



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:59 am BST

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

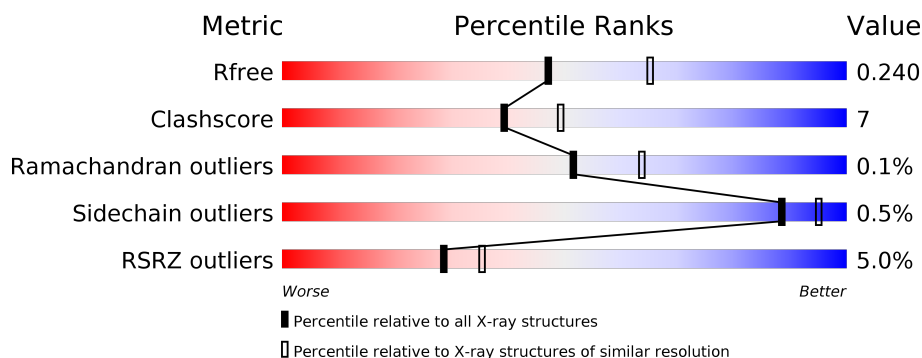
1 Overall quality at a glance

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 ≥ 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	<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;"> % 79% 13% 8% </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;"> 6% 76% 16% 8% </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;"> 2% 80% 12% 8% </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;"> 4% 80% 12% 8% </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;"> 2% 81% 11% 8% </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;"> 7% 77% 15% 8% </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	433	<div><div></div><div>12%</div><div>78%</div><div>14%</div><div>8%</div></div>
1	H	433	<div><div></div><div>2%</div><div>77%</div><div>15%</div><div>8%</div></div>
1	I	433	<div><div></div><div>7%</div><div>78%</div><div>14%</div><div>8%</div></div>
1	J	433	<div><div></div><div>8%</div><div>72%</div><div>20%</div><div>8%</div></div>
1	K	433	<div><div></div><div>%</div><div>79%</div><div>14%</div><div>8%</div></div>
1	L	433	<div><div></div><div>4%</div><div>77%</div><div>15%</div><div>8%</div></div>

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

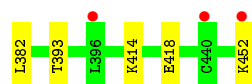
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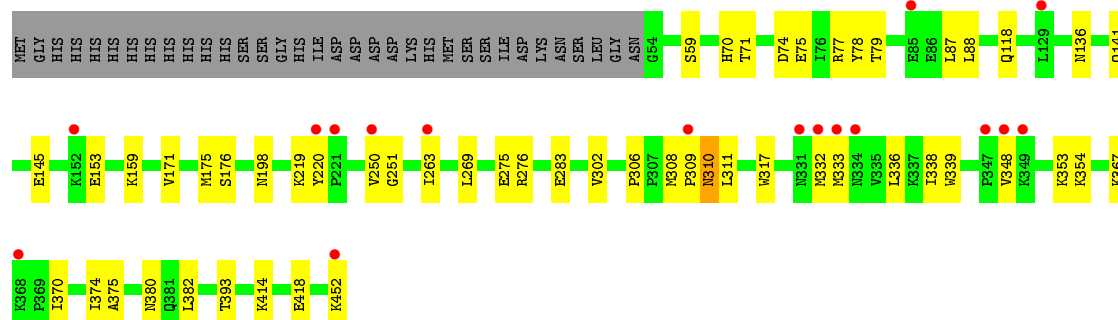
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	1	Total 1	Cl 1	0	0
2	F	1	Total 1	Cl 1	0	0

- Molecule 3 is water.

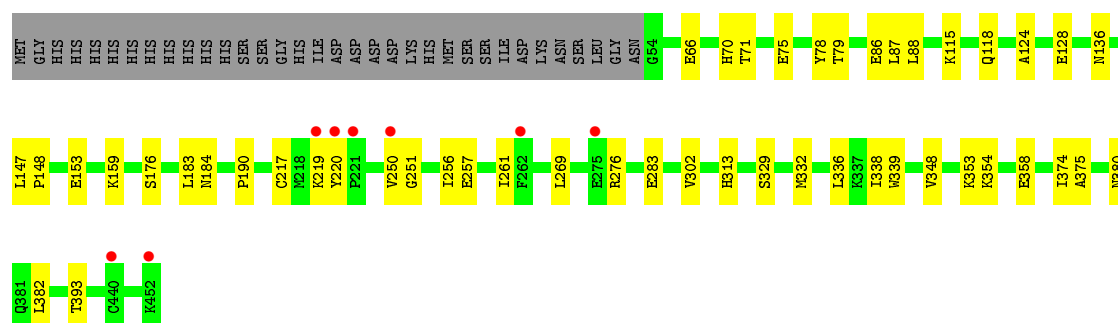
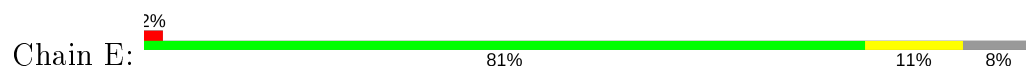
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	212	Total 212	O 212	0	0
3	B	117	Total 117	O 117	0	0
3	C	213	Total 213	O 213	0	0
3	D	142	Total 142	O 142	0	0
3	E	180	Total 180	O 180	0	0
3	F	99	Total 99	O 99	0	0
3	G	80	Total 80	O 80	0	0
3	H	140	Total 140	O 140	0	0
3	I	86	Total 86	O 86	0	0
3	J	82	Total 82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



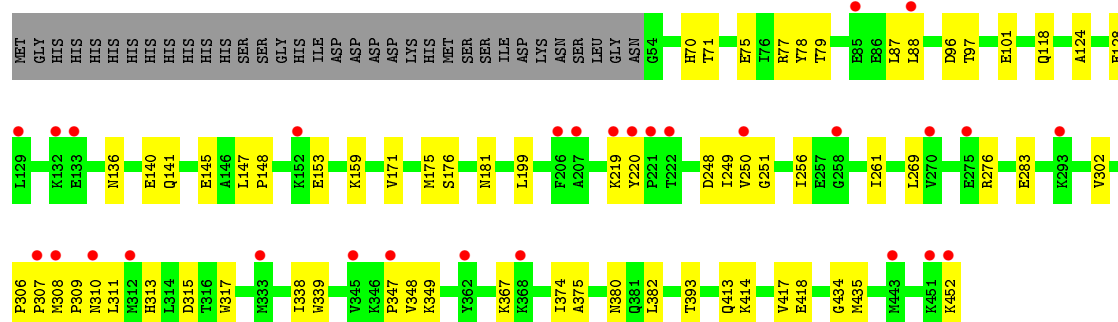
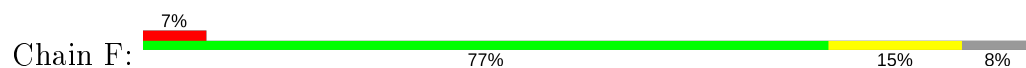
• Molecule 1: Arginine deiminase



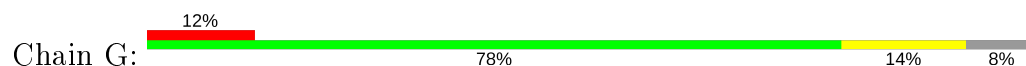
• Molecule 1: Arginine deiminase

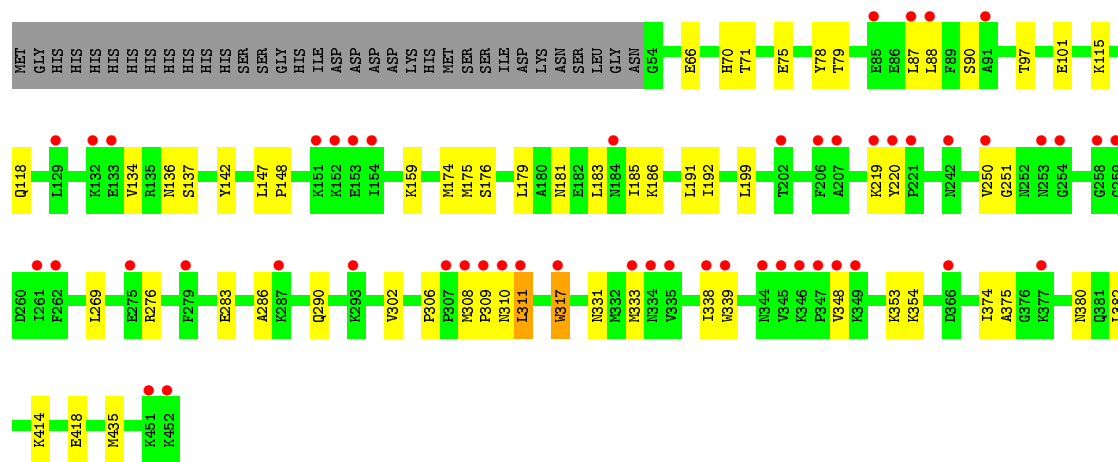


• Molecule 1: Arginine deiminase

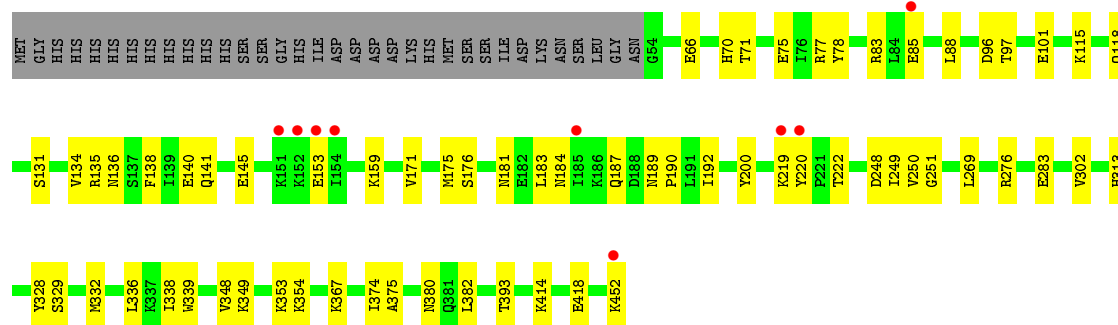
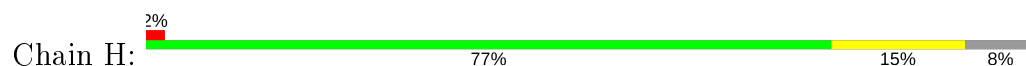


