



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:45 am GMT

PDB ID : 4E4J  
Title : Crystal structure of arginine deiminase from Mycoplasma penetrans  
Authors : Benach, J.; Gallego, P.; Planell, R.; Querol, E.; Perez Pons, J.A.; Reverter, D.  
Deposited on : 2012-03-13  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

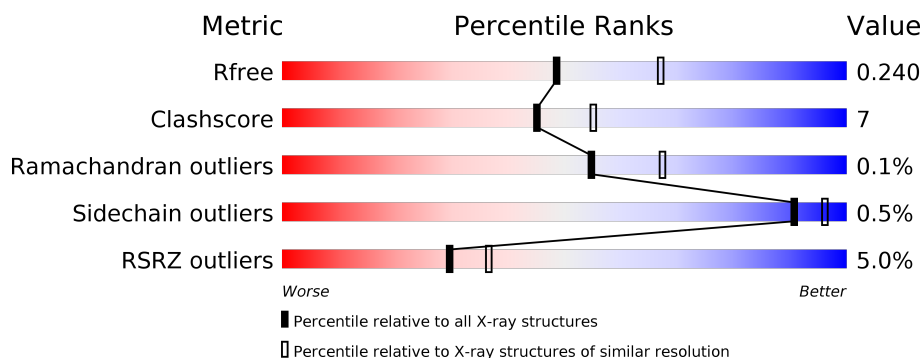
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	433	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 13%, green 79%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>79%</span> <span>13%</span> <span>8%</span> </div> </div>
1	B	433	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 1%, yellow 16%, green 76%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>6%</span> <span>76%</span> <span>16%</span> <span>8%</span> </div> </div>
1	C	433	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 12%, green 80%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>2%</span> <span>80%</span> <span>12%</span> <span>8%</span> </div> </div>
1	D	433	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 12%, green 80%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>4%</span> <span>80%</span> <span>12%</span> <span>8%</span> </div> </div>
1	E	433	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 11%, green 81%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>2%</span> <span>81%</span> <span>11%</span> <span>8%</span> </div> </div>
1	F	433	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 7%, orange 1%, yellow 15%, green 77%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>7%</span> <span>77%</span> <span>15%</span> <span>8%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	433	
1	H	433	
1	I	433	
1	J	433	
1	K	433	
1	L	433	

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	CL	D	501	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39631 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 Arginine deiminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3167	2033	525	590	19			
1	B	399	Total	C	N	O	S	0	0	0
			3167	2033	525	590	19			
1	C	399	Total	C	N	O	S	0	0	0
			3167	2033	525	590	19			
1	D	399	Total	C	N	O	S	0	0	0
			3167	2033	525	590	19			
1	E	399	Total	C	N	O	S	0	0	0
			3167	2033	525	590	19			
1	F	399	Total	C	N	O	S	0	0	0
			3167	2033	525	590	19			
1	G	399	Total	C	N	O	S	0	0	0
			3167	2033	525	590	19			
1	H	399	Total	C	N	O	S	0	0	0
			3167	2033	525	590	19			
1	I	399	Total	C	N	O	S	0	0	0
			3167	2033	525	590	19			
1	J	399	Total	C	N	O	S	0	0	0
			3167	2033	525	590	19			
1	K	399	Total	C	N	O	S	0	0	0
			3167	2033	525	590	19			
1	L	399	Total	C	N	O	S	0	0	0
			3167	2033	525	590	19			

