



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:04 PM UTC

PDB ID : 4E4J / pdb\_00004e4j  
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

<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>.

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

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

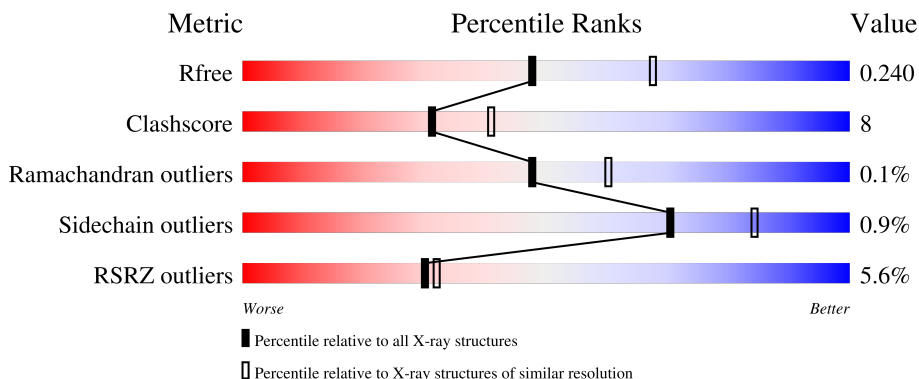
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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.



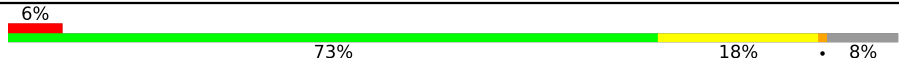
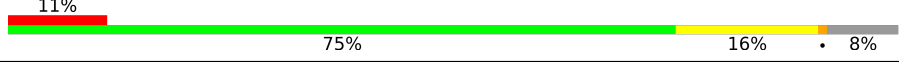
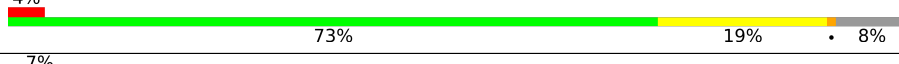
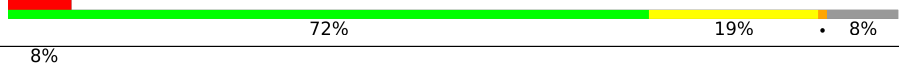

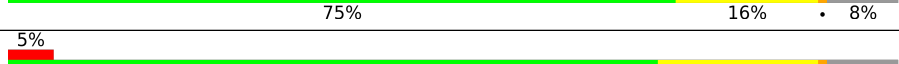
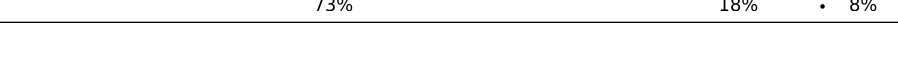
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	433	 75% 17% 8%
1	B	433	 71% 20% 8%
1	C	433	 76% 16% 8%
1	D	433	 74% 18% 8%
1	E	433	 77% 14% 8%

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Mol	Chain	Length	Quality of chain
1	F	433	 <p>6% 73% 18% • 8%</p>
1	G	433	 <p>11% 75% 16% • 8%</p>
1	H	433	 <p>4% 73% 19% • 8%</p>
1	I	433	 <p>7% 72% 19% • 8%</p>
1	J	433	 <p>8% 69% 22% • 8%</p>
1	K	433	 <p>2% 75% 16% • 8%</p>
1	L	433	 <p>5% 73% 18% • 8%</p>

## 2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	399	3167	2033	525	590	19	0	0	0
1	B	399	3167	2033	525	590	19	0	0	0
1	C	399	3167	2033	525	590	19	0	0	0
1	D	399	3167	2033	525	590	19	0	0	0
1	E	399	3167	2033	525	590	19	0	0	0
1	F	399	3167	2033	525	590	19	0	0	0
1	G	399	3167	2033	525	590	19	0	0	0
1	H	399	3167	2033	525	590	19	0	0	0
1	I	399	3167	2033	525	590	19	0	0	0
1	J	399	3167	2033	525	590	19	0	0	0
1	K	399	3167	2033	525	590	19	0	0	0
1	L	399	3167	2033	525	590	19	0	0	0

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 (CCD ID: CL) (formula: Cl).