• Molecule 1: Arginine deiminase

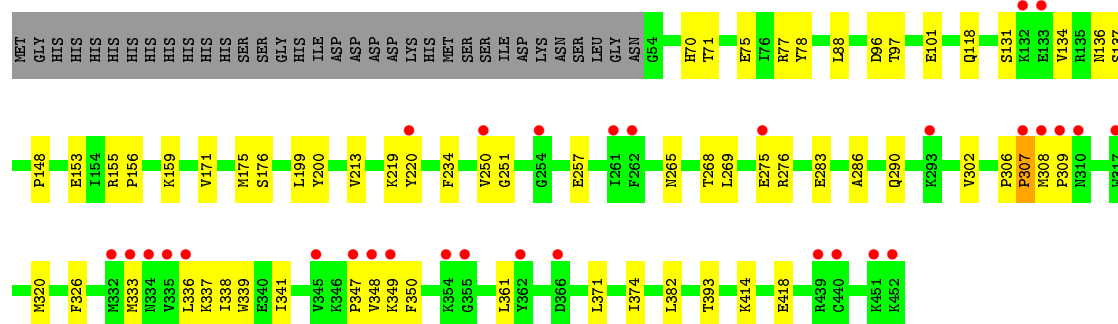
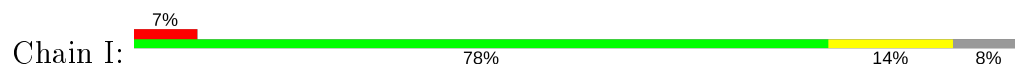




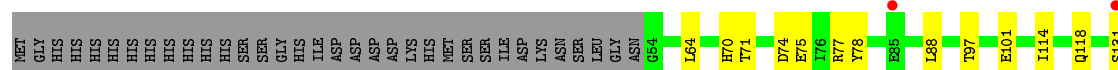
• Molecule 1: Arginine deiminase

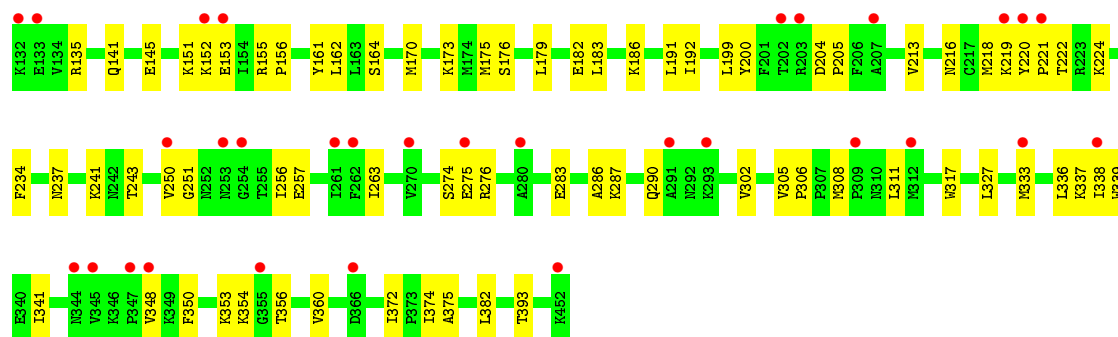


• Molecule 1: Arginine deiminase

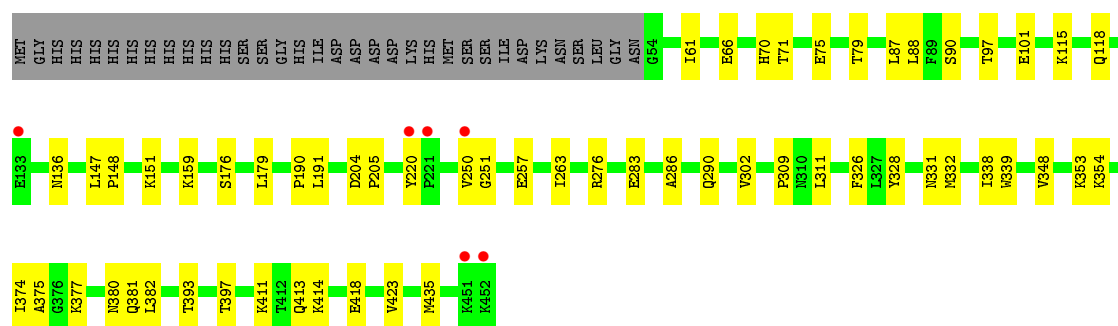
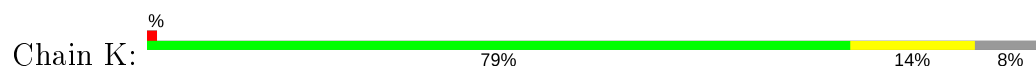


• Molecule 1: Arginine deiminase

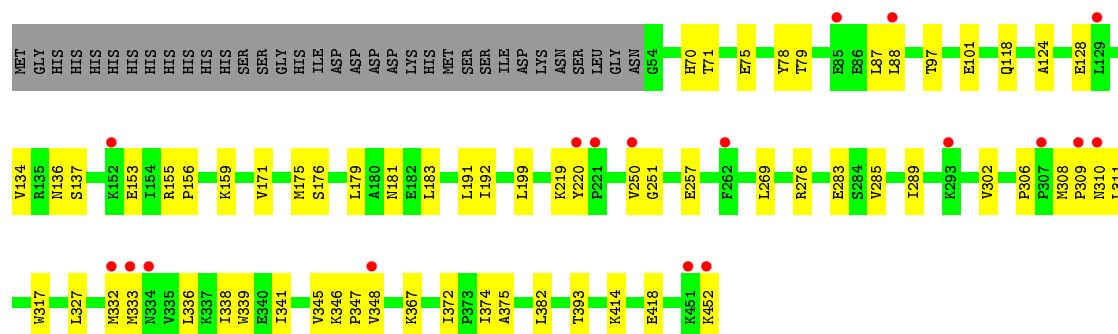
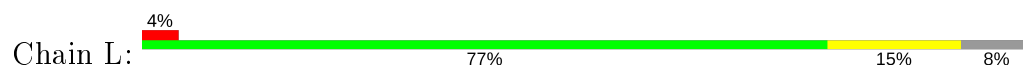




● Molecule 1: Arginine deiminase



● Molecule 1: Arginine deiminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

