wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:58 AM GMT

PDB ID	:	2EWO
Title	:	X-ray structure of putative agmatine deiminase Q8DW17, Northeast Structural Genomics target SmR6.
Authors	:	Kuzin, A.P.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2005-11-04
Resolution	:	2.90 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

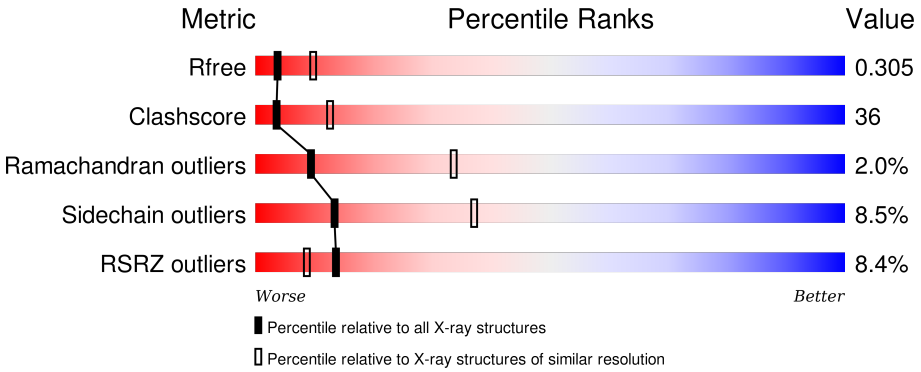
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	377	3% 40% 50% 6% ·
1	B	377	3% 41% 49% 6% ·
1	C	377	9% 41% 49% 6% ·
1	D	377	8% 40% 49% 7% ·
1	E	377	9% 40% 50% 6% ·

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Mol	Chain	Length	Quality of chain
1	F	377	5% 41% 49% 7%
1	G	377	10% 41% 49% 6%
1	H	377	4% 44% 45% 9%
1	I	377	7% 41% 48% 7%
1	J	377	12% 41% 48% 7%
1	K	377	6% 41% 49% 7%
1	L	377	18% 40% 49% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 34934 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 Putative agmatine deiminase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	B	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	C	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	D	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	E	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	F	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	G	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	H	369	Total	C	N	O	S	Se	0	0	0
			2942	1868	496	561	10	7			
1	I	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	J	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	K	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	L	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q8DW17
A	17	MSE	MET	modified residue	UNP Q8DW17
A	29	MSE	MET	modified residue	UNP Q8DW17
A	91	MSE	MET	modified residue	UNP Q8DW17
A	178	MSE	MET	modified residue	UNP Q8DW17

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Chain	Residue	Modelled	Actual	Comment	Reference
A	274	MSE	MET	modified residue	UNP Q8DW17
A	303	MSE	MET	modified residue	UNP Q8DW17
A	338	MSE	MET	modified residue	UNP Q8DW17
A	370	LEU	-	cloning artifact	UNP Q8DW17
A	371	GLU	-	cloning artifact	UNP Q8DW17
A	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
A	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
A	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
A	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
A	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
A	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
B	1	MSE	MET	modified residue	UNP Q8DW17
B	17	MSE	MET	modified residue	UNP Q8DW17
B	29	MSE	MET	modified residue	UNP Q8DW17
B	91	MSE	MET	modified residue	UNP Q8DW17
B	178	MSE	MET	modified residue	UNP Q8DW17
B	274	MSE	MET	modified residue	UNP Q8DW17
B	303	MSE	MET	modified residue	UNP Q8DW17
B	338	MSE	MET	modified residue	UNP Q8DW17
B	370	LEU	-	cloning artifact	UNP Q8DW17
B	371	GLU	-	cloning artifact	UNP Q8DW17
B	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
B	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
B	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
B	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
B	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
B	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
C	1	MSE	MET	modified residue	UNP Q8DW17
C	17	MSE	MET	modified residue	UNP Q8DW17
C	29	MSE	MET	modified residue	UNP Q8DW17
C	91	MSE	MET	modified residue	UNP Q8DW17
C	178	MSE	MET	modified residue	UNP Q8DW17
C	274	MSE	MET	modified residue	UNP Q8DW17
C	303	MSE	MET	modified residue	UNP Q8DW17
C	338	MSE	MET	modified residue	UNP Q8DW17
C	370	LEU	-	cloning artifact	UNP Q8DW17
C	371	GLU	-	cloning artifact	UNP Q8DW17
C	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
C	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
C	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
C	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
C	376	HIS	-	EXPRESSION TAG	UNP Q8DW17

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Chain	Residue	Modelled	Actual	Comment	Reference
C	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
D	1	MSE	MET	modified residue	UNP Q8DW17
D	17	MSE	MET	modified residue	UNP Q8DW17
D	29	MSE	MET	modified residue	UNP Q8DW17
D	91	MSE	MET	modified residue	UNP Q8DW17
D	178	MSE	MET	modified residue	UNP Q8DW17
D	274	MSE	MET	modified residue	UNP Q8DW17
D	303	MSE	MET	modified residue	UNP Q8DW17
D	338	MSE	MET	modified residue	UNP Q8DW17
D	370	LEU	-	cloning artifact	UNP Q8DW17
D	371	GLU	-	cloning artifact	UNP Q8DW17
D	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
D	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
D	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
D	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
D	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
D	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
E	1	MSE	MET	modified residue	UNP Q8DW17
E	17	MSE	MET	modified residue	UNP Q8DW17
E	29	MSE	MET	modified residue	UNP Q8DW17
E	91	MSE	MET	modified residue	UNP Q8DW17
E	178	MSE	MET	modified residue	UNP Q8DW17
E	274	MSE	MET	modified residue	UNP Q8DW17
E	303	MSE	MET	modified residue	UNP Q8DW17
E	338	MSE	MET	modified residue	UNP Q8DW17
E	370	LEU	-	cloning artifact	UNP Q8DW17
E	371	GLU	-	cloning artifact	UNP Q8DW17
E	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
E	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
E	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
E	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
E	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
E	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
F	1	MSE	MET	modified residue	UNP Q8DW17
F	17	MSE	MET	modified residue	UNP Q8DW17
F	29	MSE	MET	modified residue	UNP Q8DW17
F	91	MSE	MET	modified residue	UNP Q8DW17
F	178	MSE	MET	modified residue	UNP Q8DW17
F	274	MSE	MET	modified residue	UNP Q8DW17
F	303	MSE	MET	modified residue	UNP Q8DW17
F	338	MSE	MET	modified residue	UNP Q8DW17
F	370	LEU	-	cloning artifact	UNP Q8DW17

