117	HIS	3.5
1	J	260	SER	3.5
1	L	278	VAL	3.4
1	L	332	ASN	3.4
1	F	282	ASP	3.4
1	L	316	ASP	3.3
1	L	122	GLY	3.3
1	L	315	GLY	3.2
1	E	115	SER	3.2
1	M	135	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	M	271	GLU	3.1
1	H	336	ALA	3.1
1	P	310	TYR	3.1
1	P	275	LEU	3.1
1	L	291	VAL	3.0
1	M	136	GLY	3.0
1	O	272	GLY	3.0
1	M	115	SER	3.0
1	M	323	LYS	3.0
1	L	200	LYS	3.0
1	F	275	LEU	3.0
1	J	271	GLU	3.0
1	L	276	GLU	3.0
1	K	275	LEU	3.0
1	N	161	HIS	3.0
1	C	314	ALA	2.9
1	B	169	ASP	2.9
1	C	307	PRO	2.9
1	J	338	VAL	2.9
1	H	310	TYR	2.9
1	P	306	PRO	2.9
1	L	275	LEU	2.9
1	P	203	GLU	2.9
1	P	258	GLU	2.9
1	O	115	SER	2.9
1	M	176	ARG	2.9
1	J	150	LYS	2.9
1	N	138	GLU	2.8
1	N	139	VAL	2.8
1	N	280	VAL	2.8
1	P	312	PHE	2.8
1	A	277	GLY	2.8
1	F	268	PRO	2.8
1	M	203	GLU	2.8
1	L	299	GLY	2.8
1	I	301	GLU	2.8
1	J	272	GLY	2.8
1	I	276	GLU	2.8
1	L	292	ILE	2.7
1	F	301	GLU	2.7
1	B	314	ALA	2.7
1	I	331	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	116	ARG	2.7
1	B	335	SER	2.7
1	L	138	GLU	2.7
1	P	314	ALA	2.7
1	K	138	GLU	2.6
1	L	271	GLU	2.6
1	O	135	ARG	2.6
1	I	268	PRO	2.6
1	E	311	SER	2.6
1	E	336	ALA	2.6
1	O	268	PRO	2.6
1	P	133	GLU	2.6
1	J	155	SER	2.6
1	K	115	SER	2.6
1	L	147	ASN	2.6
1	M	298	ARG	2.6
1	C	315	GLY	2.6
1	K	335	SER	2.6
1	P	276	GLU	2.6
1	M	337	LEU	2.6
1	H	262	ARG	2.5
1	L	325	GLU	2.5
1	N	307	PRO	2.5
1	H	271	GLU	2.5
1	L	176	ARG	2.5
1	L	309	ASP	2.5
1	P	309	ASP	2.5
1	I	327	ILE	2.5
1	F	136	GLY	2.5
1	P	257	ALA	2.5
1	P	136	GLY	2.5
1	P	315	GLY	2.5
1	P	313	ARG	2.5
1	P	298	ARG	2.5
1	I	274	LYS	2.5
1	L	155	SER	2.5
1	E	203	GLU	2.4
1	M	247	TYR	2.4
1	O	278	VAL	2.4
1	I	312	PHE	2.4
1	M	204	SER	2.4
1	O	273	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	202	ASP	2.4
1	H	273	SER	2.4
1	O	261	THR	2.4
1	N	202	ASP	2.4
1	N	116	ARG	2.4
1	O	314	ALA	2.4
1	I	272	GLY	2.4
1	O	284	ASP	2.4
1	K	280	VAL	2.4
1	M	178	ALA	2.4
1	K	300	ASP	2.3
1	J	178	ALA	2.3
1	M	116	ARG	2.3
1	K	155	SER	2.3
1	K	176	ARG	2.3
1	E	275	LEU	2.3
1	N	225	ALA	2.3
1	I	300	ASP	2.3
1	I	303	ILE	2.3
1	J	204	SER	2.3
1	A	308	ARG	2.3
1	I	328	GLU	2.3
1	I	261	THR	2.3
1	I	336	ALA	2.3
1	P	154	ARG	2.3
1	M	300	ASP	2.3
1	O	289	THR	2.3
1	D	136	GLY	2.3
1	O	176	ARG	2.3
1	E	297	GLY	2.3
1	I	333	TYR	2.3
1	J	133	GLU	2.3
1	L	261	THR	2.3
1	M	144	GLU	2.3