All (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
1:D:71:THR:H	1:D:118:GLN:HE22	1.09	0.98
1:I:283:GLU:HG3	1:I:348:VAL:HG11	1.44	0.98
1:G:71:THR:H	1:G:118:GLN:HE22	1.11	0.97
1:J:71:THR:H	1:J:118:GLN:NE2	1.63	0.96
1:A:71:THR:H	1:A:118:GLN:HE22	1.02	0.96
1:L:71:THR:H	1:L:118:GLN:HE22	1.09	0.96
1:J:283:GLU:HG3	1:J:348:VAL:HG21	1.45	0.95
1:C:71:THR:H	1:C:118:GLN:HE22	1.14	0.95
1:E:71:THR:H	1:E:118:GLN:NE2	1.64	0.95
1:H:71:THR:H	1:H:118:GLN:HE22	1.07	0.93
1:F:71:THR:H	1:F:118:GLN:NE2	1.66	0.93
1:K:71:THR:H	1:K:118:GLN:NE2	1.65	0.93
1:E:71:THR:H	1:E:118:GLN:HE22	1.00	0.93
1:B:71:THR:H	1:B:118:GLN:HE22	0.98	0.92
1:K:71:THR:N	1:K:118:GLN:HE22	1.69	0.91
1:H:71:THR:H	1:H:118:GLN:NE2	1.68	0.90
1:D:71:THR:H	1:D:118:GLN:NE2	1.68	0.89
1:G:71:THR:H	1:G:118:GLN:NE2	1.69	0.89
1:D:283:GLU:HG3	1:D:348:VAL:HG11	1.54	0.89
1:I:71:THR:H	1:I:118:GLN:NE2	1.72	0.87
1:K:71:THR:H	1:K:118:GLN:HE22	0.89	0.87
1:F:283:GLU:HG3	1:F:348:VAL:HG11	1.55	0.87
1:C:71:THR:H	1:C:118:GLN:NE2	1.72	0.86
1:D:311:LEU:H	1:D:311:LEU:HD12	1.41	0.85
1:A:71:THR:N	1:A:118:GLN:HE22	1.75	0.83
1:E:71:THR:N	1:E:118:GLN:HE22	1.76	0.83
1:D:317:TRP:HZ3	1:D:332:MET:HA	1.43	0.82
1:D:353:LYS:HG2	1:D:354:LYS:H	1.43	0.82
1:H:276:ARG:HG3	1:H:313:HIS:HE1	1.42	0.82
1:B:71:THR:N	1:B:118:GLN:HE22	1.76	0.82
1:D:317:TRP:CZ3	1:D:332:MET:HA	2.16	0.80
1:H:184:ASN:CB	1:I:333:MET:HE2	2.12	0.80
1:G:283:GLU:HG3	1:G:348:VAL:HG11	1.63	0.79
1:F:71:THR:N	1:F:118:GLN:HE22	1.81	0.79
1:I:71:THR:H	1:I:118:GLN:HE22	1.28	0.78
1:B:283:GLU:HG3	1:B:348:VAL:HG21	1.67	0.76
1:H:184:ASN:HB3	1:I:333:MET:HG2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:71:THR:N	1:H:118:GLN:HE22	1.82	0.76
1:L:71:THR:N	1:L:118:GLN:HE22	1.82	0.76
1:D:71:THR:N	1:D:118:GLN:HE22	1.84	0.75
1:D:353:LYS:HG2	1:D:354:LYS:N	2.02	0.75
1:G:71:THR:N	1:G:118:GLN:HE22	1.85	0.72
1:K:328:TYR:HB2	1:K:332:MET:HE1	1.70	0.72
1:K:353:LYS:HG2	1:K:354:LYS:H	1.55	0.72
1:J:306:PRO:HB2	1:J:308:MET:CE	2.20	0.71
1:K:136:ASN:HD21	1:K:159:LYS:NZ	1.88	0.71
1:L:283:GLU:HG3	1:L:348:VAL:HG11	1.72	0.71
1:J:306:PRO:HG2	1:J:333:MET:SD	2.30	0.70
1:E:382:LEU:HD21	1:F:78:TYR:HA	1.73	0.70
1:K:283:GLU:HG3	1:K:348:VAL:HG11	1.73	0.70
1:F:79:THR:HG23	1:F:87:LEU:HD12	1.73	0.70
1:J:71:THR:H	1:J:118:GLN:HE22	1.36	0.70
1:G:78:TYR:HA	1:H:382:LEU:HD21	1.74	0.69
1:E:353:LYS:HG2	1:E:354:LYS:H	1.56	0.69
1:K:75:GLU:HB3	1:K:176:SER:HA	1.75	0.69
1:G:88:LEU:HD11	1:G:220:TYR:HB2	1.74	0.69
1:E:353:LYS:HG2	1:E:354:LYS:N	2.07	0.69
1:J:283:GLU:HG2	1:J:287:LYS:HE2	1.74	0.68
1:C:136:ASN:HD21	1:C:159:LYS:NZ	1.92	0.68
1:J:75:GLU:HB3	1:J:176:SER:HA	1.76	0.67
1:D:306:PRO:HG2	1:D:317:TRP:CH2	2.29	0.67
1:L:88:LEU:HD11	1:L:220:TYR:HB2	1.75	0.67
1:C:71:THR:N	1:C:118:GLN:HE22	1.88	0.67
1:I:283:GLU:HG3	1:I:348:VAL:CG1	2.23	0.67
1:J:306:PRO:HB2	1:J:308:MET:HE1	1.76	0.66
1:K:136:ASN:HD21	1:K:159:LYS:HZ1	1.43	0.66
1:J:338:ILE:HG22	1:J:339:TRP:N	2.11	0.66
1:G:75:GLU:HB3	1:G:176:SER:HA	1.77	0.66
1:C:348:VAL:HG12	3:C:622:HOH:O	1.95	0.65
1:E:88:LEU:HD11	1:E:220:TYR:HB2	1.77	0.65
1:F:75:GLU:HB3	1:F:176:SER:HA	1.78	0.65
1:J:173:LYS:HE3	1:J:182:GLU:OE2	1.97	0.65
1:D:308:MET:HG3	1:D:317:TRP:CZ2	2.31	0.65
1:G:306:PRO:HG3	1:G:333:MET:SD	2.36	0.65
1:K:151:LYS:HE3	3:K:660:HOH:O	1.97	0.64
1:L:317:TRP:HZ3	1:L:332:MET:HA	1.60	0.64
1:B:136:ASN:HD21	1:B:159:LYS:HZ1	1.43	0.64
1:L:136:ASN:HD21	1:L:159:LYS:NZ	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:136:ASN:HD21	1:H:159:LYS:NZ	1.96	0.64
1:H:88:LEU:HD11	1:H:220:TYR:HB2	1.80	0.64
1:C:283:GLU:HG3	1:C:348:VAL:HG11	1.78	0.64
1:H:276:ARG:HG3	1:H:313:HIS:CE1	2.31	0.64
1:K:70:HIS:HA	1:K:118:GLN:NE2	2.13	0.64
1:A:374:ILE:HD11	1:A:393:THR:HG22	1.80	0.63
1:A:54:GLY:N	3:A:660:HOH:O	2.31	0.63
1:F:88:LEU:HD11	1:F:220:TYR:HB2	1.80	0.63
1:L:317:TRP:CZ3	1:L:332:MET:HA	2.33	0.63
1:I:75:GLU:HB3	1:I:176:SER:HA	1.78	0.63
1:H:75:GLU:HB3	1:H:176:SER:HA	1.79	0.63
1:B:414:LYS:O	1:B:418:GLU:HG3	2.00	0.62
1:L:302:VAL:HB	1:L:339:TRP:HB2	1.81	0.62
1:L:75:GLU:HB3	1:L:176:SER:HA	1.82	0.62
1:K:328:TYR:HB2	1:K:332:MET:CE	2.29	0.62
1:K:380:ASN:HD22	1:L:181:ASN:HD21	1.46	0.62
1:B:75:GLU:HB3	1:B:176:SER:HA	1.82	0.61
1:E:283:GLU:HG3	1:E:348:VAL:HG11	1.82	0.61
1:I:71:THR:N	1:I:118:GLN:HE22	1.96	0.61
1:J:153:GLU:H	1:J:153:GLU:CD	2.03	0.61
1:A:75:GLU:HB3	1:A:176:SER:HA	1.81	0.61
1:A:71:THR:N	1:A:118:GLN:NE2	2.40	0.61
1:C:75:GLU:HB3	1:C:176:SER:HA	1.82	0.61
1:D:136:ASN:HD21	1:D:159:LYS:NZ	1.98	0.61
1:I:136:ASN:HD21	1:I:159:LYS:NZ	1.99	0.61
1:C:78:TYR:HA	1:D:382:LEU:HD21	1.83	0.61
1:G:414:LYS:O	1:G:418:GLU:HG3	2.00	0.61
1:B:88:LEU:HD11	1:B:220:TYR:HB2	1.83	0.61
1:H:97:THR:O	1:H:101:GLU:HG3	2.00	0.61
1:K:309:PRO:O	1:K:311:LEU:HD22	2.00	0.61
1:J:353:LYS:HD3	1:J:354:LYS:H	1.66	0.61
1:B:136:ASN:HD21	1:B:159:LYS:NZ	1.99	0.60
1:L:346:LYS:HG3	1:L:347:PRO:HA	1.83	0.60
1:B:86:GLU:HB2	3:B:686:HOH:O	2.02	0.60
1:E:302:VAL:HB	1:E:339:TRP:HB2	1.83	0.60
1:C:70:HIS:HA	1:C:118:GLN:NE2	2.16	0.60
1:L:306:PRO:HG3	1:L:333:MET:HG3	1.83	0.60
1:D:75:GLU:HB3	1:D:176:SER:HA	1.82	0.60
1:H:222:THR:HG22	3:H:672:HOH:O	2.01	0.60
1:F:414:LYS:O	1:F:418:GLU:HG3	2.01	0.60
1:J:338:ILE:HD12	1:J:338:ILE:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:341:ILE:HD11	1:J:350:PHE:CE1	2.37	0.60
1:I:78:TYR:HA	1:J:382:LEU:HD21	1.84	0.60
1:L:414:LYS:O	1:L:418:GLU:HG3	2.01	0.60
1:D:88:LEU:HD11	1:D:220:TYR:HB2	1.82	0.60
1:H:349:LYS:HG2	3:H:687:HOH:O	2.02	0.59
1:G:136:ASN:HD21	1:G:159:LYS:NZ	2.01	0.59
1:H:136:ASN:HD21	1:H:159:LYS:HZ1	1.51	0.59
1:J:88:LEU:HD11	1:J:220:TYR:HB2	1.85	0.59
1:E:380:ASN:HD22	1:F:181:ASN:HD21	1.50	0.59
1:J:71:THR:N	1:J:118:GLN:NE2	2.44	0.59
1:J:141:GLN:O	1:J:145:GLU:HG3	2.02	0.58
1:L:71:THR:N	1:L:118:GLN:NE2	2.42	0.58
1:G:302:VAL:HB	1:G:339:TRP:HB2	1.85	0.58
1:D:367:LYS:NZ	1:D:452:LYS:HE3	2.18	0.58
1:E:136:ASN:HD21	1:E:159:LYS:NZ	2.01	0.58
1:J:219:LYS:HD2	1:J:276:ARG:NE	2.18	0.58
1:F:171:VAL:O	1:F:175:MET:HG3	2.04	0.58
1:A:136:ASN:HD21	1:A:159:LYS:NZ	2.01	0.58
1:A:309:PRO:HG3	1:E:153:GLU:HG2	1.84	0.58
1:G:70:HIS:HA	1:G:118:GLN:NE2	2.19	0.58
1:I:347:PRO:HG2	1:I:349:LYS:HE3	1.87	0.57
1:K:414:LYS:O	1:K:418:GLU:HG3	2.04	0.57