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Chain	Residue	Modelled	Actual	Comment	Reference
F	371	GLU	-	cloning artifact	UNP Q8DW17
F	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
F	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
F	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
F	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
F	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
F	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
G	1	MSE	MET	modified residue	UNP Q8DW17
G	17	MSE	MET	modified residue	UNP Q8DW17
G	29	MSE	MET	modified residue	UNP Q8DW17
G	91	MSE	MET	modified residue	UNP Q8DW17
G	178	MSE	MET	modified residue	UNP Q8DW17
G	274	MSE	MET	modified residue	UNP Q8DW17
G	303	MSE	MET	modified residue	UNP Q8DW17
G	338	MSE	MET	modified residue	UNP Q8DW17
G	370	LEU	-	cloning artifact	UNP Q8DW17
G	371	GLU	-	cloning artifact	UNP Q8DW17
G	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
G	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
G	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
G	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
G	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
G	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
H	1	MSE	MET	modified residue	UNP Q8DW17
H	17	MSE	MET	modified residue	UNP Q8DW17
H	29	MSE	MET	modified residue	UNP Q8DW17
H	91	MSE	MET	modified residue	UNP Q8DW17
H	178	MSE	MET	modified residue	UNP Q8DW17
H	274	MSE	MET	modified residue	UNP Q8DW17
H	303	MSE	MET	modified residue	UNP Q8DW17
H	338	MSE	MET	modified residue	UNP Q8DW17
H	370	LEU	-	cloning artifact	UNP Q8DW17
H	371	GLU	-	cloning artifact	UNP Q8DW17
H	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
H	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
H	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
H	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
H	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
H	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
I	1	MSE	MET	modified residue	UNP Q8DW17
I	17	MSE	MET	modified residue	UNP Q8DW17
I	29	MSE	MET	modified residue	UNP Q8DW17

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Chain	Residue	Modelled	Actual	Comment	Reference
I	91	MSE	MET	modified residue	UNP Q8DW17
I	178	MSE	MET	modified residue	UNP Q8DW17
I	274	MSE	MET	modified residue	UNP Q8DW17
I	303	MSE	MET	modified residue	UNP Q8DW17
I	338	MSE	MET	modified residue	UNP Q8DW17
I	370	LEU	-	cloning artifact	UNP Q8DW17
I	371	GLU	-	cloning artifact	UNP Q8DW17
I	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
I	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
I	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
I	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
I	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
I	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
J	1	MSE	MET	modified residue	UNP Q8DW17
J	17	MSE	MET	modified residue	UNP Q8DW17
J	29	MSE	MET	modified residue	UNP Q8DW17
J	91	MSE	MET	modified residue	UNP Q8DW17
J	178	MSE	MET	modified residue	UNP Q8DW17
J	274	MSE	MET	modified residue	UNP Q8DW17
J	303	MSE	MET	modified residue	UNP Q8DW17
J	338	MSE	MET	modified residue	UNP Q8DW17
J	370	LEU	-	cloning artifact	UNP Q8DW17
J	371	GLU	-	cloning artifact	UNP Q8DW17
J	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
J	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
J	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
J	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
J	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
J	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
K	1	MSE	MET	modified residue	UNP Q8DW17
K	17	MSE	MET	modified residue	UNP Q8DW17
K	29	MSE	MET	modified residue	UNP Q8DW17
K	91	MSE	MET	modified residue	UNP Q8DW17
K	178	MSE	MET	modified residue	UNP Q8DW17
K	274	MSE	MET	modified residue	UNP Q8DW17
K	303	MSE	MET	modified residue	UNP Q8DW17
K	338	MSE	MET	modified residue	UNP Q8DW17
K	370	LEU	-	cloning artifact	UNP Q8DW17
K	371	GLU	-	cloning artifact	UNP Q8DW17
K	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
K	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
K	374	HIS	-	EXPRESSION TAG	UNP Q8DW17

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Chain	Residue	Modelled	Actual	Comment	Reference
K	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
K	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
K	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
L	1	MSE	MET	modified residue	UNP Q8DW17
L	17	MSE	MET	modified residue	UNP Q8DW17
L	29	MSE	MET	modified residue	UNP Q8DW17
L	91	MSE	MET	modified residue	UNP Q8DW17
L	178	MSE	MET	modified residue	UNP Q8DW17
L	274	MSE	MET	modified residue	UNP Q8DW17
L	303	MSE	MET	modified residue	UNP Q8DW17
L	338	MSE	MET	modified residue	UNP Q8DW17
L	370	LEU	-	cloning artifact	UNP Q8DW17
L	371	GLU	-	cloning artifact	UNP Q8DW17
L	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
L	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
L	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
L	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
L	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
L	377	HIS	-	EXPRESSION TAG	UNP Q8DW17

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	26	Total O 26 26	0	0
2	B	22	Total O 22 22	0	0
2	C	18	Total O 18 18	0	0
2	D	20	Total O 20 20	0	0
2	E	15	Total O 15 15	0	0
2	F	19	Total O 19 19	0	0
2	G	27	Total O 27 27	0	0
2	H	23	Total O 23 23	0	0
2	I	13	Total O 13 13	0	0
2	J	11	Total O 11 11	0	0