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

*Continued on next page...*

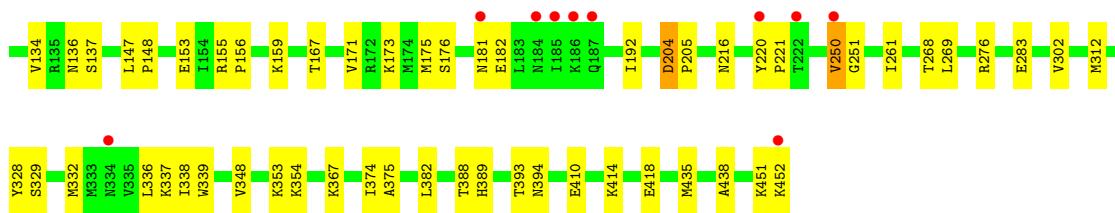
*Continued from previous page...*

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

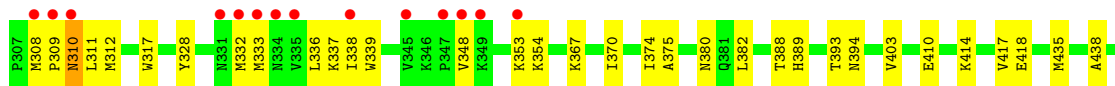
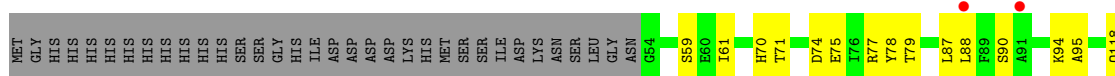
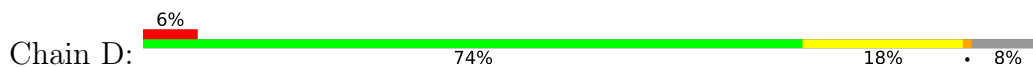
- Molecule 3 is water.

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

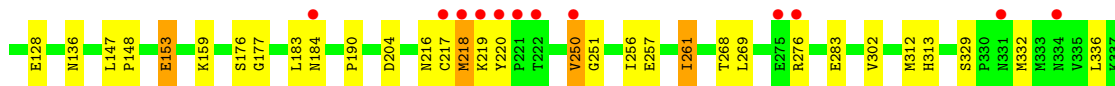
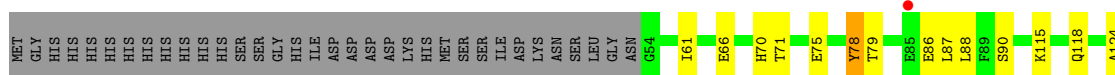
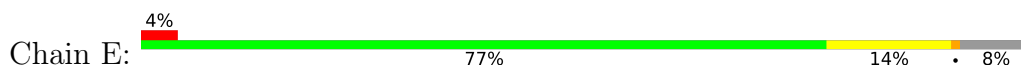




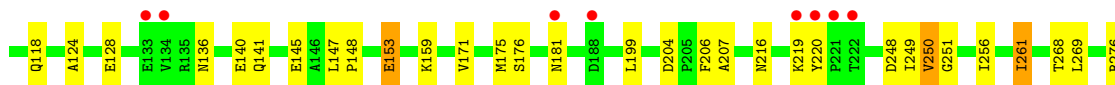
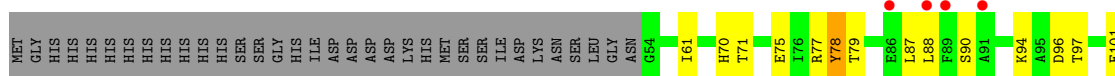
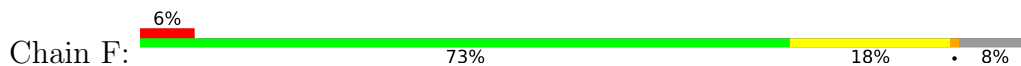
• Molecule 1: Arginine deiminase