1:G:380:ASN:HD22	1:H:181:ASN:HD21	1.53	0.57
1:C:88:LEU:HD11	1:C:220:TYR:HB2	1.86	0.57
1:I:302:VAL:HB	1:I:339:TRP:HB2	1.86	0.57
1:E:75:GLU:HB3	1:E:176:SER:HA	1.87	0.56
1:J:97:THR:O	1:J:101:GLU:HG3	2.05	0.56
1:A:374:ILE:HD11	1:A:393:THR:CG2	2.36	0.56
1:C:382:LEU:HD21	1:D:78:TYR:HA	1.88	0.56
1:K:353:LYS:HG2	1:K:354:LYS:N	2.20	0.56
1:K:257:GLU:HG3	1:K:276:ARG:HB3	1.87	0.56
1:F:97:THR:O	1:F:101:GLU:HG3	2.06	0.56
1:F:136:ASN:HD21	1:F:159:LYS:NZ	2.04	0.56
1:H:153:GLU:CG	1:I:309:PRO:HB3	2.36	0.56
1:L:79:THR:HG23	1:L:87:LEU:HD12	1.88	0.55
1:A:88:LEU:HD11	1:A:220:TYR:HB2	1.88	0.55
1:F:338:ILE:CG2	1:F:339:TRP:N	2.69	0.55
1:G:136:ASN:HD21	1:G:159:LYS:HZ1	1.53	0.55
1:C:136:ASN:HD21	1:C:159:LYS:HZ1	1.54	0.55
1:I:88:LEU:HD11	1:I:220:TYR:HB2	1.87	0.55
1:D:308:MET:HG3	1:D:317:TRP:HZ2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:LEU:HD12	1:D:311:LEU:N	2.18	0.55
1:I:306:PRO:HG3	1:I:333:MET:SD	2.47	0.55
1:J:179:LEU:HD23	1:J:191:LEU:HD23	1.87	0.55
1:C:414:LYS:O	1:C:418:GLU:HG3	2.07	0.55
1:D:414:LYS:O	1:D:418:GLU:HG3	2.06	0.55
1:K:97:THR:O	1:K:101:GLU:HG3	2.07	0.55
1:K:302:VAL:HB	1:K:339:TRP:HB2	1.89	0.54
1:F:70:HIS:HA	1:F:118:GLN:NE2	2.22	0.54
1:J:71:THR:N	1:J:118:GLN:HE22	2.02	0.54
1:J:306:PRO:HB2	1:J:308:MET:HE2	1.89	0.54
1:L:317:TRP:HE3	1:L:332:MET:HB2	1.72	0.54
1:D:70:HIS:HA	1:D:118:GLN:NE2	2.22	0.54
1:B:151:LYS:HG3	3:E:670:HOH:O	2.07	0.54
1:B:306:PRO:HG2	1:B:333:MET:SD	2.48	0.54
1:E:66:GLU:HG2	1:E:115:LYS:HB3	1.90	0.54
1:H:153:GLU:HG3	1:I:309:PRO:HB3	1.90	0.54
1:E:70:HIS:HA	1:E:118:GLN:NE2	2.23	0.54
1:G:97:THR:O	1:G:101:GLU:HG3	2.08	0.54
1:A:348:VAL:HA	3:A:792:HOH:O	2.08	0.54
1:J:175:MET:HB3	1:J:199:LEU:CD1	2.38	0.54
1:F:374:ILE:O	1:F:375:ALA:HB3	2.08	0.53
1:J:374:ILE:HD11	1:J:393:THR:HG22	1.88	0.53
1:L:136:ASN:HD21	1:L:159:LYS:HZ1	1.55	0.53
1:B:71:THR:N	1:B:118:GLN:NE2	2.44	0.53
1:B:79:THR:HG23	1:B:87:LEU:HD12	1.90	0.53
1:F:77:ARG:NH2	1:F:96:ASP:OD1	2.41	0.53
1:G:181:ASN:HD21	1:H:380:ASN:HD22	1.55	0.53
1:E:86:GLU:HB2	3:E:682:HOH:O	2.08	0.53
1:L:374:ILE:HD11	1:L:393:THR:HG22	1.90	0.53
1:H:302:VAL:HB	1:H:339:TRP:HB2	1.90	0.53
1:A:302:VAL:HB	1:A:339:TRP:HB2	1.90	0.53
1:A:308:MET:C	1:E:153:GLU:HG3	2.28	0.53
1:K:286:ALA:O	1:K:290:GLN:HG3	2.09	0.53
1:C:302:VAL:HB	1:C:339:TRP:HB2	1.91	0.53
1:I:338:ILE:CG2	1:I:339:TRP:N	2.70	0.53
1:G:353:LYS:HD3	1:G:354:LYS:N	2.24	0.53
1:I:148:PRO:HG3	3:I:662:HOH:O	2.09	0.53
1:J:218:MET:HB2	1:J:224:LYS:HG2	1.91	0.53
1:L:310:ASN:C	1:L:311:LEU:HD12	2.29	0.52
1:I:97:THR:O	1:I:101:GLU:HG3	2.09	0.52
1:B:151:LYS:HE3	3:E:682:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:HIS:HA	1:B:118:GLN:NE2	2.25	0.52
1:L:219:LYS:HD2	1:L:276:ARG:NE	2.24	0.52
1:F:302:VAL:HB	1:F:339:TRP:HB2	1.90	0.52
1:H:283:GLU:HG3	1:H:348:VAL:HG11	1.91	0.52
1:E:219:LYS:HD2	1:E:276:ARG:NE	2.25	0.52
1:J:302:VAL:HB	1:J:339:TRP:HB2	1.92	0.52
1:A:118:GLN:HG3	3:A:602:HOH:O	2.09	0.52
1:B:250:VAL:HG13	1:B:251:GLY:N	2.24	0.52
1:H:219:LYS:HD2	1:H:276:ARG:NE	2.25	0.52
1:J:338:ILE:CG2	1:J:339:TRP:N	2.73	0.52
1:D:302:VAL:HB	1:D:339:TRP:HB2	1.92	0.52
1:G:181:ASN:ND2	1:H:380:ASN:HD22	2.08	0.52
1:E:79:THR:HG23	1:E:87:LEU:HD12	1.91	0.52
1:G:179:LEU:HD23	1:G:191:LEU:HD23	1.92	0.52
1:D:136:ASN:HD21	1:D:159:LYS:HZ1	1.58	0.51
1:G:338:ILE:CG2	1:G:339:TRP:N	2.74	0.51
1:H:70:HIS:HA	1:H:118:GLN:NE2	2.26	0.51
1:D:374:ILE:O	1:D:375:ALA:HB3	2.10	0.51
1:A:78:TYR:HA	1:B:382:LEU:HD21	1.93	0.51
1:D:311:LEU:H	1:D:311:LEU:CD1	2.18	0.51
1:G:88:LEU:HD11	1:G:220:TYR:CB	2.38	0.51
1:K:88:LEU:HD11	1:K:220:TYR:CG	2.46	0.51
1:K:374:ILE:O	1:K:375:ALA:HB3	2.11	0.51
1:B:338:ILE:CG2	1:B:339:TRP:N	2.73	0.51
1:I:219:LYS:HD2	1:I:276:ARG:NE	2.25	0.51
1:K:79:THR:HG23	1:K:87:LEU:HD12	1.93	0.51
1:B:341:ILE:HD11	1:B:350:PHE:CE1	2.46	0.51
1:I:250:VAL:HG13	1:I:251:GLY:N	2.26	0.51
1:I:341:ILE:HD11	1:I:350:PHE:CE1	2.45	0.51
1:D:338:ILE:CG2	1:D:339:TRP:N	2.73	0.51
1:F:71:THR:N	1:F:118:GLN:NE2	2.48	0.51
1:J:70:HIS:CD2	1:J:199:LEU:HB3	2.46	0.51
1:J:70:HIS:HA	1:J:118:GLN:HE21	1.76	0.51
1:F:118:GLN:HG3	3:F:605:HOH:O	2.11	0.50
1:A:70:HIS:HA	1:A:118:GLN:NE2	2.26	0.50
1:B:136:ASN:ND2	1:B:159:LYS:HZ1	2.08	0.50
1:D:317:TRP:HE3	1:D:332:MET:HB2	1.76	0.50
1:G:382:LEU:HD21	1:H:78:TYR:HA	1.93	0.50
1:L:306:PRO:HG2	1:L:317:TRP:CH2	2.46	0.50
1:A:414:LYS:O	1:A:418:GLU:HG3	2.12	0.50
1:E:78:TYR:HA	1:F:382:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:140:GLU:OE2	1:H:159:LYS:NZ	2.44	0.50
1:J:118:GLN:HG3	3:J:633:HOH:O	2.10	0.50
1:F:219:LYS:HD2	1:F:276:ARG:NE	2.27	0.50
1:J:336:LEU:N	1:J:336:LEU:HD12	2.26	0.50
1:C:367:LYS:NZ	1:C:452:LYS:HE3	2.26	0.50
1:L:310:ASN:O	1:L:311:LEU:HD12	2.11	0.50
1:E:256:ILE:HD11	1:E:261:ILE:HD11	1.94	0.50
1:F:308:MET:HB3	1:F:309:PRO:HD2	1.93	0.50
1:C:337:LYS:C	1:C:338:ILE:HD12	2.32	0.49
1:F:250:VAL:HG13	1:F:251:GLY:N	2.26	0.49
1:B:302:VAL:HB	1:B:339:TRP:HB2	1.94	0.49
1:K:328:TYR:HD1	1:K:332:MET:HE3	1.76	0.49
1:F:248:ASP:OD1	1:F:249:ILE:N	2.44	0.49
1:L:306:PRO:HB3	1:L:333:MET:SD	2.52	0.49
1:G:118:GLN:HG3	3:G:610:HOH:O	2.12	0.49
1:H:353:LYS:HG2	1:H:354:LYS:H	1.77	0.49
1:D:306:PRO:HG3	1:D:333:MET:HG3	1.94	0.49
1:J:155:ARG:N	1:J:156:PRO:HD2	2.27	0.49
1:A:181:ASN:HD21	1:B:380:ASN:HD22	1.60	0.49
1:E:358:GLU:HB2	3:E:732:HOH:O	2.13	0.49
1:I:382:LEU:HD21	1:J:78:TYR:HA	1.95	0.49
1:K:136:ASN:ND2	1:K:159:LYS:HZ1	2.08	0.49
1:L:317:TRP:CE3	1:L:332:MET:HB2	2.48	0.49
1:A:367:LYS:NZ	1:A:452:LYS:HE3	2.28	0.49
1:H:374:ILE:O	1:H:375:ALA:HB3	2.12	0.49
1:F:308:MET:HE2	1:F:311:LEU:HD22	1.94	0.49
1:G:311:LEU:N	1:G:311:LEU:HD12	2.28	0.49
1:L:183:LEU:HD12	1:L:192:ILE:HG13	1.95	0.48
1:L:338:ILE:CG2	1:L:339:TRP:N	2.75	0.48
1:L:88:LEU:HD11	1:L:220:TYR:CB	2.41	0.48
1:J:374:ILE:HD11	1:J:393:THR:CG2	2.43	0.48
1:D:317:TRP:CE3	1:D:332:MET:HB2	2.48	0.48
1:G:308:MET:HB3	1:G:309:PRO:CD	2.42	0.48
1:B:219:LYS:HD2	1:B:276:ARG:NE	2.28	0.48
1:D:250:VAL:HG13	1:D:251:GLY:N	2.28	0.48
1:F:175:MET:HB3	1:F:199:LEU:CD1	2.42	0.48
1:A:338:ILE:CG2	1:A:339:TRP:N	2.77	0.48
1:F:347:PRO:O	1:F:349:LYS:HG3	2.13	0.48
1:H:171:VAL:O	1:H:175:MET:HG3	2.14	0.48
1:I:275:GLU:HG2	1:I:275:GLU:O	2.13	0.48