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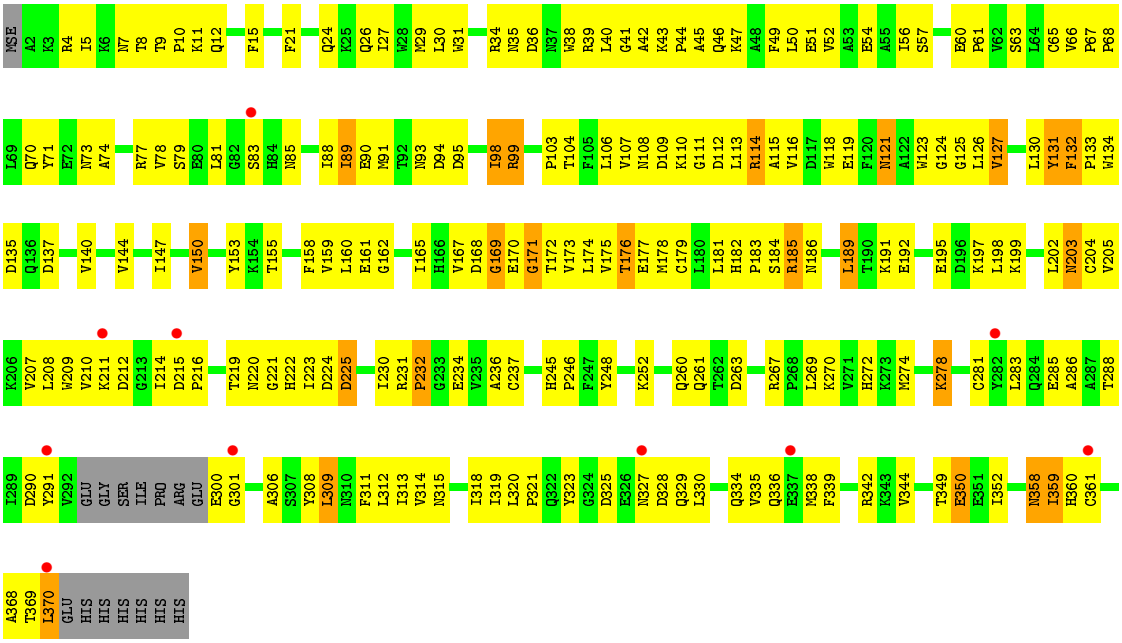
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	17	Total O 17 17	0	0
2	L	13	Total O 13 13	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

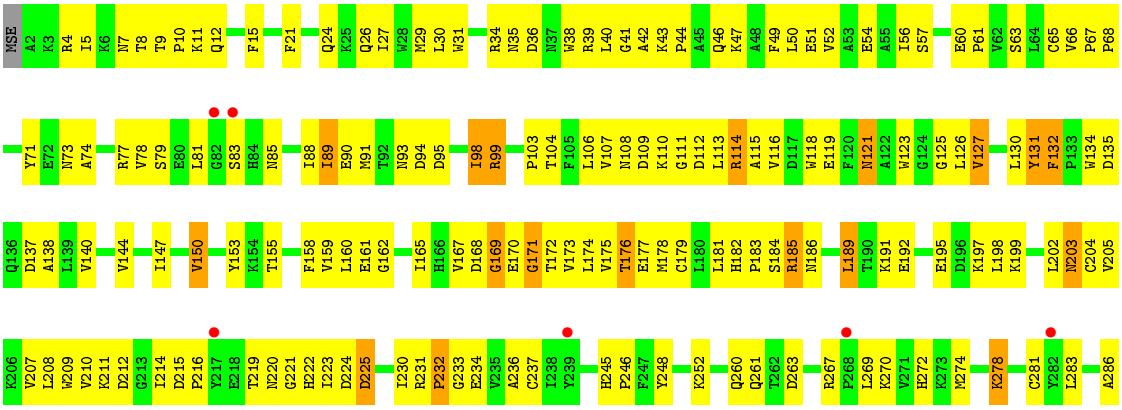
- Molecule 1: Putative agmatine deiminase

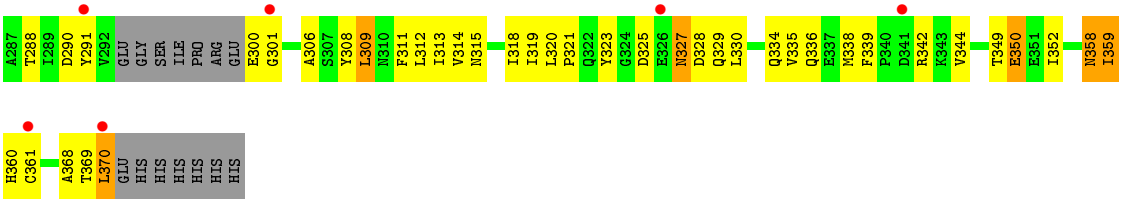
Chain A:



- Molecule 1: Putative agmatine deiminase

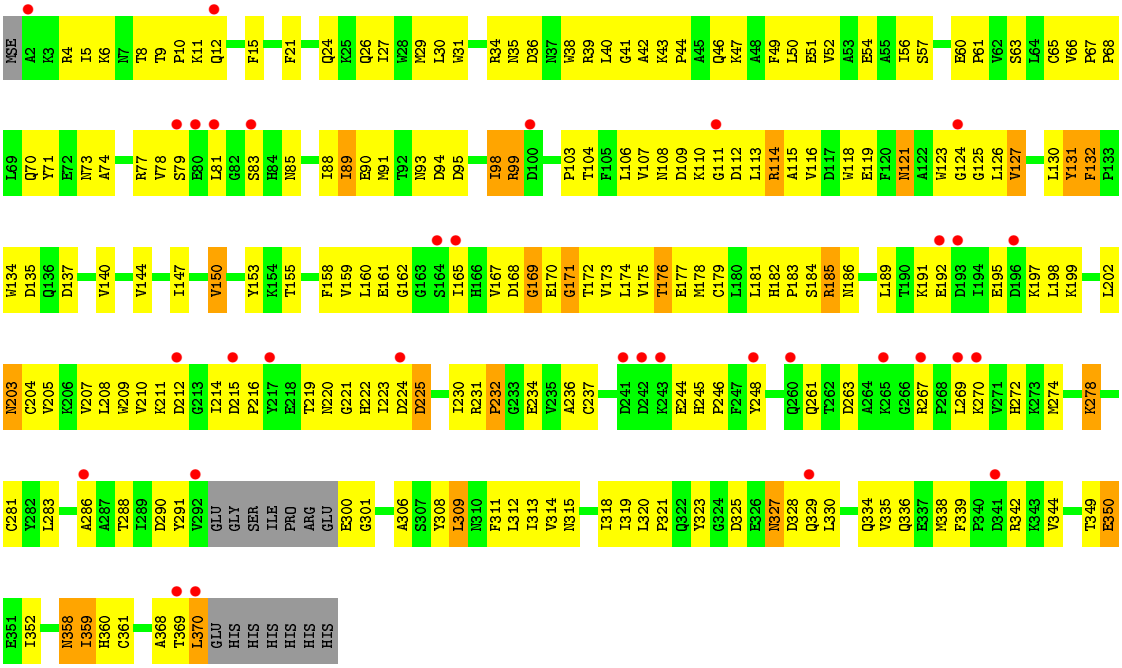
Chain B:





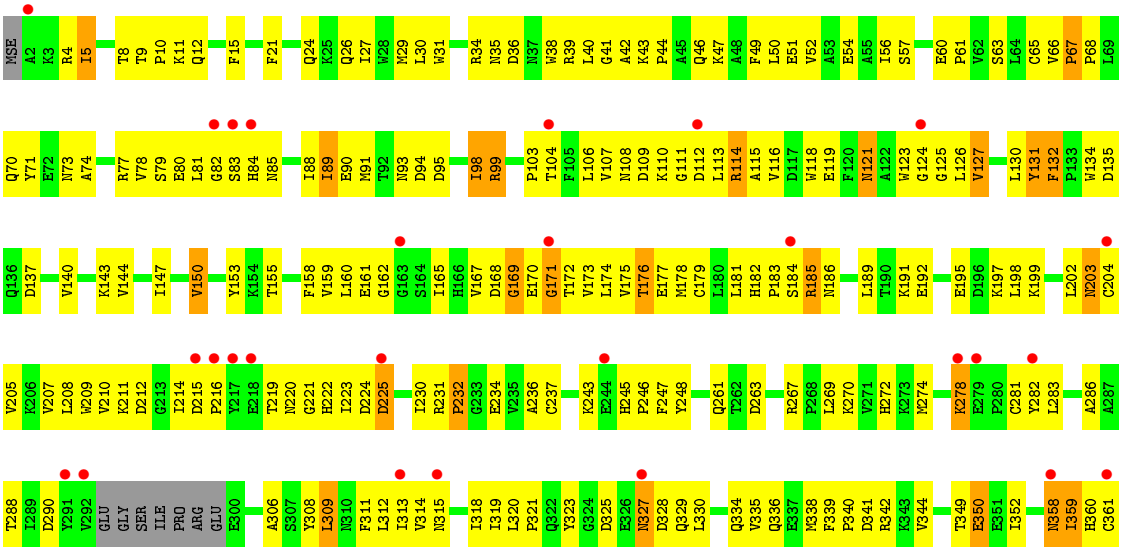
- Molecule 1: Putative agmatine deiminase

Chain C:



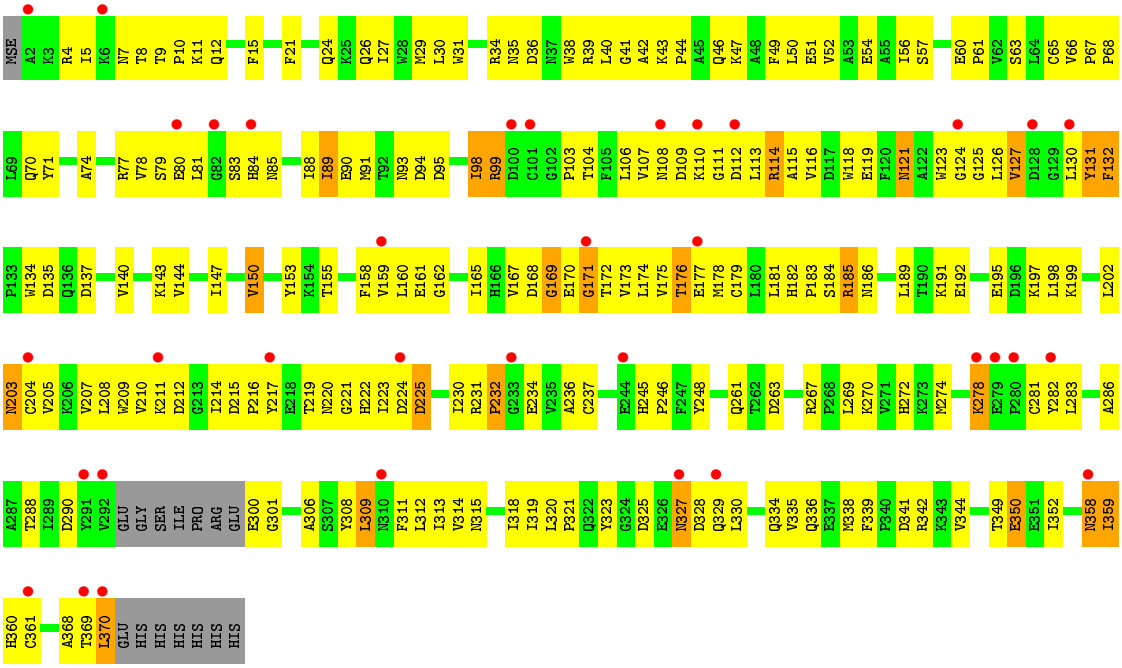
- Molecule 1: Putative agmatine deiminase

Chain D:



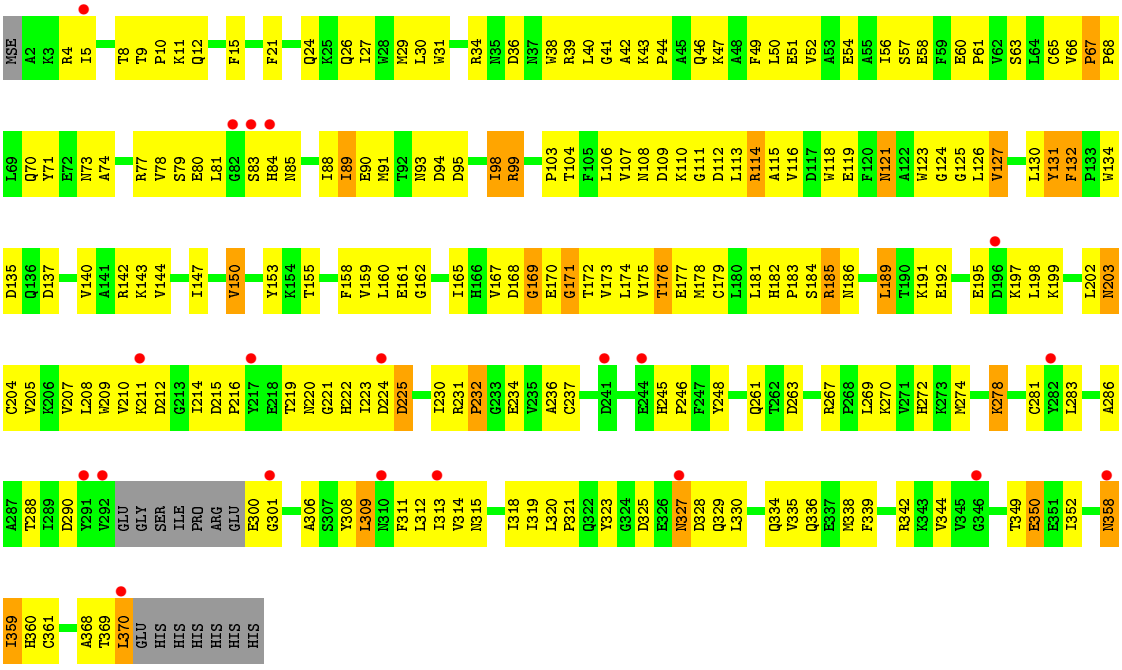
• Molecule 1: Putative agmatine deiminase

Chain E:



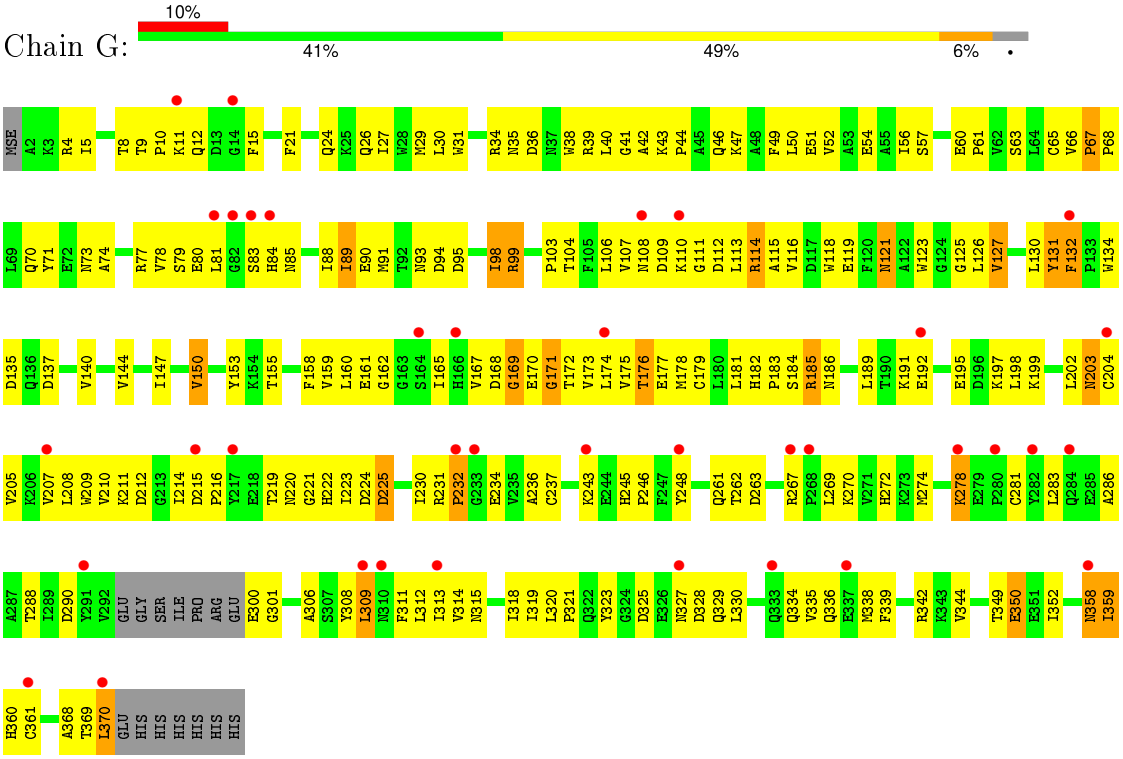
• Molecule 1: Putative agmatine deiminase

Chain F:



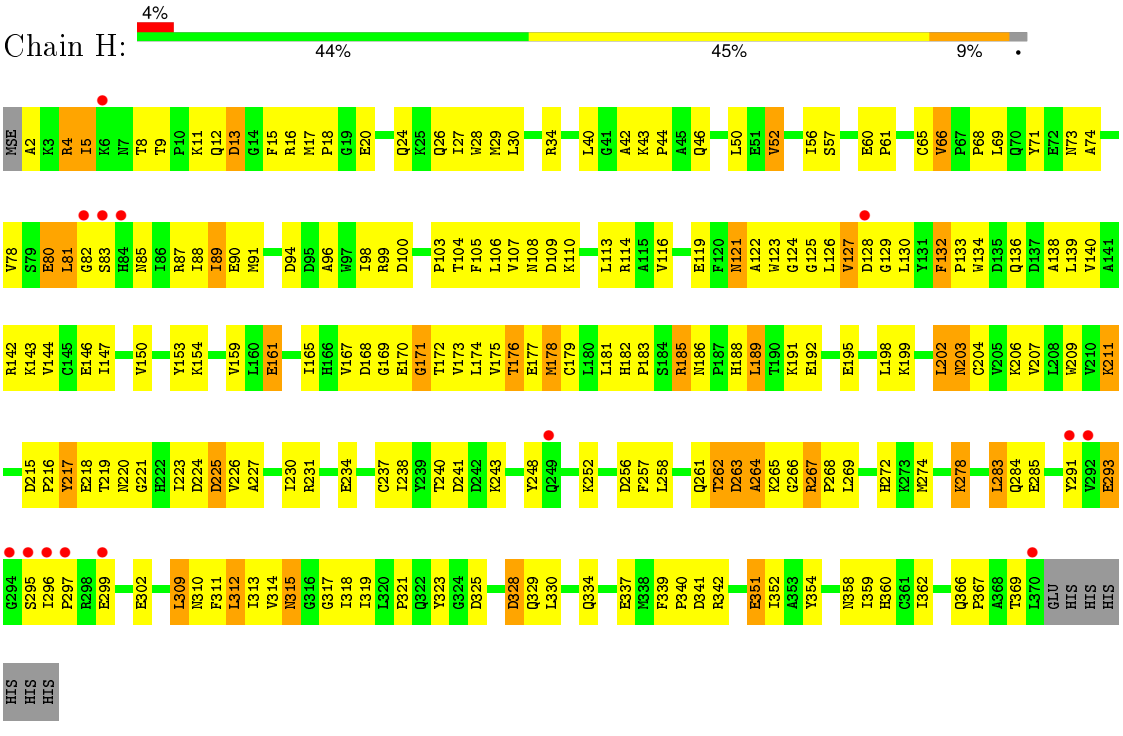
• Molecule 1: Putative agmatine deiminase

Chain G:



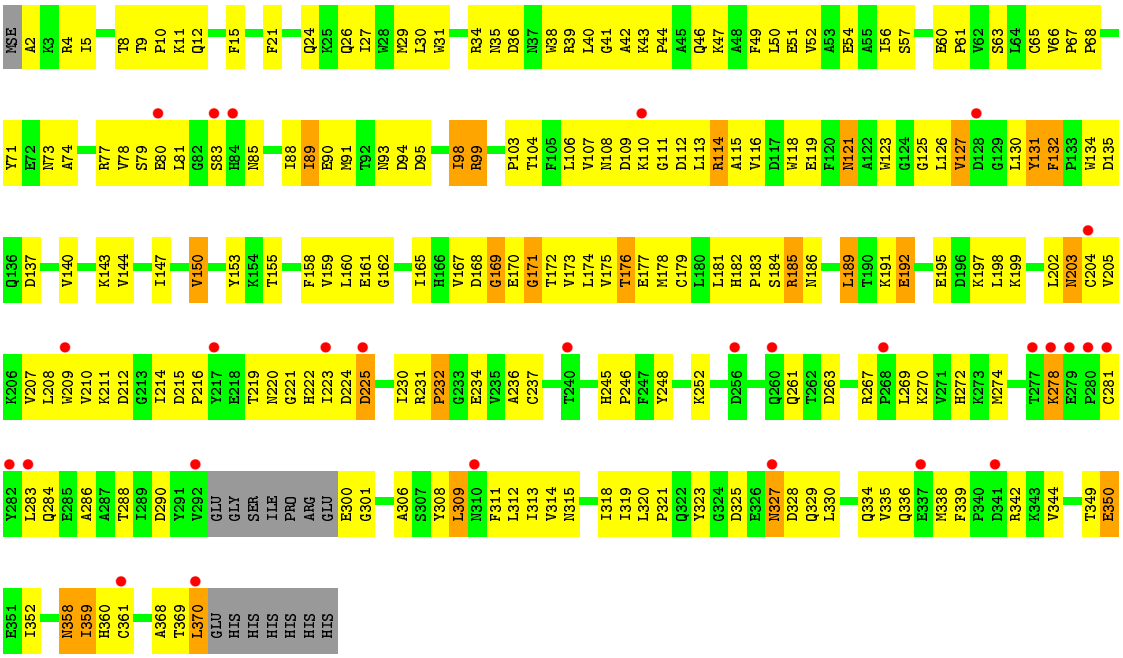
• Molecule 1: Putative agmatine deiminase

Chain H:



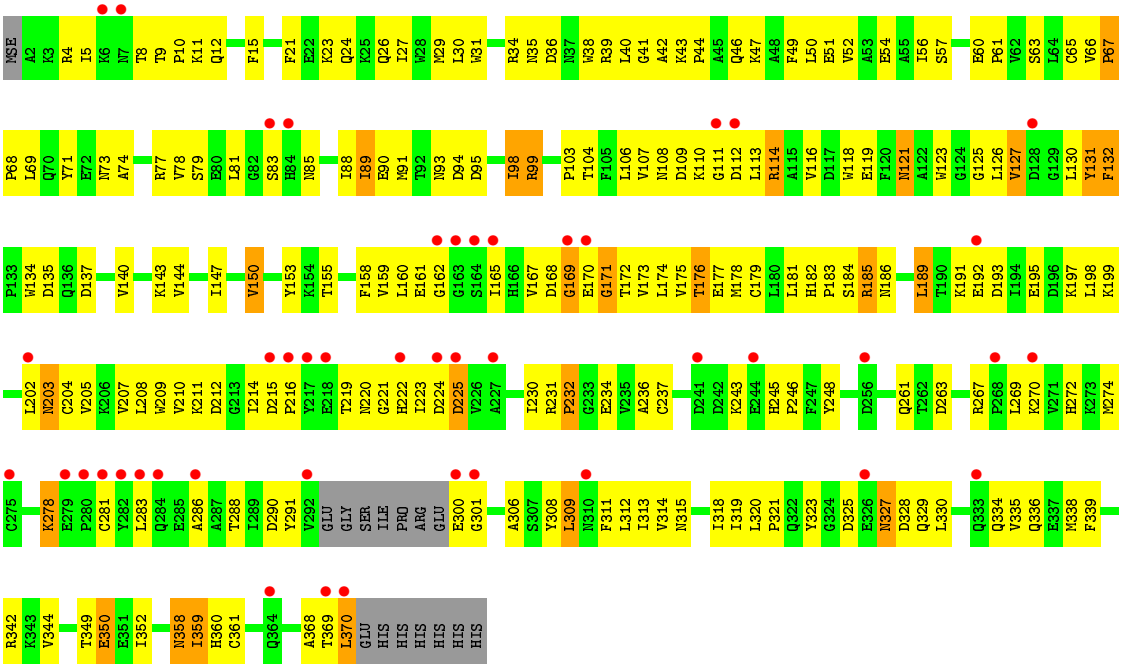
• Molecule 1: Putative agmatine deiminase