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	EXPRESSION TAG	UNP Q8EVF6
A	21	GLY	-	EXPRESSION TAG	UNP Q8EVF6
A	22	HIS	-	EXPRESSION TAG	UNP Q8EVF6
A	23	HIS	-	EXPRESSION TAG	UNP Q8EVF6
A	24	HIS	-	EXPRESSION TAG	UNP Q8EVF6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	25	HIS	-	EXPRESSION TAG	UNP Q8EVF6
A	26	HIS	-	EXPRESSION TAG	UNP Q8EVF6
A	27	HIS	-	EXPRESSION TAG	UNP Q8EVF6
A	28	HIS	-	EXPRESSION TAG	UNP Q8EVF6
A	29	HIS	-	EXPRESSION TAG	UNP Q8EVF6
A	30	HIS	-	EXPRESSION TAG	UNP Q8EVF6
A	31	HIS	-	EXPRESSION TAG	UNP Q8EVF6
A	32	SER	-	EXPRESSION TAG	UNP Q8EVF6
A	33	SER	-	EXPRESSION TAG	UNP Q8EVF6
A	34	GLY	-	EXPRESSION TAG	UNP Q8EVF6
A	35	HIS	-	EXPRESSION TAG	UNP Q8EVF6
A	36	ILE	-	EXPRESSION TAG	UNP Q8EVF6
A	37	ASP	-	EXPRESSION TAG	UNP Q8EVF6
A	38	ASP	-	EXPRESSION TAG	UNP Q8EVF6
A	39	ASP	-	EXPRESSION TAG	UNP Q8EVF6
A	40	ASP	-	EXPRESSION TAG	UNP Q8EVF6
A	41	LYS	-	EXPRESSION TAG	UNP Q8EVF6
A	42	HIS	-	EXPRESSION TAG	UNP Q8EVF6
B	20	MET	-	EXPRESSION TAG	UNP Q8EVF6
B	21	GLY	-	EXPRESSION TAG	UNP Q8EVF6
B	22	HIS	-	EXPRESSION TAG	UNP Q8EVF6
B	23	HIS	-	EXPRESSION TAG	UNP Q8EVF6
B	24	HIS	-	EXPRESSION TAG	UNP Q8EVF6
B	25	HIS	-	EXPRESSION TAG	UNP Q8EVF6
B	26	HIS	-	EXPRESSION TAG	UNP Q8EVF6
B	27	HIS	-	EXPRESSION TAG	UNP Q8EVF6
B	28	HIS	-	EXPRESSION TAG	UNP Q8EVF6
B	29	HIS	-	EXPRESSION TAG	UNP Q8EVF6
B	30	HIS	-	EXPRESSION TAG	UNP Q8EVF6
B	31	HIS	-	EXPRESSION TAG	UNP Q8EVF6
B	32	SER	-	EXPRESSION TAG	UNP Q8EVF6
B	33	SER	-	EXPRESSION TAG	UNP Q8EVF6
B	34	GLY	-	EXPRESSION TAG	UNP Q8EVF6
B	35	HIS	-	EXPRESSION TAG	UNP Q8EVF6
B	36	ILE	-	EXPRESSION TAG	UNP Q8EVF6
B	37	ASP	-	EXPRESSION TAG	UNP Q8EVF6
B	38	ASP	-	EXPRESSION TAG	UNP Q8EVF6
B	39	ASP	-	EXPRESSION TAG	UNP Q8EVF6
B	40	ASP	-	EXPRESSION TAG	UNP Q8EVF6
B	41	LYS	-	EXPRESSION TAG	UNP Q8EVF6
B	42	HIS	-	EXPRESSION TAG	UNP Q8EVF6
C	20	MET	-	EXPRESSION TAG	UNP Q8EVF6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	GLY	-	EXPRESSION TAG	UNP Q8EVF6
C	22	HIS	-	EXPRESSION TAG	UNP Q8EVF6
C	23	HIS	-	EXPRESSION TAG	UNP Q8EVF6
C	24	HIS	-	EXPRESSION TAG	UNP Q8EVF6
C	25	HIS	-	EXPRESSION TAG	UNP Q8EVF6
C	26	HIS	-	EXPRESSION TAG	UNP Q8EVF6
C	27	HIS	-	EXPRESSION TAG	UNP Q8EVF6
C	28	HIS	-	EXPRESSION TAG	UNP Q8EVF6
C	29	HIS	-	EXPRESSION TAG	UNP Q8EVF6
C	30	HIS	-	EXPRESSION TAG	UNP Q8EVF6
C	31	HIS	-	EXPRESSION TAG	UNP Q8EVF6
C	32	SER	-	EXPRESSION TAG	UNP Q8EVF6
C	33	SER	-	EXPRESSION TAG	UNP Q8EVF6
C	34	GLY	-	EXPRESSION TAG	UNP Q8EVF6
C	35	HIS	-	EXPRESSION TAG	UNP Q8EVF6
C	36	ILE	-	EXPRESSION TAG	UNP Q8EVF6
C	37	ASP	-	EXPRESSION TAG	UNP Q8EVF6
C	38	ASP	-	EXPRESSION TAG	UNP Q8EVF6
C	39	ASP	-	EXPRESSION TAG	UNP Q8EVF6
C	40	ASP	-	EXPRESSION TAG	UNP Q8EVF6
C	41	LYS	-	EXPRESSION TAG	UNP Q8EVF6
C	42	HIS	-	EXPRESSION TAG	UNP Q8EVF6
D	20	MET	-	EXPRESSION TAG	UNP Q8EVF6
D	21	GLY	-	EXPRESSION TAG	UNP Q8EVF6
D	22	HIS	-	EXPRESSION TAG	UNP Q8EVF6
D	23	HIS	-	EXPRESSION TAG	UNP Q8EVF6
D	24	HIS	-	EXPRESSION TAG	UNP Q8EVF6
D	25	HIS	-	EXPRESSION TAG	UNP Q8EVF6
D	26	HIS	-	EXPRESSION TAG	UNP Q8EVF6
D	27	HIS	-	EXPRESSION TAG	UNP Q8EVF6
D	28	HIS	-	EXPRESSION TAG	UNP Q8EVF6
D	29	HIS	-	EXPRESSION TAG	UNP Q8EVF6
D	30	HIS	-	EXPRESSION TAG	UNP Q8EVF6
D	31	HIS	-	EXPRESSION TAG	UNP Q8EVF6
D	32	SER	-	EXPRESSION TAG	UNP Q8EVF6
D	33	SER	-	EXPRESSION TAG	UNP Q8EVF6
D	34	GLY	-	EXPRESSION TAG	UNP Q8EVF6
D	35	HIS	-	EXPRESSION TAG	UNP Q8EVF6
D	36	ILE	-	EXPRESSION TAG	UNP Q8EVF6
D	37	ASP	-	EXPRESSION TAG	UNP Q8EVF6
D	38	ASP	-	EXPRESSION TAG	UNP Q8EVF6
D	39	ASP	-	EXPRESSION TAG	UNP Q8EVF6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	40	ASP	-	EXPRESSION TAG	UNP Q8EVF6
D	41	LYS	-	EXPRESSION TAG	UNP Q8EVF6
D	42	HIS	-	EXPRESSION TAG	UNP Q8EVF6
E	20	MET	-	EXPRESSION TAG	UNP Q8EVF6
E	21	GLY	-	EXPRESSION TAG	UNP Q8EVF6
E	22	HIS	-	EXPRESSION TAG	UNP Q8EVF6
E	23	HIS	-	EXPRESSION TAG	UNP Q8EVF6
E	24	HIS	-	EXPRESSION TAG	UNP Q8EVF6
E	25	HIS	-	EXPRESSION TAG	UNP Q8EVF6
E	26	HIS	-	EXPRESSION TAG	UNP Q8EVF6
E	27	HIS	-	EXPRESSION TAG	UNP Q8EVF6
E	28	HIS	-	EXPRESSION TAG	UNP Q8EVF6
E	29	HIS	-	EXPRESSION TAG	UNP Q8EVF6
E	30	HIS	-	EXPRESSION TAG	UNP Q8EVF6
E	31	HIS	-	EXPRESSION TAG	UNP Q8EVF6
E	32	SER	-	EXPRESSION TAG	UNP Q8EVF6
E	33	SER	-	EXPRESSION TAG	UNP Q8EVF6
E	34	GLY	-	EXPRESSION TAG	UNP Q8EVF6
E	35	HIS	-	EXPRESSION TAG	UNP Q8EVF6
E	36	ILE	-	EXPRESSION TAG	UNP Q8EVF6
E	37	ASP	-	EXPRESSION TAG	UNP Q8EVF6
E	38	ASP	-	EXPRESSION TAG	UNP Q8EVF6
E	39	ASP	-	EXPRESSION TAG	UNP Q8EVF6
E	40	ASP	-	EXPRESSION TAG	UNP Q8EVF6
E	41	LYS	-	EXPRESSION TAG	UNP Q8EVF6
E	42	HIS	-	EXPRESSION TAG	UNP Q8EVF6
F	20	MET	-	EXPRESSION TAG	UNP Q8EVF6
F	21	GLY	-	EXPRESSION TAG	UNP Q8EVF6
F	22	HIS	-	EXPRESSION TAG	UNP Q8EVF6
F	23	HIS	-	EXPRESSION TAG	UNP Q8EVF6
F	24	HIS	-	EXPRESSION TAG	UNP Q8EVF6
F	25	HIS	-	EXPRESSION TAG	UNP Q8EVF6
F	26	HIS	-	EXPRESSION TAG	UNP Q8EVF6
F	27	HIS	-	EXPRESSION TAG	UNP Q8EVF6
F	28	HIS	-	EXPRESSION TAG	UNP Q8EVF6
F	29	HIS	-	EXPRESSION TAG	UNP Q8EVF6
F	30	HIS	-	EXPRESSION TAG	UNP Q8EVF6
F	31	HIS	-	EXPRESSION TAG	UNP Q8EVF6
F	32	SER	-	EXPRESSION TAG	UNP Q8EVF6