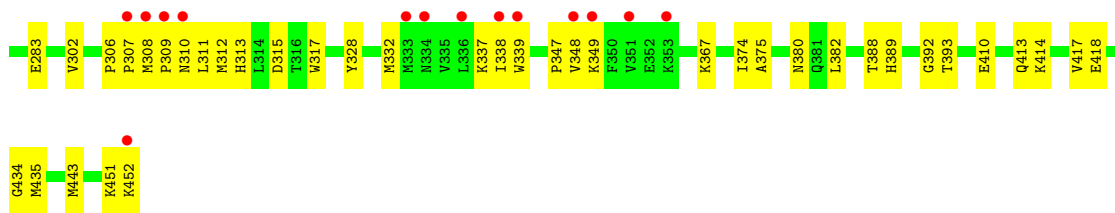


• Molecule 1: Arginine deiminase

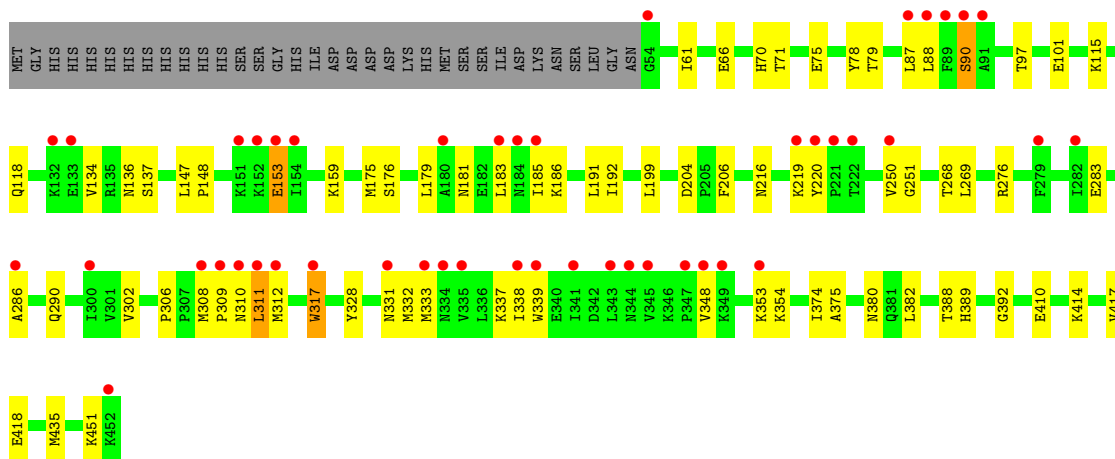
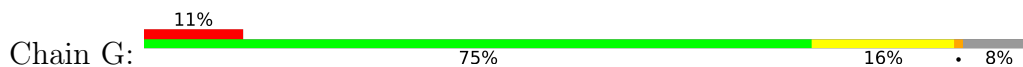


• Molecule 1: Arginine deiminase

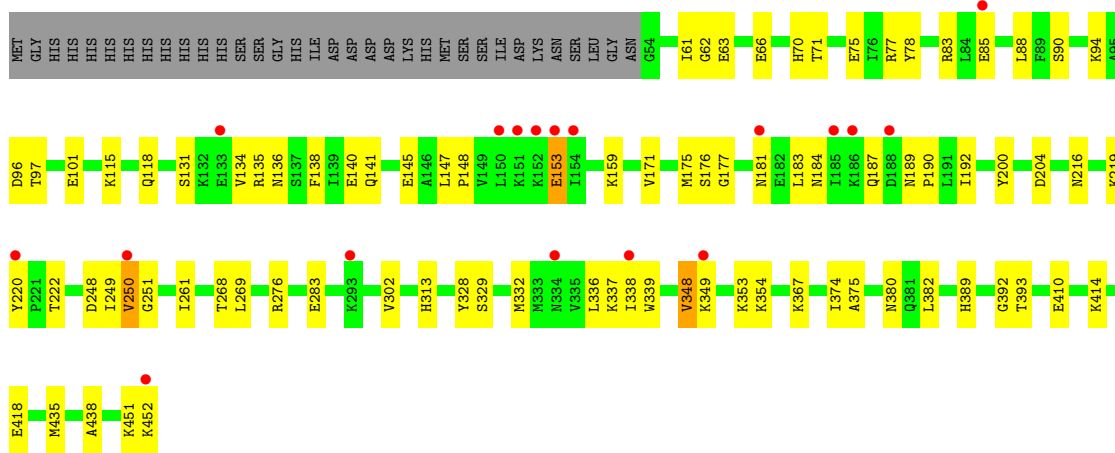
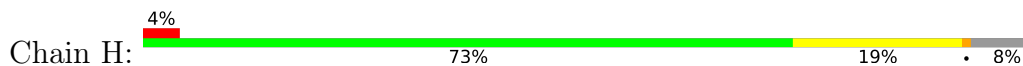