1:K:382:LEU:HD21	1:L:78:TYR:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:131:SER:O	1:J:135:ARG:HG3	2.14	0.48
1:K:250:VAL:HG13	1:K:251:GLY:N	2.28	0.48
1:J:250:VAL:HG13	1:J:251:GLY:N	2.29	0.48
1:G:380:ASN:HB2	1:H:190:PRO:HB3	1.95	0.48
1:E:329:SER:O	1:E:332:MET:HG2	2.14	0.48
1:G:134:VAL:O	1:G:137:SER:HB3	2.14	0.48
1:H:83:ARG:HD3	3:H:632:HOH:O	2.14	0.48
1:I:341:ILE:HG23	1:I:348:VAL:HG23	1.96	0.48
1:I:374:ILE:HD11	1:I:393:THR:CG2	2.44	0.47
1:J:336:LEU:HB2	1:J:338:ILE:HD11	1.96	0.47
1:C:374:ILE:HD11	1:C:393:THR:HG22	1.96	0.47
1:I:171:VAL:O	1:I:175:MET:HG3	2.14	0.47
1:J:183:LEU:HD12	1:J:192:ILE:HG13	1.95	0.47
1:D:370:ILE:HD13	3:D:689:HOH:O	2.13	0.47
1:E:374:ILE:HD11	1:E:393:THR:HG22	1.96	0.47
1:I:134:VAL:O	1:I:137:SER:HB3	2.14	0.47
1:A:313:HIS:HB2	1:A:315:ASP:OD1	2.14	0.47
1:F:313:HIS:HB2	1:F:315:ASP:OD1	2.15	0.47
1:G:175:MET:HB3	1:G:199:LEU:CD1	2.45	0.47
1:A:309:PRO:N	1:E:153:GLU:HG3	2.30	0.47
1:E:374:ILE:O	1:E:375:ALA:HB3	2.14	0.47
1:K:374:ILE:HD11	1:K:393:THR:HG22	1.97	0.47
1:C:70:HIS:HA	1:C:118:GLN:HE21	1.80	0.47
1:J:356:THR:O	1:J:360:VAL:HG23	2.14	0.47
1:B:361:LEU:HD12	1:B:371:LEU:HD21	1.96	0.46
1:B:88:LEU:HD11	1:B:220:TYR:CB	2.45	0.46
1:H:184:ASN:HB3	1:I:333:MET:CG	2.42	0.46
1:C:353:LYS:HG2	1:C:354:LYS:H	1.81	0.46
1:E:71:THR:N	1:E:118:GLN:NE2	2.46	0.46
1:E:257:GLU:HG3	1:E:276:ARG:HB3	1.98	0.46
1:F:88:LEU:HD11	1:F:220:TYR:CB	2.45	0.46
1:L:124:ALA:O	1:L:128:GLU:HG2	2.15	0.46
1:L:250:VAL:HG13	1:L:251:GLY:N	2.31	0.46
1:F:153:GLU:CD	1:F:153:GLU:H	2.19	0.46
1:F:256:ILE:HD11	1:F:261:ILE:HD11	1.98	0.46
1:F:367:LYS:NZ	1:F:452:LYS:HE3	2.31	0.46
1:F:136:ASN:HD21	1:F:159:LYS:HZ1	1.64	0.46
1:J:213:VAL:HG11	1:J:234:PHE:CZ	2.51	0.46
1:C:338:ILE:CG2	1:C:339:TRP:N	2.78	0.46
1:E:136:ASN:HD21	1:E:159:LYS:HZ1	1.63	0.46
1:G:250:VAL:HG13	1:G:251:GLY:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:222:THR:HB	3:J:642:HOH:O	2.16	0.46
1:G:331:ASN:OD1	1:J:186:LYS:HD3	2.16	0.46
1:D:88:LEU:HD11	1:D:220:TYR:CB	2.44	0.46
1:E:336:LEU:HB3	1:E:338:ILE:CD1	2.45	0.46
1:I:320:MET:HG3	1:I:326:PHE:CE2	2.51	0.46
1:I:70:HIS:HA	1:I:118:GLN:NE2	2.30	0.46
1:J:151:LYS:HB3	1:J:153:GLU:OE2	2.16	0.46
1:K:66:GLU:HG2	1:K:115:LYS:HB3	1.97	0.46
1:L:341:ILE:HG23	1:L:348:VAL:HG23	1.98	0.46
1:K:136:ASN:ND2	1:K:159:LYS:NZ	2.62	0.46
1:A:136:ASN:HD21	1:A:159:LYS:HZ3	1.64	0.46
1:E:256:ILE:CD1	1:E:261:ILE:HD11	2.46	0.46
1:G:308:MET:HB3	1:G:309:PRO:HD2	1.97	0.45
1:K:71:THR:N	1:K:118:GLN:NE2	2.45	0.45
1:K:377:LYS:HG3	3:K:634:HOH:O	2.15	0.45
1:A:66:GLU:HG2	1:A:115:LYS:HB3	1.99	0.45
1:A:77:ARG:NH2	1:A:96:ASP:OD1	2.50	0.45
1:I:153:GLU:H	1:I:153:GLU:CD	2.20	0.45
1:A:337:LYS:C	1:A:338:ILE:HD12	2.36	0.45
1:C:77:ARG:NH2	1:C:96:ASP:OD1	2.49	0.45
1:F:79:THR:HB	3:F:634:HOH:O	2.16	0.45
1:L:171:VAL:O	1:L:175:MET:HG3	2.16	0.45
1:C:181:ASN:HD21	1:D:380:ASN:HD22	1.64	0.45
1:C:348:VAL:HG13	1:C:348:VAL:O	2.17	0.45
1:D:141:GLN:O	1:D:145:GLU:HG3	2.17	0.45
1:G:338:ILE:HG23	1:G:339:TRP:N	2.32	0.45
1:H:183:LEU:HD12	1:H:192:ILE:HG13	1.97	0.45
1:D:74:ASP:OD1	1:D:77:ARG:NH1	2.49	0.45
1:I:257:GLU:HG3	1:I:276:ARG:HB3	1.98	0.45
1:L:257:GLU:HG3	1:L:276:ARG:HB3	1.98	0.45
1:B:308:MET:HG2	1:B:311:LEU:HD23	1.98	0.45
1:G:79:THR:HG23	1:G:87:LEU:HD12	1.97	0.45
1:I:336:LEU:HB3	1:I:338:ILE:CD1	2.46	0.45
1:L:345:VAL:HG12	1:L:346:LYS:N	2.32	0.45
1:L:374:ILE:O	1:L:375:ALA:HB3	2.16	0.45
1:H:338:ILE:CG2	1:H:339:TRP:N	2.79	0.45
1:K:147:LEU:HA	1:K:148:PRO:C	2.37	0.45
1:A:183:LEU:HD12	1:A:192:ILE:HG13	1.99	0.45
1:B:77:ARG:NH2	1:B:96:ASP:OD1	2.50	0.45
1:C:97:THR:O	1:C:101:GLU:HG3	2.17	0.45
1:H:367:LYS:NZ	1:H:452:LYS:HE3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:70:HIS:HA	1:I:118:GLN:HE21	1.82	0.45
1:A:134:VAL:O	1:A:137:SER:HB3	2.17	0.45
1:A:329:SER:O	1:A:332:MET:HG2	2.16	0.45
1:B:155:ARG:N	1:B:156:PRO:HD2	2.31	0.45
1:C:374:ILE:O	1:C:375:ALA:HB3	2.17	0.45
1:G:374:ILE:O	1:G:375:ALA:HB3	2.17	0.45
1:A:361:LEU:HD12	1:A:371:LEU:HD21	1.99	0.45
1:G:185:ILE:HG22	1:G:186:LYS:N	2.31	0.45
1:I:175:MET:HB3	1:I:199:LEU:CD1	2.47	0.45
1:A:353:LYS:HG2	1:A:354:LYS:H	1.81	0.44
1:G:66:GLU:HG2	1:G:115:LYS:HB3	1.99	0.44
1:I:155:ARG:N	1:I:156:PRO:HD2	2.31	0.44
1:A:341:ILE:HD11	1:A:350:PHE:CE1	2.53	0.44
1:B:97:THR:O	1:B:101:GLU:HG3	2.18	0.44
1:B:337:LYS:C	1:B:338:ILE:HD12	2.38	0.44
1:K:263:ILE:N	1:K:263:ILE:HD12	2.32	0.44
1:C:348:VAL:HG13	3:C:730:HOH:O	2.17	0.44
1:F:141:GLN:O	1:F:145:GLU:HG3	2.18	0.44
1:H:374:ILE:HD11	1:H:393:THR:HG22	1.98	0.44
1:I:136:ASN:HD21	1:I:159:LYS:HZ1	1.65	0.44
1:J:305:VAL:HG13	1:J:311:LEU:HD21	1.98	0.44
1:C:336:LEU:HB3	1:C:338:ILE:CD1	2.47	0.44
1:D:198:ASN:HB2	3:D:651:HOH:O	2.16	0.44
1:D:275:GLU:O	1:D:275:GLU:HG2	2.17	0.44
1:F:309:PRO:O	1:F:310:ASN:HB2	2.17	0.44
1:K:331:ASN:HD21	1:K:381:GLN:HE22	1.65	0.44
1:B:132:LYS:HG3	3:B:683:HOH:O	2.17	0.44
1:E:374:ILE:HD11	1:E:393:THR:CG2	2.48	0.44
1:H:336:LEU:HB3	1:H:338:ILE:CD1	2.47	0.44
1:J:213:VAL:HG13	1:J:243:THR:HG21	2.00	0.44
1:F:374:ILE:HD11	1:F:393:THR:CG2	2.47	0.44
1:I:70:HIS:HB3	1:I:200:TYR:HA	2.00	0.44
1:K:413:GLN:HG3	1:K:423:VAL:HG11	1.99	0.44
1:C:136:ASN:HD21	1:C:159:LYS:HZ3	1.65	0.44
1:C:250:VAL:HG13	1:C:251:GLY:N	2.33	0.44
1:C:337:LYS:HG3	1:C:354:LYS:HZ2	1.83	0.44
1:D:336:LEU:HB3	1:D:338:ILE:CD1	2.48	0.44
1:E:88:LEU:HD11	1:E:220:TYR:CB	2.45	0.44
1:G:70:HIS:HA	1:G:118:GLN:HE21	1.81	0.44
1:I:286:ALA:O	1:I:290:GLN:HG3	2.17	0.44
1:I:306:PRO:HA	1:I:307:PRO:HD3	1.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:179:LEU:HD23	1:L:191:LEU:HD23	2.00	0.44
1:K:190:PRO:HG3	1:L:382:LEU:HB2	2.00	0.44
1:C:88:LEU:HD11	1:C:220:TYR:CB	2.47	0.44
1:G:382:LEU:HB2	1:H:190:PRO:HG3	1.98	0.44
1:I:213:VAL:HG11	1:I:234:PHE:CZ	2.52	0.44
1:L:70:HIS:HA	1:L:118:GLN:NE2	2.33	0.44
1:B:140:GLU:OE2	1:B:159:LYS:NZ	2.49	0.43
1:F:147:LEU:HA	1:F:148:PRO:C	2.38	0.43
1:J:274:SER:HB2	3:J:663:HOH:O	2.16	0.43
1:L:134:VAL:O	1:L:137:SER:HB3	2.18	0.43
1:A:305:VAL:HG13	1:A:317:TRP:CE2	2.53	0.43
1:B:66:GLU:HG2	1:B:115:LYS:HB3	2.00	0.43
1:D:219:LYS:HD2	1:D:276:ARG:NE	2.32	0.43
1:C:134:VAL:O	1:C:137:SER:HB3	2.18	0.43
1:D:118:GLN:HG3	3:D:616:HOH:O	2.17	0.43
1:J:336:LEU:CB	1:J:338:ILE:HD11	2.48	0.43