F	33	SER	-	EXPRESSION TAG	UNP Q8EVF6
F	34	GLY	-	EXPRESSION TAG	UNP Q8EVF6
F	35	HIS	-	EXPRESSION TAG	UNP Q8EVF6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	36	ILE	-	EXPRESSION TAG	UNP Q8EVF6
F	37	ASP	-	EXPRESSION TAG	UNP Q8EVF6
F	38	ASP	-	EXPRESSION TAG	UNP Q8EVF6
F	39	ASP	-	EXPRESSION TAG	UNP Q8EVF6
F	40	ASP	-	EXPRESSION TAG	UNP Q8EVF6
F	41	LYS	-	EXPRESSION TAG	UNP Q8EVF6
F	42	HIS	-	EXPRESSION TAG	UNP Q8EVF6
G	20	MET	-	EXPRESSION TAG	UNP Q8EVF6
G	21	GLY	-	EXPRESSION TAG	UNP Q8EVF6
G	22	HIS	-	EXPRESSION TAG	UNP Q8EVF6
G	23	HIS	-	EXPRESSION TAG	UNP Q8EVF6
G	24	HIS	-	EXPRESSION TAG	UNP Q8EVF6
G	25	HIS	-	EXPRESSION TAG	UNP Q8EVF6
G	26	HIS	-	EXPRESSION TAG	UNP Q8EVF6
G	27	HIS	-	EXPRESSION TAG	UNP Q8EVF6
G	28	HIS	-	EXPRESSION TAG	UNP Q8EVF6
G	29	HIS	-	EXPRESSION TAG	UNP Q8EVF6
G	30	HIS	-	EXPRESSION TAG	UNP Q8EVF6
G	31	HIS	-	EXPRESSION TAG	UNP Q8EVF6
G	32	SER	-	EXPRESSION TAG	UNP Q8EVF6
G	33	SER	-	EXPRESSION TAG	UNP Q8EVF6
G	34	GLY	-	EXPRESSION TAG	UNP Q8EVF6
G	35	HIS	-	EXPRESSION TAG	UNP Q8EVF6
G	36	ILE	-	EXPRESSION TAG	UNP Q8EVF6
G	37	ASP	-	EXPRESSION TAG	UNP Q8EVF6
G	38	ASP	-	EXPRESSION TAG	UNP Q8EVF6
G	39	ASP	-	EXPRESSION TAG	UNP Q8EVF6
G	40	ASP	-	EXPRESSION TAG	UNP Q8EVF6
G	41	LYS	-	EXPRESSION TAG	UNP Q8EVF6
G	42	HIS	-	EXPRESSION TAG	UNP Q8EVF6
H	20	MET	-	EXPRESSION TAG	UNP Q8EVF6
H	21	GLY	-	EXPRESSION TAG	UNP Q8EVF6
H	22	HIS	-	EXPRESSION TAG	UNP Q8EVF6
H	23	HIS	-	EXPRESSION TAG	UNP Q8EVF6
H	24	HIS	-	EXPRESSION TAG	UNP Q8EVF6
H	25	HIS	-	EXPRESSION TAG	UNP Q8EVF6
H	26	HIS	-	EXPRESSION TAG	UNP Q8EVF6
H	27	HIS	-	EXPRESSION TAG	UNP Q8EVF6
H	28	HIS	-	EXPRESSION TAG	UNP Q8EVF6
H	29	HIS	-	EXPRESSION TAG	UNP Q8EVF6
H	30	HIS	-	EXPRESSION TAG	UNP Q8EVF6
H	31	HIS	-	EXPRESSION TAG	UNP Q8EVF6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	32	SER	-	EXPRESSION TAG	UNP Q8EVF6
H	33	SER	-	EXPRESSION TAG	UNP Q8EVF6
H	34	GLY	-	EXPRESSION TAG	UNP Q8EVF6
H	35	HIS	-	EXPRESSION TAG	UNP Q8EVF6
H	36	ILE	-	EXPRESSION TAG	UNP Q8EVF6
H	37	ASP	-	EXPRESSION TAG	UNP Q8EVF6
H	38	ASP	-	EXPRESSION TAG	UNP Q8EVF6
H	39	ASP	-	EXPRESSION TAG	UNP Q8EVF6
H	40	ASP	-	EXPRESSION TAG	UNP Q8EVF6
H	41	LYS	-	EXPRESSION TAG	UNP Q8EVF6
H	42	HIS	-	EXPRESSION TAG	UNP Q8EVF6
I	20	MET	-	EXPRESSION TAG	UNP Q8EVF6
I	21	GLY	-	EXPRESSION TAG	UNP Q8EVF6
I	22	HIS	-	EXPRESSION TAG	UNP Q8EVF6
I	23	HIS	-	EXPRESSION TAG	UNP Q8EVF6
I	24	HIS	-	EXPRESSION TAG	UNP Q8EVF6
I	25	HIS	-	EXPRESSION TAG	UNP Q8EVF6
I	26	HIS	-	EXPRESSION TAG	UNP Q8EVF6
I	27	HIS	-	EXPRESSION TAG	UNP Q8EVF6
I	28	HIS	-	EXPRESSION TAG	UNP Q8EVF6
I	29	HIS	-	EXPRESSION TAG	UNP Q8EVF6
I	30	HIS	-	EXPRESSION TAG	UNP Q8EVF6
I	31	HIS	-	EXPRESSION TAG	UNP Q8EVF6
I	32	SER	-	EXPRESSION TAG	UNP Q8EVF6
I	33	SER	-	EXPRESSION TAG	UNP Q8EVF6
I	34	GLY	-	EXPRESSION TAG	UNP Q8EVF6
I	35	HIS	-	EXPRESSION TAG	UNP Q8EVF6
I	36	ILE	-	EXPRESSION TAG	UNP Q8EVF6
I	37	ASP	-	EXPRESSION TAG	UNP Q8EVF6
I	38	ASP	-	EXPRESSION TAG	UNP Q8EVF6
I	39	ASP	-	EXPRESSION TAG	UNP Q8EVF6
I	40	ASP	-	EXPRESSION TAG	UNP Q8EVF6
I	41	LYS	-	EXPRESSION TAG	UNP Q8EVF6
I	42	HIS	-	EXPRESSION TAG	UNP Q8EVF6
J	20	MET	-	EXPRESSION TAG	UNP Q8EVF6
J	21	GLY	-	EXPRESSION TAG	UNP Q8EVF6
J	22	HIS	-	EXPRESSION TAG	UNP Q8EVF6
J	23	HIS	-	EXPRESSION TAG	UNP Q8EVF6
J	24	HIS	-	EXPRESSION TAG	UNP Q8EVF6
J	25	HIS	-	EXPRESSION TAG	UNP Q8EVF6
J	26	HIS	-	EXPRESSION TAG	UNP Q8EVF6
J	27	HIS	-	EXPRESSION TAG	UNP Q8EVF6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	28	HIS	-	EXPRESSION TAG	UNP Q8EVF6
J	29	HIS	-	EXPRESSION TAG	UNP Q8EVF6
J	30	HIS	-	EXPRESSION TAG	UNP Q8EVF6
J	31	HIS	-	EXPRESSION TAG	UNP Q8EVF6
J	32	SER	-	EXPRESSION TAG	UNP Q8EVF6
J	33	SER	-	EXPRESSION TAG	UNP Q8EVF6
J	34	GLY	-	EXPRESSION TAG	UNP Q8EVF6
J	35	HIS	-	EXPRESSION TAG	UNP Q8EVF6
J	36	ILE	-	EXPRESSION TAG	UNP Q8EVF6
J	37	ASP	-	EXPRESSION TAG	UNP Q8EVF6
J	38	ASP	-	EXPRESSION TAG	UNP Q8EVF6
J	39	ASP	-	EXPRESSION TAG	UNP Q8EVF6
J	40	ASP	-	EXPRESSION TAG	UNP Q8EVF6
J	41	LYS	-	EXPRESSION TAG	UNP Q8EVF6
J	42	HIS	-	EXPRESSION TAG	UNP Q8EVF6
K	20	MET	-	EXPRESSION TAG	UNP Q8EVF6
K	21	GLY	-	EXPRESSION TAG	UNP Q8EVF6
K	22	HIS	-	EXPRESSION TAG	UNP Q8EVF6
K	23	HIS	-	EXPRESSION TAG	UNP Q8EVF6
K	24	HIS	-	EXPRESSION TAG	UNP Q8EVF6
K	25	HIS	-	EXPRESSION TAG	UNP Q8EVF6
K	26	HIS	-	EXPRESSION TAG	UNP Q8EVF6
K	27	HIS	-	EXPRESSION TAG	UNP Q8EVF6
K	28	HIS	-	EXPRESSION TAG	UNP Q8EVF6
K	29	HIS	-	EXPRESSION TAG	UNP Q8EVF6
K	30	HIS	-	EXPRESSION TAG	UNP Q8EVF6
K	31	HIS	-	EXPRESSION TAG	UNP Q8EVF6
K	32	SER	-	EXPRESSION TAG	UNP Q8EVF6
K	33	SER	-	EXPRESSION TAG	UNP Q8EVF6
K	34	GLY	-	EXPRESSION TAG	UNP Q8EVF6
K	35	HIS	-	EXPRESSION TAG	UNP Q8EVF6
K	36	ILE	-	EXPRESSION TAG	UNP Q8EVF6
K	37	ASP	-	EXPRESSION TAG	UNP Q8EVF6
K	38	ASP	-	EXPRESSION TAG	UNP Q8EVF6
K	39	ASP	-	EXPRESSION TAG	UNP Q8EVF6
K	40	ASP	-	EXPRESSION TAG	UNP Q8EVF6
K	41	LYS	-	EXPRESSION TAG	UNP Q8EVF6
K	42	HIS	-	EXPRESSION TAG	UNP Q8EVF6
L	20	MET	-	EXPRESSION TAG	UNP Q8EVF6
L	21	GLY	-	EXPRESSION TAG	UNP Q8EVF6
L	22	HIS	-	EXPRESSION TAG	UNP Q8EVF6
L	23	HIS	-	EXPRESSION TAG	UNP Q8EVF6