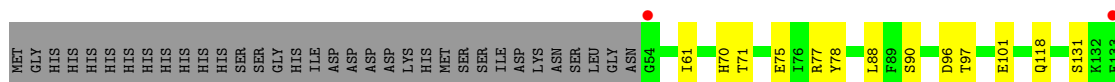
- Molecule 1: Arginine deiminase



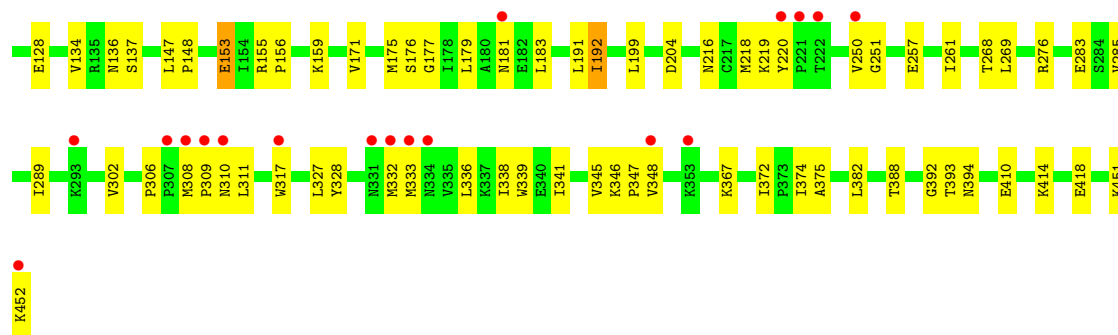
- Molecule 1: Arginine deiminase



- 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 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.9 (30.00-2.30) 97.5 (30.00-2.30)	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)	Xtrriage
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%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtrriage
Anisotropy	0.284	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	39631	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage'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	0.46	0/3226	0.94	14/4362 (0.3%)
1	B	0.42	0/3226	0.93	15/4362 (0.3%)
1	C	0.46	0/3226	0.94	17/4362 (0.4%)
1	D	0.41	0/3226	0.93	16/4362 (0.4%)
1	E	0.45	0/3226	0.97	14/4362 (0.3%)
1	F	0.41	0/3226	0.93	13/4362 (0.3%)
1	G	0.39	0/3226	0.91	9/4362 (0.2%)
1	H	0.43	0/3226	0.95	13/4362 (0.3%)
1	I	0.39	0/3226	0.92	14/4362 (0.3%)
1	J	0.39	0/3226	0.91	14/4362 (0.3%)
1	K	0.45	0/3226	0.97	17/4362 (0.4%)
1	L	0.41	0/3226	0.94	14/4362 (0.3%)
All	All	0.42	0/38712	0.94	170/52344 (0.3%)

There are no bond length outliers.

The worst 5 of 170 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	250	VAL	N-CA-C	11.34	120.58	111.62
1	H	250	VAL	N-CA-C	11.19	120.46	111.62
1	E	250	VAL	N-CA-C	10.41	119.84	111.62
1	G	90	SER	N-CA-C	8.86	123.88	112.89
1	K	90	SER	N-CA-C	8.79	123.30	112.23

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	3167	0	3243	47	0
1	B	3167	0	3243	55	0
1	C	3167	0	3243	49	0
1	D	3167	0	3243	59	0
1	E	3167	0	3243	45	0
1	F	3167	0	3243	55	0
1	G	3167	0	3243	54	0
1	H	3167	0	3243	63	0
1	I	3167	0	3243	66	0
1	J	3167	0	3243	68	0
1	K	3167	0	3243	48	0
1	L	3167	0	3243	58	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	628	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 628 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:J:306:PRO:HB2	1:J:308:MET:HE2	1.37	1.03
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:B:71:THR:H	1:B:118:GLN:NE2	1.61	0.98