1	I	271	GLU	2.2
1	I	277	GLY	2.2
1	C	147	ASN	2.2
1	N	204	SER	2.2
1	I	176	ARG	2.2
1	K	146	GLU	2.2
1	P	301	GLU	2.2
1	M	137	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	N	299	GLY	2.2
1	M	261	THR	2.2
1	N	135	ARG	2.2
1	D	186	GLU	2.2
1	A	145	ASP	2.2
1	F	270	PRO	2.2
1	H	299	GLY	2.2
1	N	260	SER	2.2
1	N	310	TYR	2.1
1	L	295	GLY	2.1
1	K	131	LEU	2.1
1	I	335	SER	2.1
1	M	123	TRP	2.1
1	B	136	GLY	2.1
1	I	315	GLY	2.1
1	K	315	GLY	2.1
1	M	324	PRO	2.1
1	J	118	VAL	2.1
1	H	272	GLY	2.1
1	O	312	PHE	2.1
1	B	278	VAL	2.1
1	O	144	GLU	2.1
1	H	309	ASP	2.1
1	M	334	ILE	2.1
1	I	281	LEU	2.1
1	J	299	GLY	2.1
1	I	116	ARG	2.1
1	I	257	ALA	2.1
1	J	139	VAL	2.1
1	L	223	ALA	2.1
1	D	224	GLY	2.1
1	B	133	GLU	2.1
1	K	332	ASN	2.1
1	A	122	GLY	2.1
1	B	273	SER	2.1
1	F	332	ASN	2.0
1	L	263	ARG	2.0
1	G	147	ASN	2.0
1	N	118	VAL	2.0
1	J	136	GLY	2.0
1	K	271	GLU	2.0
1	N	186	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BA	I	403	1/1	-0.07	0.32	297,297,297,297	0
2	BA	D	404	1/1	0.02	0.20	251,251,251,251	0
2	BA	K	404	1/1	0.18	0.36	276,276,276,276	0
2	BA	B	404	1/1	0.23	0.56	355,355,355,355	0
2	BA	D	405	1/1	0.26	0.29	254,254,254,254	0
2	BA	L	402	1/1	0.27	0.13	320,320,320,320	0
2	BA	M	401	1/1	0.33	0.15	290,290,290,290	0
2	BA	F	403	1/1	0.37	0.12	262,262,262,262	0
2	BA	J	401	1/1	0.48	0.22	269,269,269,269	0
2	BA	M	404	1/1	0.50	0.20	306,306,306,306	0
2	BA	M	402	1/1	0.51	0.10	237,237,237,237	0
2	BA	A	404	1/1	0.53	0.11	265,265,265,265	0
2	BA	C	403	1/1	0.53	0.09	256,256,256,256	0
2	BA	B	403	1/1	0.54	0.29	245,245,245,245	0
2	BA	F	401	1/1	0.54	0.13	222,222,222,222	0
2	BA	K	402	1/1	0.57	0.18	271,271,271,271	0
2	BA	G	404	1/1	0.57	0.15	259,259,259,259	0
2	BA	P	403	1/1	0.58	0.12	276,276,276,276	0
2	BA	O	403	1/1	0.59	0.42	313,313,313,313	0
2	BA	A	405	1/1	0.61	0.15	241,241,241,241	0
2	BA	E	404	1/1	0.62	0.09	256,256,256,256	0
2	BA	O	402	1/1	0.64	0.10	248,248,248,248	0
2	BA	D	402	1/1	0.64	0.07	250,250,250,250	0
2	BA	J	402	1/1	0.64	0.13	282,282,282,282	0
2	BA	A	403	1/1	0.65	0.12	230,230,230,230	0
2	BA	D	403	1/1	0.66	0.10	229,229,229,229	0
2	BA	F	402	1/1	0.67	0.17	253,253,253,253	0

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

6.5 Other polymers (i)

There are no such residues in this entry.