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Chain	Residue	Modelled	Actual	Comment	Reference
L	24	HIS	-	EXPRESSION TAG	UNP Q8EVF6
L	25	HIS	-	EXPRESSION TAG	UNP Q8EVF6
L	26	HIS	-	EXPRESSION TAG	UNP Q8EVF6
L	27	HIS	-	EXPRESSION TAG	UNP Q8EVF6
L	28	HIS	-	EXPRESSION TAG	UNP Q8EVF6
L	29	HIS	-	EXPRESSION TAG	UNP Q8EVF6
L	30	HIS	-	EXPRESSION TAG	UNP Q8EVF6
L	31	HIS	-	EXPRESSION TAG	UNP Q8EVF6
L	32	SER	-	EXPRESSION TAG	UNP Q8EVF6
L	33	SER	-	EXPRESSION TAG	UNP Q8EVF6
L	34	GLY	-	EXPRESSION TAG	UNP Q8EVF6
L	35	HIS	-	EXPRESSION TAG	UNP Q8EVF6
L	36	ILE	-	EXPRESSION TAG	UNP Q8EVF6
L	37	ASP	-	EXPRESSION TAG	UNP Q8EVF6
L	38	ASP	-	EXPRESSION TAG	UNP Q8EVF6
L	39	ASP	-	EXPRESSION TAG	UNP Q8EVF6
L	40	ASP	-	EXPRESSION TAG	UNP Q8EVF6
L	41	LYS	-	EXPRESSION TAG	UNP Q8EVF6
L	42	HIS	-	EXPRESSION TAG	UNP Q8EVF6