Chain I:



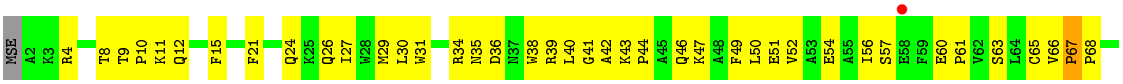
• Molecule 1: Putative agmatine deiminase

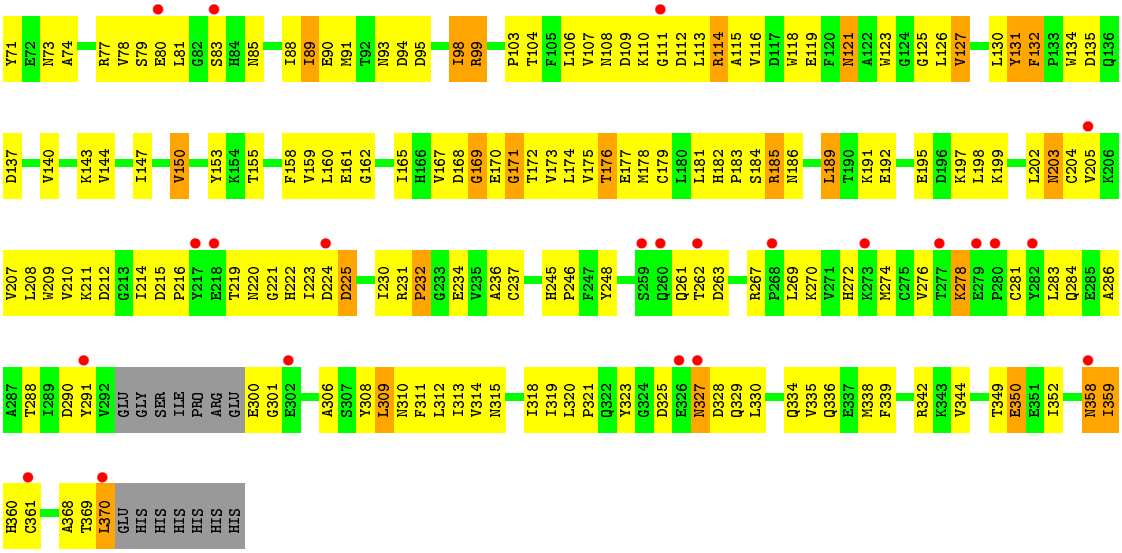
Chain J:



• Molecule 1: Putative agmatine deiminase

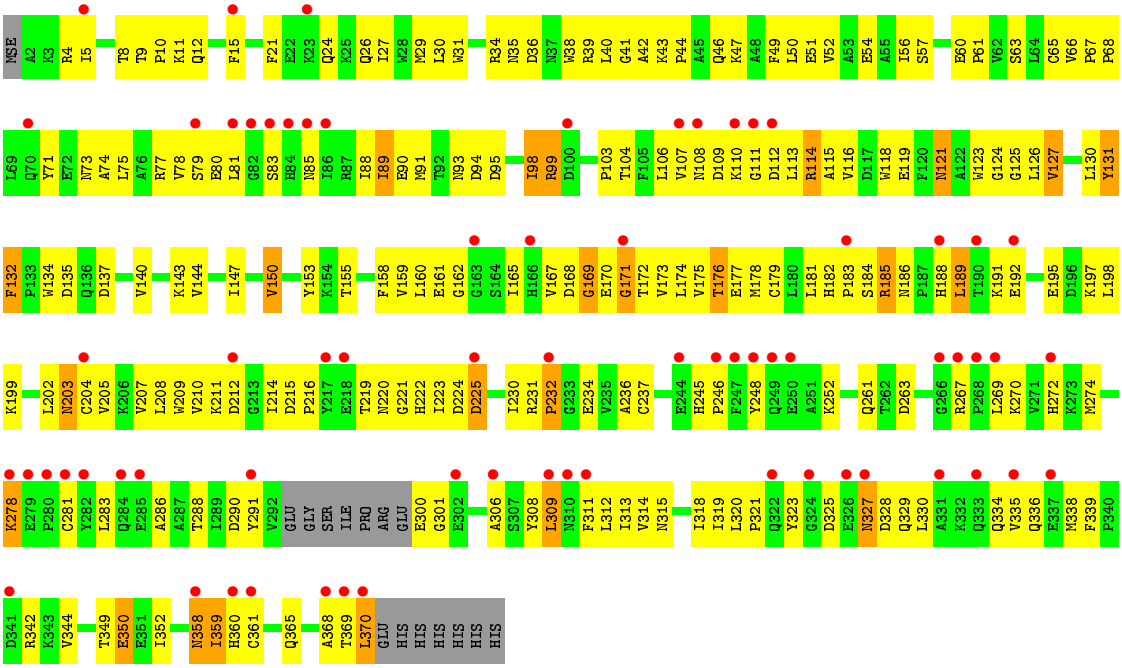
Chain K:





• Molecule 1: Putative agmatine deiminase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.52Å 203.69Å 139.54Å 90.00° 104.72° 90.00°	Depositor
Resolution (Å)	19.99 – 2.90 29.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	83.8 (19.99-2.90) 98.5 (29.95-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.269 0.282 , 0.305	Depositor DCC
R_{free} test set	5222 reflections (4.93%)	DCC
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 20.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 218714 reflections	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	34934	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.48	0/2950	0.65	0/3992
1	B	0.48	0/2950	0.65	0/3992
1	C	0.48	0/2950	0.65	0/3992
1	D	0.48	0/2950	0.65	0/3992
1	E	0.48	0/2950	0.65	0/3992
1	F	0.48	0/2950	0.65	0/3992
1	G	0.48	0/2950	0.65	0/3992
1	H	0.48	0/3006	0.68	1/4069 (0.0%)
1	I	0.48	0/2950	0.65	0/3992
1	J	0.48	0/2950	0.65	0/3992
1	K	0.48	0/2950	0.65	0/3992
1	L	0.48	0/2950	0.65	0/3992
All	All	0.48	0/35456	0.65	1/47981 (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	H	267	ARG	NE-CZ-NH2	6.56	123.58	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2888	0	2800	236	8
1	B	2888	0	2800	207	11
1	C	2888	0	2800	205	2
1	D	2888	0	2800	258	6
1	E	2888	0	2800	207	19
1	F	2888	0	2800	227	2
1	G	2888	0	2800	213	5
1	H	2942	0	2852	212	2
1	I	2888	0	2800	211	3
1	J	2888	0	2800	211	8
1	K	2888	0	2800	210	3
1	L	2888	0	2800	210	1
2	A	26	0	0	10	0
2	B	22	0	0	5	0
2	C	18	0	0	5	0
2	D	20	0	0	9	0
2	E	15	0	0	5	0
2	F	19	0	0	6	0
2	G	27	0	0	13	0
2	H	23	0	0	6	0
2	I	13	0	0	3	0
2	J	11	0	0	5	0
2	K	17	0	0	4	0
2	L	13	0	0	4	0
All	All	34934	0	33652	2456	35

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 36.

The worst 5 of 2456 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ASN:ND2	1:D:84:HIS:CE1	1.86	1.40
1:A:7:ASN:ND2	1:D:84:HIS:HE1	1.16	1.36
1:A:7:ASN:CG	1:D:84:HIS:CE1	2.06	1.28
1:A:7:ASN:CB	1:D:84:HIS:CE1	2.23	1.21
1:G:211:LYS:HG2	1:G:211:LYS:O	1.41	1.16

The worst 5 of 35 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:LYS:NZ	1:K:284:GLN:NE2[1_556]	1.07	1.13
1:B:329:GLN:CB	1:D:282:TYR:OH[1_455]	1.18	1.02
1:A:329:GLN:CB	1:E:282:TYR:OH[2_646]	1.22	0.98
1:A:260:GLN:OE1	1:H:323:TYR:O[2_646]	1.34	0.86
1:E:217:TYR:OH	1:J:267:ARG:NE[2_655]	1.47	0.73

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	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	9	33
1	B	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	9	33
1	C	358/377 (95%)	291 (81%)	60 (17%)	7 (2%)	9	33
1	D	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	9	33
1	E	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	9	33
1	F	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	9	33
1	G	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	9	33
1	H	367/377 (97%)	303 (83%)	54 (15%)	10 (3%)	6	25
1	I	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	9	33
1	J	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	9	33
1	K	358/377 (95%)	293 (82%)	58 (16%)	7 (2%)	9	33
1	L	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	9	33
All	All	4305/4524 (95%)	3515 (82%)	703 (16%)	87 (2%)	9	33

5 of 87 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	GLY
1	B	171	GLY
1	C	171	GLY

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Mol	Chain	Res	Type
1	D	171	GLY
1	E	171	GLY

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	310/316 (98%)	284 (92%)	26 (8%)	14	37
1	B	310/316 (98%)	284 (92%)	26 (8%)	14	37
1	C	310/316 (98%)	284 (92%)	26 (8%)	14	37
1	D	310/316 (98%)	284 (92%)	26 (8%)	14	37
1	E	310/316 (98%)	284 (92%)	26 (8%)	14	37
1	F	310/316 (98%)	284 (92%)	26 (8%)	14	37
1	G	310/316 (98%)	284 (92%)	26 (8%)	14	37
1	H	316/316 (100%)	286 (90%)	30 (10%)	11	31
1	I	310/316 (98%)	284 (92%)	26 (8%)	14	37
1	J	310/316 (98%)	284 (92%)	26 (8%)	14	37
1	K	310/316 (98%)	285 (92%)	25 (8%)	15	39
1	L	310/316 (98%)	284 (92%)	26 (8%)	14	37
All	All	3726/3792 (98%)	3411 (92%)	315 (8%)	13	37

5 of 315 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	178	MSE
1	G	278	LYS
1	L	36	ASP
1	F	197	LYS
1	G	67	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 255 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	203	ASN
1	G	315	ASN
1	L	26	GLN
1	F	261	GLN
1	G	26	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	355/377 (94%)	0.36	10 (2%) 56 50	10, 17, 47, 60	1 (0%)
1	B	355/377 (94%)	0.31	12 (3%) 49 41	10, 20, 54, 60	1 (0%)
1	C	355/377 (94%)	0.66	33 (9%) 11 7	10, 40, 60, 60	1 (0%)
1	D	355/377 (94%)	0.59	30 (8%) 13 8	10, 34, 60, 60	1 (0%)
1	E	355/377 (94%)	0.63	35 (9%) 9 5	10, 35, 60, 60	1 (0%)
1	F	355/377 (94%)	0.58	20 (5%) 28 21	10, 36, 60, 60	1 (0%)
1	G	355/377 (94%)	0.70	37 (10%) 8 5	10, 37, 60, 60	1 (0%)
1	H	362/377 (96%)	0.19	14 (3%) 43 36	10, 33, 59, 60	1 (0%)
1	I	355/377 (94%)	0.56	28 (7%) 15 10	10, 38, 60, 60	1 (0%)
1	J	355/377 (94%)	0.80	45 (12%) 5 3	11, 49, 60, 60	1 (0%)
1	K	355/377 (94%)	0.56	24 (6%) 20 14	10, 45, 60, 60	1 (0%)
1	L	355/377 (94%)	1.10	69 (19%) 1 1	15, 56, 60, 60	1 (0%)
All	All	4267/4524 (94%)	0.59	357 (8%) 14 9	10, 37, 60, 60	12 (0%)

The worst 5 of 357 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	294	GLY	6.9
1	B	370	LEU	6.4
1	C	370	LEU	6.3
1	E	217	TYR	6.3
1	J	83	SER	6.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.