1:C:147:LEU:HA	1:C:148:PRO:C	2.39	0.43
1:D:306:PRO:HG2	1:D:317:TRP:CZ2	2.52	0.43
1:H:250:VAL:HG13	1:H:251:GLY:N	2.33	0.43
1:H:85:GLU:HB2	3:H:716:HOH:O	2.19	0.43
1:J:64:LEU:HD23	1:J:114:ILE:HD13	2.01	0.43
1:B:346:LYS:HA	1:B:347:PRO:C	2.39	0.43
1:E:183:LEU:O	1:E:184:ASN:HB2	2.18	0.43
1:B:213:VAL:HG11	1:B:234:PHE:CZ	2.53	0.43
1:G:311:LEU:HD23	1:G:317:TRP:CD1	2.54	0.43
1:I:338:ILE:HG23	1:I:339:TRP:N	2.33	0.43
1:A:380:ASN:HD22	1:B:181:ASN:HD21	1.65	0.43
1:B:275:GLU:HG2	1:B:275:GLU:O	2.19	0.43
1:F:124:ALA:O	1:F:128:GLU:HG2	2.18	0.43
1:J:275:GLU:O	1:J:275:GLU:HG2	2.19	0.43
1:C:155:ARG:N	1:C:156:PRO:HD2	2.34	0.43
1:G:219:LYS:HD2	1:G:276:ARG:NE	2.34	0.43
1:L:283:GLU:HG3	1:L:348:VAL:CG1	2.45	0.43
1:I:131:SER:OG	1:I:134:VAL:HG23	2.19	0.43
1:J:152:LYS:HG3	1:J:153:GLU:N	2.33	0.43
1:K:338:ILE:CG2	1:K:339:TRP:N	2.81	0.43
1:L:336:LEU:HB3	1:L:338:ILE:CD1	2.49	0.43
1:L:338:ILE:HG23	1:L:339:TRP:N	2.34	0.43
1:C:79:THR:HG23	1:C:87:LEU:HD12	2.00	0.43
1:H:414:LYS:O	1:H:418:GLU:HG3	2.19	0.43
1:H:88:LEU:HD11	1:H:220:TYR:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:TYR:HA	1:C:221:PRO:HD3	1.95	0.42
1:D:153:GLU:CD	1:D:153:GLU:H	2.21	0.42
1:D:367:LYS:HZ2	1:D:452:LYS:HE3	1.83	0.42
1:E:276:ARG:HG3	1:E:313:HIS:CE1	2.54	0.42
1:B:147:LEU:HA	1:B:148:PRO:C	2.39	0.42
1:B:336:LEU:HB3	1:B:338:ILE:CD1	2.49	0.42
1:D:374:ILE:HD11	1:D:393:THR:CG2	2.49	0.42
1:I:275:GLU:HB2	1:I:307:PRO:HG3	2.00	0.42
1:K:338:ILE:HG23	1:K:339:TRP:N	2.34	0.42
1:L:155:ARG:N	1:L:156:PRO:HD2	2.34	0.42
1:E:124:ALA:O	1:E:128:GLU:HG2	2.19	0.42
1:J:74:ASP:OD1	1:J:77:ARG:HD2	2.19	0.42
1:K:204:ASP:HB2	1:K:205:PRO:HD3	2.00	0.42
1:A:382:LEU:HD21	1:B:78:TYR:HA	2.01	0.42
1:B:153:GLU:H	1:B:153:GLU:CD	2.23	0.42
1:F:338:ILE:HG23	1:F:339:TRP:N	2.34	0.42
1:J:237:ASN:O	1:J:241:LYS:HB2	2.19	0.42
1:J:216:ASN:HB3	1:J:256:ILE:O	2.20	0.42
1:J:337:LYS:C	1:J:338:ILE:HD12	2.40	0.42
1:B:276:ARG:HH11	1:B:276:ARG:HG3	1.84	0.42
1:J:161:TYR:O	1:J:164:SER:OG	2.34	0.42
1:B:204:ASP:HB2	1:B:205:PRO:HD3	2.01	0.42
1:D:79:THR:HG23	1:D:87:LEU:HD12	2.01	0.42
1:F:413:GLN:O	1:F:417:VAL:HG13	2.19	0.42
1:H:153:GLU:HG2	1:I:309:PRO:HB3	2.01	0.42
1:J:257:GLU:HG3	1:J:276:ARG:HB3	2.02	0.42
1:L:153:GLU:H	1:L:153:GLU:CD	2.22	0.42
1:D:310:ASN:HD22	1:D:311:LEU:CD1	2.33	0.42
1:H:248:ASP:OD1	1:H:249:ILE:N	2.50	0.42
1:H:77:ARG:NH2	1:H:96:ASP:OD1	2.53	0.42
1:I:337:LYS:C	1:I:338:ILE:HD12	2.40	0.42
1:K:326:PHE:N	1:K:326:PHE:CD1	2.88	0.42
1:L:175:MET:HB3	1:L:199:LEU:CD1	2.50	0.42
1:D:338:ILE:HG23	1:D:339:TRP:N	2.34	0.42
1:H:131:SER:OG	1:H:134:VAL:HG23	2.20	0.42
1:H:187:GLN:HG3	1:H:189:ASN:O	2.20	0.42
1:L:97:THR:O	1:L:101:GLU:HG3	2.20	0.42
1:B:118:GLN:HG3	3:B:608:HOH:O	2.19	0.41
1:C:276:ARG:HG3	1:C:276:ARG:HH11	1.85	0.41
1:G:309:PRO:O	1:G:310:ASN:HB2	2.19	0.41
1:I:88:LEU:HD11	1:I:220:TYR:CB	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:MET:HB3	1:A:199:LEU:CD1	2.50	0.41
1:A:338:ILE:HG23	1:A:339:TRP:N	2.36	0.41
1:B:175:MET:HB3	1:B:199:LEU:CD1	2.50	0.41
1:F:306:PRO:HA	1:F:307:PRO:HD3	1.84	0.41
1:F:434:GLY:O	1:F:435:MET:HB2	2.21	0.41
1:H:329:SER:O	1:H:332:MET:HG2	2.19	0.41
1:J:162:LEU:O	1:J:170:MET:HG3	2.20	0.41
1:J:374:ILE:O	1:J:375:ALA:HB3	2.20	0.41
1:B:134:VAL:O	1:B:137:SER:HB3	2.21	0.41
1:C:337:LYS:O	1:C:338:ILE:HD12	2.21	0.41
1:J:263:ILE:N	1:J:263:ILE:HD12	2.34	0.41
1:J:327:LEU:HD12	1:J:372:ILE:O	2.20	0.41
1:A:147:LEU:HA	1:A:148:PRO:C	2.40	0.41
1:E:190:PRO:HB3	1:F:380:ASN:HB2	2.02	0.41
1:L:285:VAL:O	1:L:289:ILE:HG13	2.20	0.41
1:L:374:ILE:HD11	1:L:393:THR:CG2	2.49	0.41
1:E:147:LEU:HA	1:E:148:PRO:C	2.40	0.41
1:E:338:ILE:CG2	1:E:339:TRP:N	2.83	0.41
1:G:90:SER:OG	1:G:435:MET:HG3	2.20	0.41
1:G:183:LEU:HD12	1:G:192:ILE:HG13	2.03	0.41
1:J:70:HIS:HB3	1:J:200:TYR:HA	2.03	0.41
1:A:171:VAL:O	1:A:175:MET:HG3	2.20	0.41
1:B:326:PHE:CD1	1:B:326:PHE:N	2.89	0.41
1:C:171:VAL:O	1:C:175:MET:HG3	2.20	0.41
1:C:338:ILE:HG23	1:C:339:TRP:N	2.35	0.41
1:D:310:ASN:HD22	1:D:311:LEU:HD12	1.86	0.41
1:G:147:LEU:HA	1:G:148:PRO:C	2.41	0.41
1:J:286:ALA:O	1:J:290:GLN:HG3	2.21	0.41
1:K:90:SER:OG	1:K:435:MET:HG3	2.20	0.41
1:D:171:VAL:O	1:D:175:MET:HG3	2.21	0.41
1:K:179:LEU:HD23	1:K:191:LEU:HD23	2.02	0.41
1:G:286:ALA:O	1:G:290:GLN:HG3	2.21	0.41
1:I:77:ARG:NH2	1:I:96:ASP:OD1	2.53	0.41
1:K:61:ILE:HG22	1:K:397:THR:HG21	2.03	0.41
1:C:204:ASP:HB2	1:C:205:PRO:HD3	2.02	0.41
1:C:329:SER:O	1:C:332:MET:HG2	2.20	0.41
1:H:135:ARG:O	1:H:138:PHE:HB3	2.21	0.41
1:H:70:HIS:HB3	1:H:200:TYR:HA	2.03	0.41
1:L:308:MET:CE	1:L:309:PRO:HD2	2.51	0.41
1:C:88:LEU:HD11	1:C:220:TYR:CG	2.56	0.40
1:C:353:LYS:HG2	3:C:717:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:SER:HA	1:D:263:ILE:O	2.21	0.40
1:D:79:THR:HB	3:D:636:HOH:O	2.20	0.40
1:E:380:ASN:HD22	1:F:181:ASN:ND2	2.17	0.40
1:I:265:ASN:OD1	1:I:268:THR:N	2.53	0.40
1:I:361:LEU:HD12	1:I:371:LEU:HD21	2.03	0.40
1:K:375:ALA:HA	1:K:411:LYS:HB2	2.03	0.40
1:A:79:THR:HG23	1:A:87:LEU:HD12	2.02	0.40
1:A:88:LEU:HD11	1:A:220:TYR:CB	2.49	0.40
1:B:171:VAL:O	1:B:175:MET:HG3	2.21	0.40
1:G:71:THR:N	1:G:118:GLN:NE2	2.50	0.40
1:G:88:LEU:HD11	1:G:220:TYR:CG	2.56	0.40
1:I:374:ILE:HD11	1:I:393:THR:HG22	2.03	0.40
1:J:204:ASP:HB2	1:J:205:PRO:HD3	2.03	0.40
1:J:220:TYR:HA	1:J:221:PRO:HD3	1.92	0.40
1:L:88:LEU:CD1	1:L:220:TYR:HB2	2.49	0.40
1:L:367:LYS:NZ	1:L:452:LYS:HE3	2.35	0.40
1:B:353:LYS:HD3	1:B:354:LYS:N	2.37	0.40
1:B:70:HIS:HB3	1:B:200:TYR:HA	2.04	0.40
1:D:70:HIS:HA	1:D:118:GLN:HE21	1.85	0.40
1:E:250:VAL:HG13	1:E:251:GLY:N	2.35	0.40
1:F:256:ILE:CD1	1:F:261:ILE:HD11	2.52	0.40
1:H:141:GLN:O	1:H:145:GLU:HG3	2.21	0.40
1:A:124:ALA:O	1:A:128:GLU:HG2	2.21	0.40
1:C:71:THR:N	1:C:118:GLN:NE2	2.53	0.40
1:G:142:TYR:CG	1:G:174:MET:HE2	2.56	0.40
1:G:283:GLU:HG3	1:G:348:VAL:CG1	2.43	0.40
1:H:328:TYR:HB2	1:H:332:MET:CE	2.51	0.40
1:I:414:LYS:HE2	1:I:418:GLU:OE2	2.21	0.40
1:K:118:GLN:HG3	3:K:612:HOH:O	2.21	0.40
1:A:70:HIS:HB3	1:A:200:TYR:HA	2.04	0.40
1:A:374:ILE:O	1:A:375:ALA:HB3	2.22	0.40
1:C:328:TYR:HB2	1:C:332:MET:CE	2.51	0.40
1:C:328:TYR:HB2	1:C:332:MET:HE3	2.04	0.40
1:F:140:GLU:OE2	1:F:159:LYS:NZ	2.53	0.40
1:H:66:GLU:HG2	1:H:115:LYS:HB3	2.02	0.40
1:L:327:LEU:HD12	1:L:372:ILE:O	2.21	0.40