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Cl 1 1	0	0
2	J	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	K	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	I	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	1	Total 1	Cl 1	0	0
2	F	1	Total 1	Cl 1	0	0

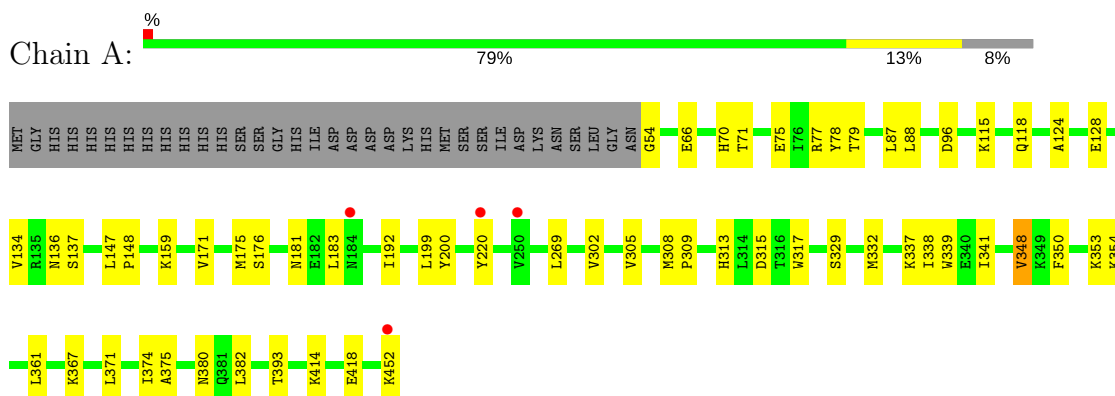
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	212	Total 212	O 212	0	0
3	B	117	Total 117	O 117	0	0
3	C	213	Total 213	O 213	0	0
3	D	142	Total 142	O 142	0	0
3	E	180	Total 180	O 180	0	0
3	F	99	Total 99	O 99	0	0
3	G	80	Total 80	O 80	0	0
3	H	140	Total 140	O 140	0	0
3	I	86	Total 86	O 86	0	0
3	J	82	Total 82	O 82	0	0
3	K	160	Total 160	O 160	0	0
3	L	104	Total 104	O 104	0	0

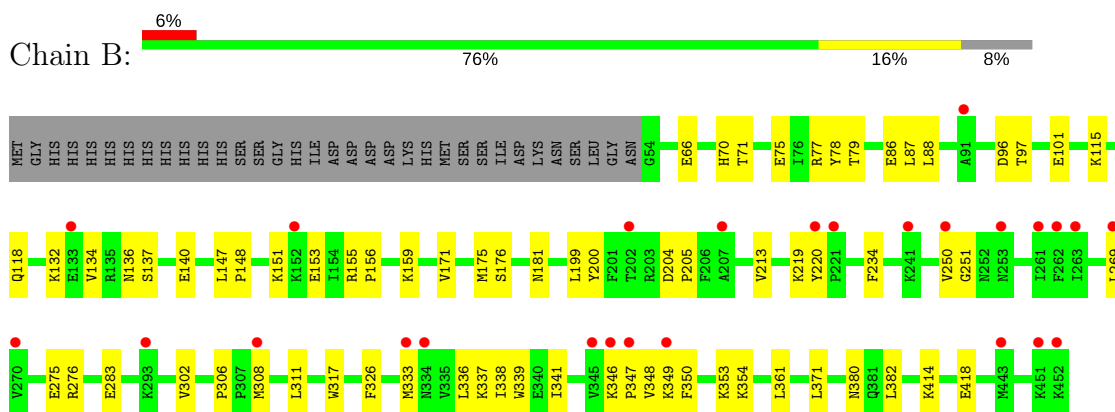
### 3 Residue-property plots [i](#)

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

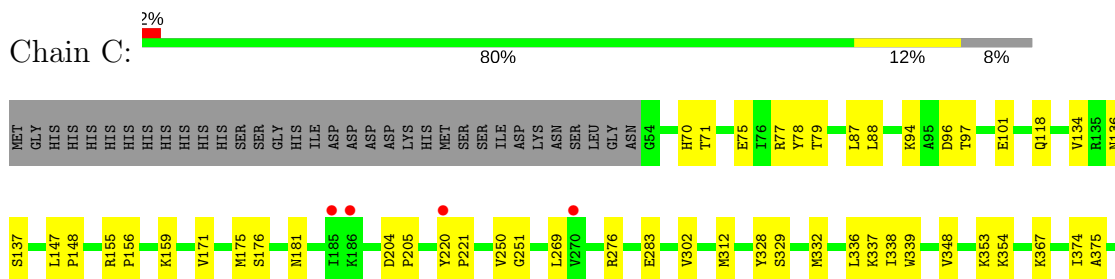
#### • Molecule 1: Arginine deiminase

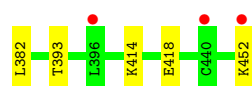


#### • Molecule 1: Arginine deiminase

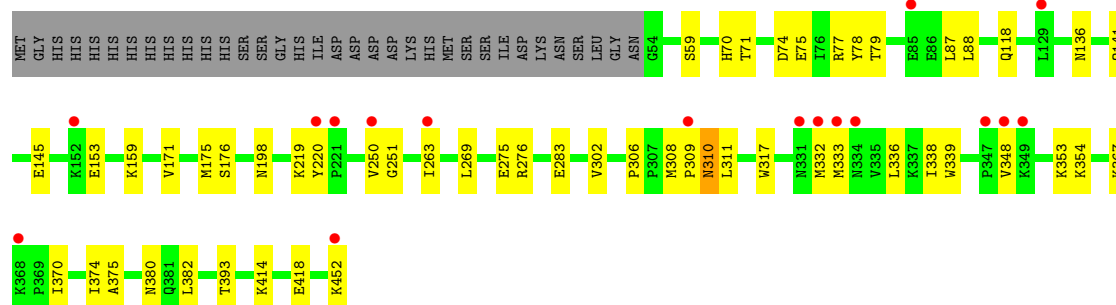
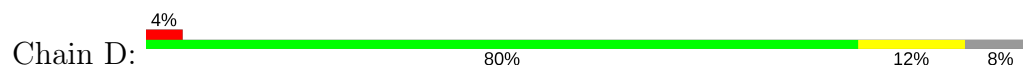