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	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%)	36	46
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%)	36	46
1	H	397/433 (92%)	383 (96%)	14 (4%)	0	100	100
1	I	397/433 (92%)	375 (94%)	21 (5%)	1 (0%)	36	46
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%)	48	60

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 [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	357/388 (92%)	354 (99%)	3 (1%)	73 86
1	B	357/388 (92%)	353 (99%)	4 (1%)	65 81
1	C	357/388 (92%)	354 (99%)	3 (1%)	73 86
1	D	357/388 (92%)	353 (99%)	4 (1%)	65 81
1	E	357/388 (92%)	353 (99%)	4 (1%)	65 81
1	F	357/388 (92%)	354 (99%)	3 (1%)	73 86
1	G	357/388 (92%)	353 (99%)	4 (1%)	65 81
1	H	357/388 (92%)	354 (99%)	3 (1%)	73 86
1	I	357/388 (92%)	354 (99%)	3 (1%)	73 86
1	J	357/388 (92%)	355 (99%)	2 (1%)	78 89
1	K	357/388 (92%)	355 (99%)	2 (1%)	78 89
1	L	357/388 (92%)	355 (99%)	2 (1%)	78 89
All	All	4284/4656 (92%)	4247 (99%)	37 (1%)	70 84

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	153	GLU
1	L	153	GLU
1	I	269	LEU
1	J	317	TRP
1	D	310	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	181	ASN
1	H	331	ASN
1	L	413	GLN
1	K	413	GLN
1	G	273	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 oligosaccharides 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

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%)	-0.40	6 (1%) 72 73	12, 23, 41, 64	0
1	B	399/433 (92%)	0.14	22 (5%) 30 32	18, 34, 59, 74	0
1	C	399/433 (92%)	-0.34	10 (2%) 58 60	14, 23, 43, 66	0
1	D	399/433 (92%)	0.05	25 (6%) 26 28	16, 31, 57, 77	0
1	E	399/433 (92%)	-0.14	16 (4%) 42 44	16, 26, 43, 69	0
1	F	399/433 (92%)	0.27	26 (6%) 25 27	16, 36, 62, 75	0
1	G	399/433 (92%)	0.67	46 (11%) 9 10	21, 42, 70, 82	0
1	H	399/433 (92%)	0.01	18 (4%) 38 40	17, 30, 55, 73	0
1	I	399/433 (92%)	0.38	31 (7%) 19 21	22, 39, 71, 87	0
1	J	399/433 (92%)	0.51	36 (9%) 15 16	22, 43, 70, 81	0
1	K	399/433 (92%)	-0.21	9 (2%) 61 63	18, 28, 46, 70	0
1	L	399/433 (92%)	0.11	22 (5%) 30 32	17, 33, 56, 77	0
All	All	4788/5196 (92%)	0.09	267 (5%) 30 32	12, 31, 61, 87	0

The worst 5 of 267 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	333	MET	7.0
1	L	333	MET	6.7
1	G	220	TYR	5.6
1	B	333	MET	5.4
1	B	220	TYR	5.4

### 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 oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	F	501	1/1	0.99	0.06	19,19,19,19	0
2	CL	G	501	1/1	0.99	0.05	24,24,24,24	0
2	CL	H	501	1/1	0.99	0.02	24,24,24,24	0
2	CL	I	501	1/1	0.99	0.03	28,28,28,28	0
2	CL	K	501	1/1	0.99	0.03	21,21,21,21	0
2	CL	L	501	1/1	0.99	0.03	20,20,20,20	0
2	CL	B	501	1/1	1.00	0.01	20,20,20,20	0
2	CL	C	501	1/1	1.00	0.02	21,21,21,21	0
2	CL	D	501	1/1	1.00	0.01	21,21,21,21	0
2	CL	J	501	1/1	1.00	0.01	24,24,24,24	0
2	CL	E	501	1/1	1.00	0.02	20,20,20,20	0
2	CL	A	501	1/1	1.00	0.01	19,19,19,19	0

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

There are no such residues in this entry.