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%)	41	50
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%)	41	50
1	H	397/433 (92%)	383 (96%)	14 (4%)	0	100	100
1	I	397/433 (92%)	375 (94%)	21 (5%)	1 (0%)	41	50
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%)	51	64

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%)	86	94
1	B	357/388 (92%)	354 (99%)	3 (1%)	81	91
1	C	357/388 (92%)	355 (99%)	2 (1%)	86	94
1	D	357/388 (92%)	355 (99%)	2 (1%)	86	94
1	E	357/388 (92%)	355 (99%)	2 (1%)	86	94
1	F	357/388 (92%)	355 (99%)	2 (1%)	86	94
1	G	357/388 (92%)	355 (99%)	2 (1%)	86	94
1	H	357/388 (92%)	356 (100%)	1 (0%)	92	97
1	I	357/388 (92%)	355 (99%)	2 (1%)	86	94
1	J	357/388 (92%)	356 (100%)	1 (0%)	92	97
1	K	357/388 (92%)	357 (100%)	0	100	100
1	L	357/388 (92%)	356 (100%)	1 (0%)	92	97
All	All	4284/4656 (92%)	4264 (100%)	20 (0%)	88	95

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	LEU
1	A	348	VAL
1	B	269	LEU
1	B	317	TRP
1	B	349	LYS
1	C	269	LEU
1	C	312	MET
1	D	269	LEU
1	D	310	ASN
1	E	217	CYS
1	E	269	LEU
1	F	269	LEU
1	F	317	TRP
1	G	269	LEU
1	G	317	TRP
1	H	269	LEU
1	I	269	LEU
1	I	308	MET
1	J	317	TRP
1	L	269	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	136	ASN
1	A	181	ASN
1	A	184	ASN
1	A	216	ASN
1	A	288	ASN
1	A	331	ASN
1	B	110	GLN
1	B	118	GLN
1	B	136	ASN
1	B	181	ASN
1	B	216	ASN
1	B	288	ASN
1	B	389	HIS
1	C	110	GLN
1	C	118	GLN
1	C	136	ASN
1	C	181	ASN
1	C	216	ASN
1	C	288	ASN
1	C	331	ASN
1	D	118	GLN
1	D	136	ASN
1	D	181	ASN
1	D	216	ASN
1	D	288	ASN
1	D	310	ASN
1	D	413	GLN
1	E	110	GLN
1	E	118	GLN
1	E	136	ASN
1	E	181	ASN
1	E	216	ASN
1	E	288	ASN
1	E	310	ASN
1	F	118	GLN
1	F	136	ASN
1	F	181	ASN
1	F	216	ASN
1	F	288	ASN
1	F	310	ASN
1	G	110	GLN