#### • Molecule 1: Arginine deiminase

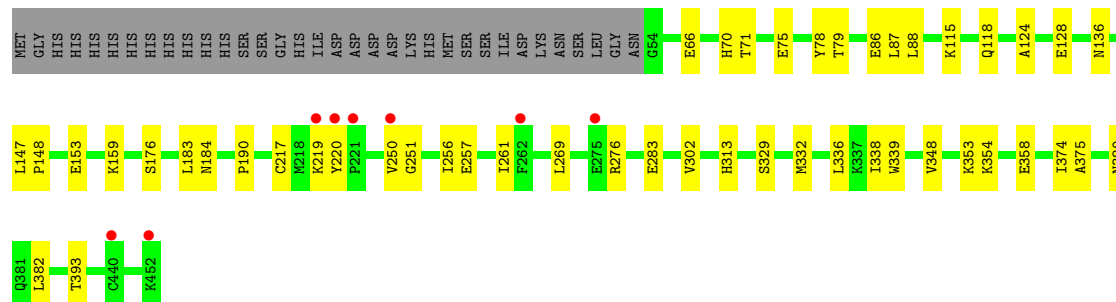
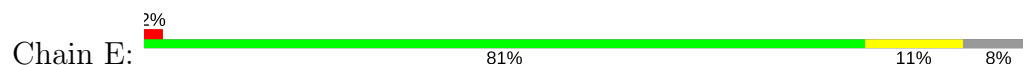




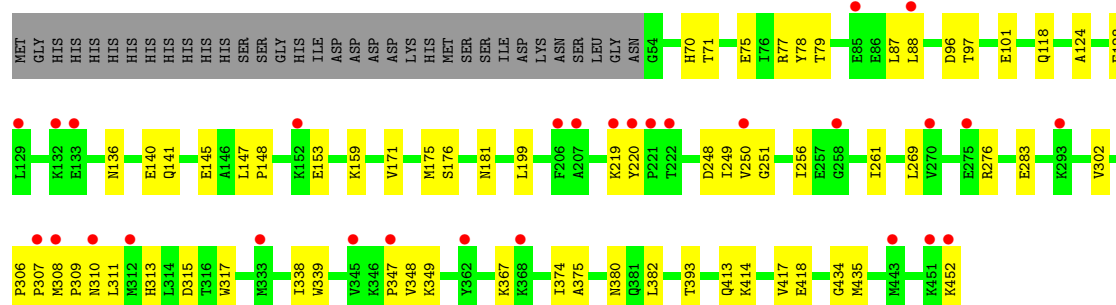
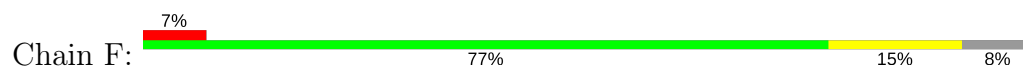
- Molecule 1: Arginine deiminase



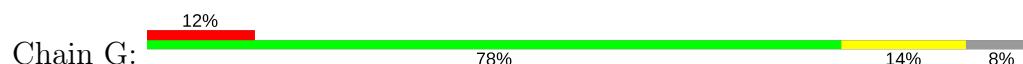
- Molecule 1: Arginine deiminase

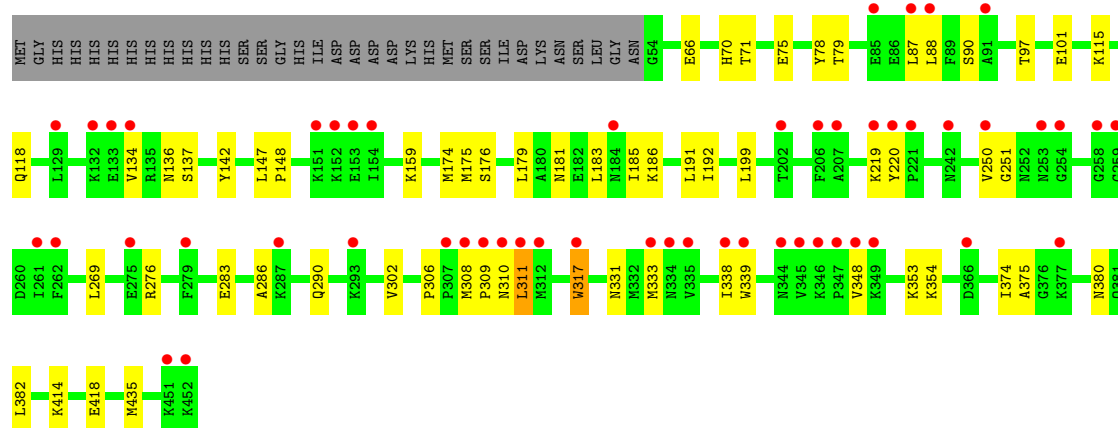


- Molecule 1: Arginine deiminase

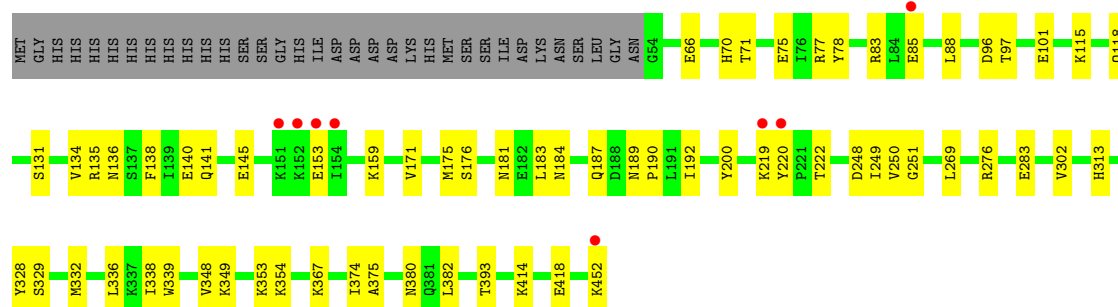
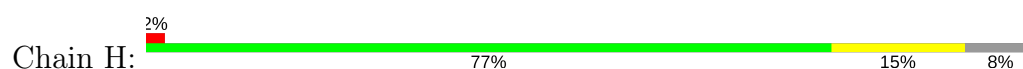


- Molecule 1: Arginine deiminase

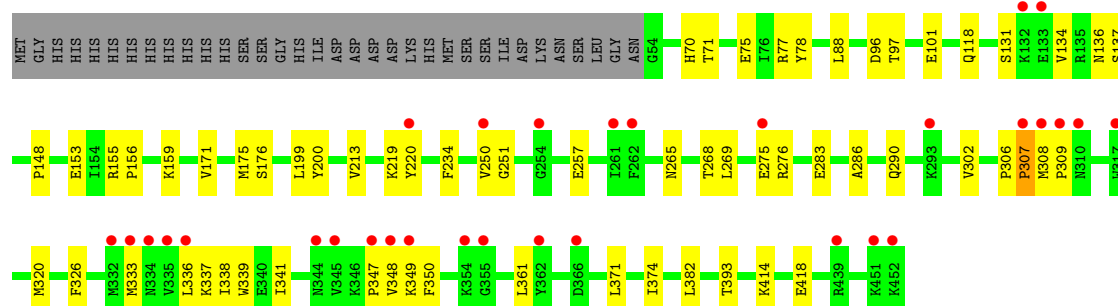
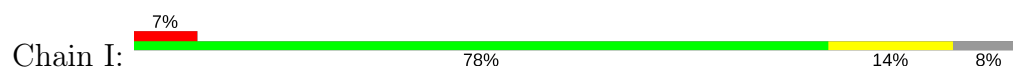




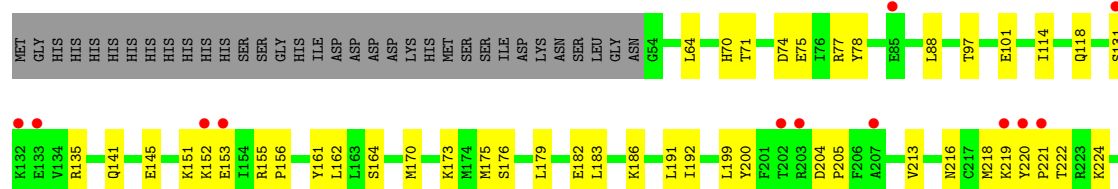
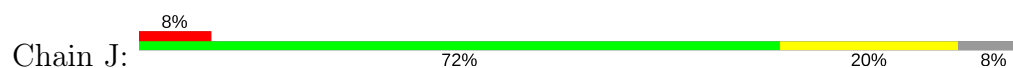
• Molecule 1: Arginine deiminase

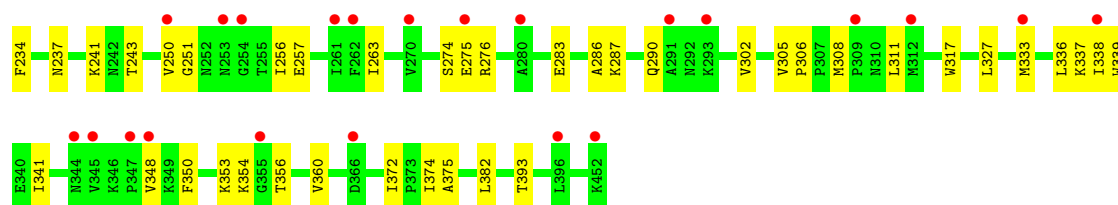


• Molecule 1: Arginine deiminase

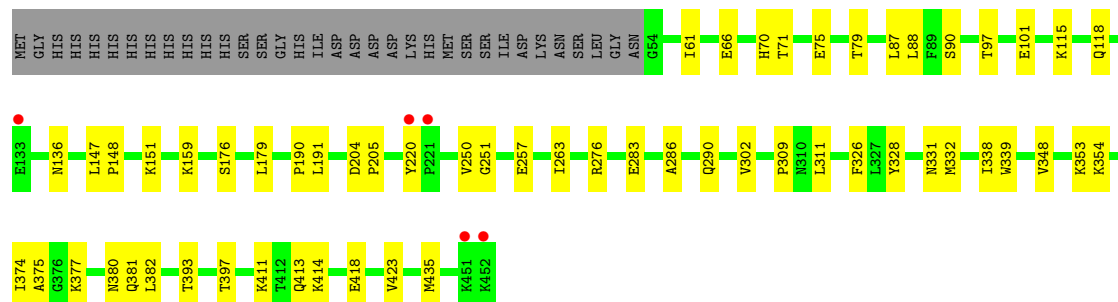
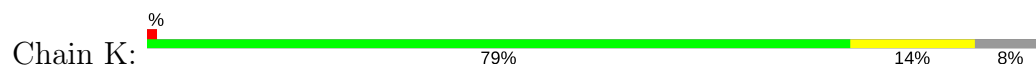


• Molecule 1: Arginine deiminase

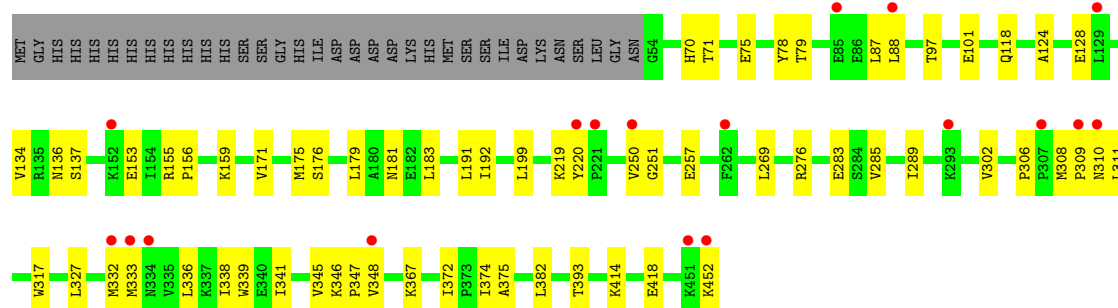
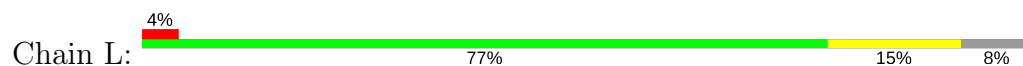




• Molecule 1: Arginine deiminase



• Molecule 1: Arginine deiminase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.55Å 128.88Å 220.28Å 90.00° 91.41° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.92 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.9 (30.00-2.30) 97.5 (29.92-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.31Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.210 , 0.238 0.211 , 0.240	Depositor DCC
$R_{free}$ test set	14720 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	39631	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.40	0/3226	0.65	0/4362
1	B	0.36	0/3226	0.61	0/4362
1	C	0.40	0/3226	0.64	1/4362 (0.0%)
1	D	0.35	0/3226	0.62	0/4362
1	E	0.39	0/3226	0.64	0/4362
1	F	0.36	0/3226	0.61	0/4362
1	G	0.34	0/3226	0.60	0/4362
1	H	0.38	0/3226	0.63	0/4362
1	I	0.34	0/3226	0.60	0/4362
1	J	0.34	0/3226	0.60	0/4362
1	K	0.39	0/3226	0.65	0/4362
1	L	0.36	0/3226	0.62	0/4362
All	All	0.37	0/38712	0.62	1/52344 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	94	LYS	N-CA-C	-5.32	96.65	111.00