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Mol	Chain	Res	Type
1	G	118	GLN
1	G	136	ASN
1	G	181	ASN
1	G	216	ASN
1	G	288	ASN
1	G	389	HIS
1	H	118	GLN
1	H	136	ASN
1	H	181	ASN
1	H	184	ASN
1	H	216	ASN
1	H	288	ASN
1	H	313	HIS
1	H	331	ASN
1	H	389	HIS
1	I	110	GLN
1	I	118	GLN
1	I	136	ASN
1	I	181	ASN
1	I	216	ASN
1	I	288	ASN
1	I	331	ASN
1	I	389	HIS
1	J	56	ASN
1	J	118	GLN
1	J	136	ASN
1	J	216	ASN
1	J	288	ASN
1	K	110	GLN
1	K	118	GLN
1	K	136	ASN
1	K	181	ASN
1	K	216	ASN
1	K	288	ASN
1	K	310	ASN
1	K	331	ASN
1	K	413	GLN
1	L	110	GLN
1	L	118	GLN
1	L	136	ASN
1	L	181	ASN
1	L	216	ASN

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Mol	Chain	Res	Type
1	L	288	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 ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	399/433 (92%)	-0.22	4 (1%) 82 86	12, 23, 41, 64	0
1	B	399/433 (92%)	0.17	26 (6%) 18 24	18, 34, 59, 74	0
1	C	399/433 (92%)	-0.18	7 (1%) 68 74	14, 23, 43, 66	0
1	D	399/433 (92%)	0.09	17 (4%) 35 42	16, 31, 57, 77	0
1	E	399/433 (92%)	-0.09	8 (2%) 65 71	16, 26, 43, 69	0
1	F	399/433 (92%)	0.23	29 (7%) 15 20	16, 36, 62, 75	0
1	G	399/433 (92%)	0.54	51 (12%) 3 5	21, 42, 70, 82	0
1	H	399/433 (92%)	0.00	9 (2%) 60 67	17, 30, 55, 73	0
1	I	399/433 (92%)	0.32	31 (7%) 13 17	22, 39, 71, 87	0
1	J	399/433 (92%)	0.42	33 (8%) 11 15	22, 43, 70, 81	0
1	K	399/433 (92%)	-0.14	6 (1%) 73 79	18, 28, 46, 70	0
1	L	399/433 (92%)	0.05	18 (4%) 33 40	17, 33, 56, 77	0
All	All	4788/5196 (92%)	0.10	239 (4%) 28 35	12, 31, 61, 87	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	333	MET	9.7
1	L	333	MET	8.9
1	I	333	MET	6.8
1	L	220	TYR	6.3
1	J	220	TYR	6.1
1	G	220	TYR	5.5
1	H	220	TYR	5.4
1	I	250	VAL	5.4
1	B	220	TYR	5.3
1	F	452	LYS	5.0
1	K	220	TYR	4.9

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Mol	Chain	Res	Type	RSRZ
1	I	307	PRO	4.8
1	I	309	PRO	4.8
1	I	220	TYR	4.8
1	H	151	LYS	4.7
1	D	220	TYR	4.6
1	J	345	VAL	4.6
1	J	452	LYS	4.6
1	J	221	PRO	4.5
1	I	452	LYS	4.5
1	G	308	MET	4.5
1	J	250	VAL	4.5
1	G	311	LEU	4.5
1	J	347	PRO	4.5
1	B	250	VAL	4.4
1	L	250	VAL	4.3
1	E	220	TYR	4.3
1	C	452	LYS	4.3
1	F	220	TYR	4.2
1	I	334	ASN	4.2
1	G	152	LYS	4.2
1	G	309	PRO	4.1
1	D	452	LYS	4.1
1	H	152	LYS	4.1
1	K	452	LYS	4.1
1	G	293	LYS	4.1
1	J	333	MET	4.1
1	G	153	GLU	4.0
1	D	309	PRO	4.0
1	G	154	ILE	4.0
1	G	333	MET	4.0
1	H	154	ILE	3.9
1	G	250	VAL	3.8
1	D	250	VAL	3.7
1	C	220	TYR	3.7
1	J	293	LYS	3.7
1	J	309	PRO	3.7
1	B	91	ALA	3.7
1	B	333	MET	3.7
1	J	133	GLU	3.6
1	I	451	LYS	3.6
1	G	87	LEU	3.6
1	G	452	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	250	VAL	3.5
1	I	293	LYS	3.4
1	I	254	GLY	3.4
1	E	452	LYS	3.4
1	A	452	LYS	3.4
1	D	221	PRO	3.4
1	G	221	PRO	3.3
1	G	91	ALA	3.3
1	G	184	ASN	3.3
1	J	261	ILE	3.3
1	G	348	VAL	3.3
1	J	344	ASN	3.3
1	I	261	ILE	3.3
1	F	333	MET	3.3
1	G	347	PRO	3.3
1	B	152	LYS	3.2
1	J	152	LYS	3.2
1	L	293	LYS	3.2
1	I	354	LYS	3.2
1	H	219	LYS	3.2
1	D	347	PRO	3.2
1	A	220	TYR	3.1
1	G	219	LYS	3.1
1	G	310	ASN	3.1
1	L	451	LYS	3.1
1	G	133	GLU	3.1
1	A	250	VAL	3.0
1	G	345	VAL	3.0
1	L	334	ASN	3.0
1	L	452	LYS	3.0
1	D	334	ASN	3.0
1	J	253	ASN	3.0
1	J	366	ASP	3.0
1	H	85	GLU	3.0
1	I	310	ASN	3.0
1	G	88	LEU	3.0
1	I	332	MET	3.0
1	F	132	LYS	3.0
1	H	153	GLU	3.0
1	L	221	PRO	3.0
1	B	293	LYS	3.0
1	B	452	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	219	LYS	2.9
1	B	347	PRO	2.9
1	J	219	LYS	2.9
1	J	312	MET	2.9
1	I	347	PRO	2.9
1	F	221	PRO	2.8
1	G	344	ASN	2.8
1	B	308	MET	2.8
1	L	332	MET	2.8
1	B	261	ILE	2.8
1	G	151	LYS	2.8
1	L	348	VAL	2.8
1	J	202	THR	2.8
1	F	310	ASN	2.8
1	G	451	LYS	2.8
1	G	335	VAL	2.8
1	D	349	LYS	2.8
1	B	263	ILE	2.7
1	G	261	ILE	2.7
1	J	254	GLY	2.6
1	F	347	PRO	2.6
1	G	85	GLU	2.6
1	K	451	LYS	2.6
1	L	85	GLU	2.6
1	I	348	VAL	2.6
1	G	334	ASN	2.6
1	J	207	ALA	2.6
1	D	331	ASN	2.6
1	G	242	ASN	2.6
1	B	262	PHE	2.6
1	I	362	TYR	2.6
1	I	317	TRP	2.6
1	B	270	VAL	2.6
1	D	348	VAL	2.6
1	F	451	LYS	2.6
1	J	132	LYS	2.6
1	G	287	LYS	2.5
1	I	366	ASP	2.5
1	B	349	LYS	2.5
1	C	186	LYS	2.5
1	H	452	LYS	2.5
1	J	270	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	334	ASN	2.5
1	D	85	GLU	2.5
1	I	262	PHE	2.5
1	L	309	PRO	2.5
1	F	368	LYS	2.5
1	J	291	ALA	2.5
1	F	222	THR	2.5
1	G	307	PRO	2.5
1	C	185	ILE	2.5
1	A	184	ASN	2.5
1	B	221	PRO	2.5
1	I	336	LEU	2.5
1	G	207	ALA	2.4
1	F	129	LEU	2.4
1	B	345	VAL	2.4
1	F	133	GLU	2.4
1	F	219	LYS	2.4
1	F	270	VAL	2.4
1	B	269	LEU	2.4
1	E	221	PRO	2.4
1	K	221	PRO	2.4
1	B	451	LYS	2.3
1	J	203	ARG	2.3
1	J	338	ILE	2.3
1	I	133	GLU	2.3
1	I	349	LYS	2.3
1	E	250	VAL	2.3
1	J	262	PHE	2.3
1	F	258	GLY	2.3
1	E	440	CYS	2.3
1	G	317	TRP	2.3
1	I	335	VAL	2.3
1	I	345	VAL	2.3
1	G	259	GLY	2.3
1	G	262	PHE	2.3
1	F	307	PRO	2.3
1	G	253	ASN	2.3
1	C	440	CYS	2.3
1	F	345	VAL	2.3
1	G	279	PHE	2.3
1	F	275	GLU	2.2
1	I	355	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	153	GLU	2.2
1	D	368	LYS	2.2
1	G	349	LYS	2.2
1	F	206	PHE	2.2
1	F	88	LEU	2.2
1	G	132	LYS	2.2
1	E	262	PHE	2.2
1	G	206	PHE	2.2
1	J	85	GLU	2.2
1	L	129	LEU	2.2
1	E	275	GLU	2.2
1	F	85	GLU	2.2
1	K	133	GLU	2.2
1	D	332	MET	2.2
1	G	366	ASP	2.2
1	B	443	MET	2.2
1	F	312	MET	2.2
1	L	307	PRO	2.2
1	J	275	GLU	2.2
1	J	280	ALA	2.2
1	G	339	TRP	2.2
1	I	275	GLU	2.2
1	J	131	SER	2.2
1	G	346	LYS	2.1
1	G	377	LYS	2.1
1	F	362	TYR	2.1
1	B	202	THR	2.1
1	G	338	ILE	2.1
1	B	133	GLU	2.1
1	B	207	ALA	2.1
1	B	346	LYS	2.1
1	G	202	THR	2.1
1	I	439	ARG	2.1
1	G	254	GLY	2.1
1	I	308	MET	2.1
1	J	348	VAL	2.1
1	G	275	GLU	2.1
1	L	310	ASN	2.1
1	J	355	GLY	2.1
1	G	129	LEU	2.1
1	B	253	ASN	2.1
1	C	270	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	152	LYS	2.1
1	F	293	LYS	2.1
1	D	129	LEU	2.1
1	G	258	GLY	2.1
1	H	185	ILE	2.0
1	I	132	LYS	2.0
1	F	207	ALA	2.0
1	L	262	PHE	2.0
1	C	396	LEU	2.0
1	L	88	LEU	2.0
1	F	443	MET	2.0
1	K	250	VAL	2.0
1	I	440	CYS	2.0
1	D	263	ILE	2.0
1	F	308	MET	2.0
1	B	241	LYS	2.0
1	D	152	LYS	2.0
1	L	152	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CL	K	501	1/1	0.99	0.10	21,21,21,21	0
2	CL	I	501	1/1	0.99	0.09	28,28,28,28	0
2	CL	H	501	1/1	0.99	0.11	24,24,24,24	0
2	CL	F	501	1/1	0.99	0.07	19,19,19,19	0
2	CL	E	501	1/1	0.99	0.11	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CL	G	501	1/1	1.00	0.06	24,24,24,24	0
2	CL	J	501	1/1	1.00	0.10	24,24,24,24	0
2	CL	L	501	1/1	1.00	0.09	20,20,20,20	0
2	CL	D	501	1/1	1.00	0.13	21,21,21,21	0
2	CL	C	501	1/1	1.00	0.11	21,21,21,21	0
2	CL	B	501	1/1	1.00	0.09	20,20,20,20	0
2	CL	A	501	1/1	1.00	0.11	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.