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	3167	0	3243	45	0
1	B	3167	0	3243	51	0
1	C	3167	0	3243	47	0
1	D	3167	0	3243	52	0
1	E	3167	0	3243	41	0
1	F	3167	0	3243	48	0
1	G	3167	0	3243	49	0
1	H	3167	0	3243	54	0
1	I	3167	0	3243	54	0
1	J	3167	0	3243	65	0
1	K	3167	0	3243	46	0
1	L	3167	0	3243	53	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	212	0	0	3	0
3	B	117	0	0	3	0
3	C	213	0	0	3	0
3	D	142	0	0	4	0
3	E	180	0	0	4	0
3	F	99	0	0	2	0
3	G	80	0	0	1	0
3	H	140	0	0	4	0
3	I	86	0	0	1	0
3	J	82	0	0	3	0
3	K	160	0	0	3	0
3	L	104	0	0	0	0
All	All	39631	0	38916	570	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 570 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:71:THR:H	1:A:118:GLN:NE2	1.58	1.01
1:F:71:THR:H	1:F:118:GLN:HE22	1.05	1.01
1:L:71:THR:H	1:L:118:GLN:NE2	1.59	1.00
1:H:184:ASN:HB2	1:I:333:MET:HE2	1.42	1.00
1:B:71:THR:H	1:B:118:GLN:NE2	1.61	0.98

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	397/433 (92%)	382 (96%)	15 (4%)	0	100	100
1	B	397/433 (92%)	379 (96%)	18 (4%)	0	100	100
1	C	397/433 (92%)	383 (96%)	14 (4%)	0	100	100
1	D	397/433 (92%)	377 (95%)	19 (5%)	1 (0%)	44	55
1	E	397/433 (92%)	379 (96%)	18 (4%)	0	100	100
1	F	397/433 (92%)	378 (95%)	19 (5%)	0	100	100
1	G	397/433 (92%)	376 (95%)	20 (5%)	1 (0%)	44	55
1	H	397/433 (92%)	383 (96%)	14 (4%)	0	100	100
1	I	397/433 (92%)	375 (94%)	21 (5%)	1 (0%)	44	55
1	J	397/433 (92%)	378 (95%)	19 (5%)	0	100	100
1	K	397/433 (92%)	379 (96%)	18 (4%)	0	100	100
1	L	397/433 (92%)	378 (95%)	19 (5%)	0	100	100
All	All	4764/5196 (92%)	4547 (95%)	214 (4%)	3 (0%)	55	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	311	LEU
1	D	309	PRO
1	I	307	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	357/388 (92%)	355 (99%)	2 (1%)	89	95
1	B	357/388 (92%)	354 (99%)	3 (1%)	85	93
1	C	357/388 (92%)	355 (99%)	2 (1%)	89	95
1	D	357/388 (92%)	355 (99%)	2 (1%)	89	95
1	E	357/388 (92%)	355 (99%)	2 (1%)	89	95
1	F	357/388 (92%)	355 (99%)	2 (1%)	89	95
1	G	357/388 (92%)	355 (99%)	2 (1%)	89	95
1	H	357/388 (92%)	356 (100%)	1 (0%)	94	97
1	I	357/388 (92%)	355 (99%)	2 (1%)	89	95
1	J	357/388 (92%)	356 (100%)	1 (0%)	94	97
1	K	357/388 (92%)	357 (100%)	0	100	100
1	L	357/388 (92%)	356 (100%)	1 (0%)	94	97
All	All	4284/4656 (92%)	4264 (100%)	20 (0%)	91	96

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	217	CYS
1	E	269	LEU
1	I	269	LEU
1	D	269	LEU
1	D	310	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	216	ASN
1	G	389	HIS
1	K	413	GLN
1	F	288	ASN
1	G	136	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	399/433 (92%)	-0.22	4 (1%) 82 86	12, 23, 41, 64	0
1	B	399/433 (92%)	0.17	26 (6%) 20 26	18, 34, 59, 74	0
1	C	399/433 (92%)	-0.18	7 (1%) 69 74	14, 23, 43, 66	0
1	D	399/433 (92%)	0.09	17 (4%) 36 43	16, 31, 57, 77	0
1	E	399/433 (92%)	-0.09	8 (2%) 65 72	16, 26, 43, 69	0
1	F	399/433 (92%)	0.23	29 (7%) 16 21	16, 36, 62, 75	0
1	G	399/433 (92%)	0.54	53 (13%) 4 5	21, 42, 70, 82	0
1	H	399/433 (92%)	0.00	8 (2%) 65 72	17, 30, 55, 73	0
1	I	399/433 (92%)	0.32	31 (7%) 14 19	22, 39, 71, 87	0
1	J	399/433 (92%)	0.42	34 (8%) 11 16	22, 43, 70, 81	0
1	K	399/433 (92%)	-0.14	5 (1%) 77 81	18, 28, 46, 70	0
1	L	399/433 (92%)	0.05	18 (4%) 34 41	17, 33, 56, 77	0
All	All	4788/5196 (92%)	0.10	240 (5%) 30 36	12, 31, 61, 87	0

The worst 5 of 240 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	333	MET	9.6
1	L	333	MET	8.9
1	I	333	MET	6.8
1	L	220	TYR	6.3
1	J	220	TYR	6.1

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	D	501	1/1	1.00	0.13	2.23	21,21,21,21	0
2	CL	A	501	1/1	1.00	0.11	1.22	19,19,19,19	0
2	CL	K	501	1/1	0.99	0.10	1.11	21,21,21,21	0
2	CL	J	501	1/1	1.00	0.10	0.96	24,24,24,24	0
2	CL	E	501	1/1	0.99	0.11	0.79	20,20,20,20	0
2	CL	C	501	1/1	1.00	0.11	0.78	21,21,21,21	0
2	CL	H	501	1/1	1.00	0.11	0.56	24,24,24,24	0
2	CL	L	501	1/1	1.00	0.09	-0.29	20,20,20,20	0
2	CL	I	501	1/1	0.99	0.09	-0.31	28,28,28,28	0
2	CL	B	501	1/1	1.00	0.09	-0.50	20,20,20,20	0
2	CL	G	501	1/1	1.00	0.06	-2.27	24,24,24,24	0
2	CL	F	501	1/1	0.99	0.07	-2.68	19,19,19,19	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.