



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:07 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (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

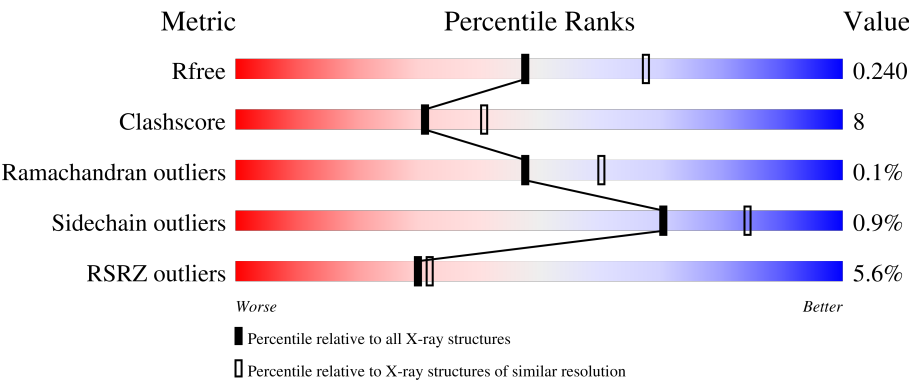
1 Overall quality at a glance i

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 ≥ 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	0% 75%17%8%
1	B	433	5% 71%20%8%
1	C	433	2% 76%16%8%
1	D	433	6% 74%18%8%
1	E	433	4% 77%14%8%

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

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 (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

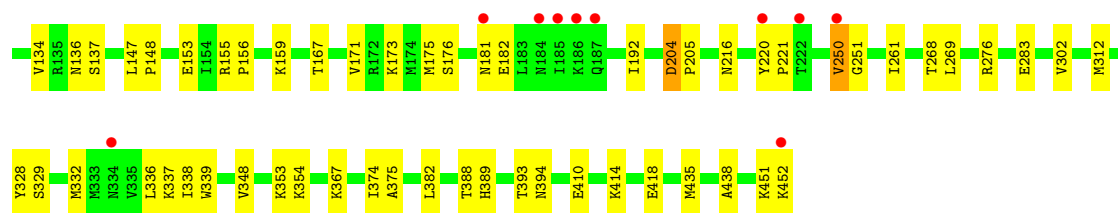
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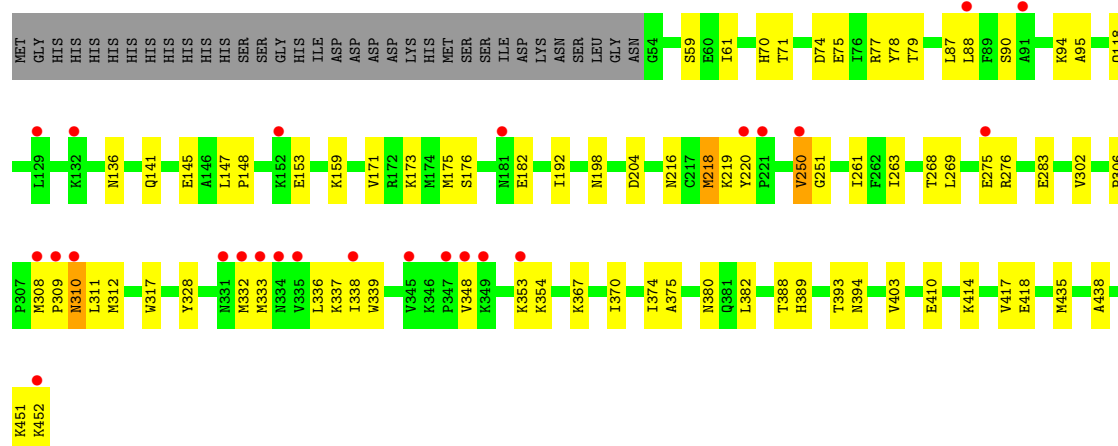
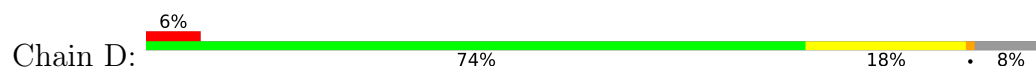
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	1	Total 1	Cl 1	0	0
2	L	1	Total 1	Cl 1	0	0

- Molecule 3 is water.

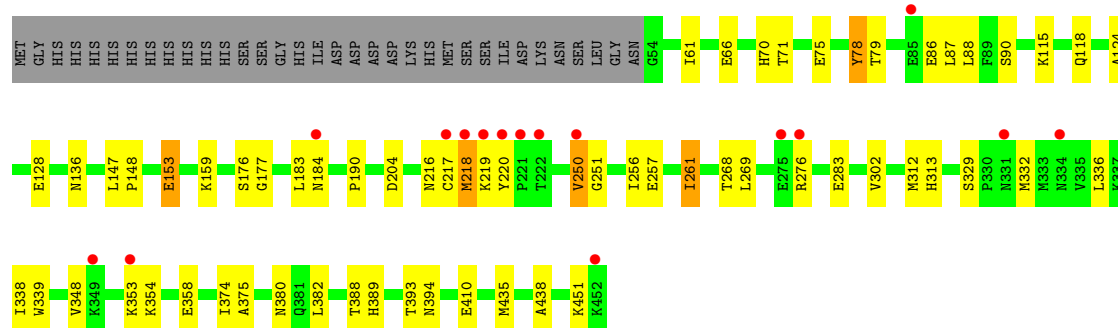
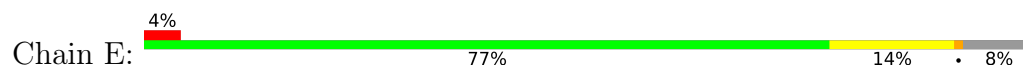
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	212	Total 212	O 212	0	0
3	B	117	Total 117	O 117	0	0
3	C	213	Total 213	O 213	0	0
3	D	142	Total 142	O 142	0	0
3	E	180	Total 180	O 180	0	0
3	F	99	Total 99	O 99	0	0
3	G	80	Total 80	O 80	0	0
3	H	140	Total 140	O 140	0	0
3	I	86	Total 86	O 86	0	0
3	J	82	Total 82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



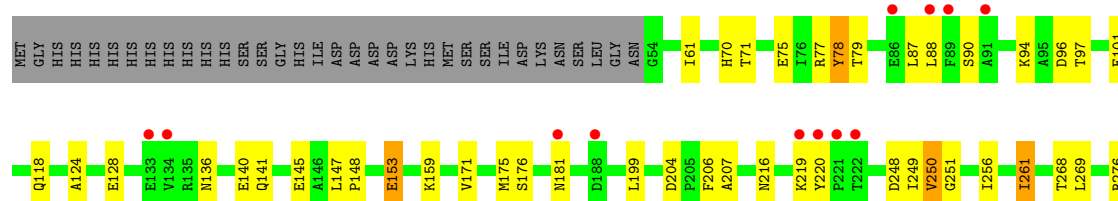
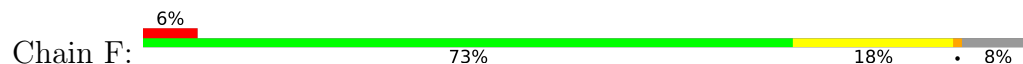
• Molecule 1: Arginine deiminase

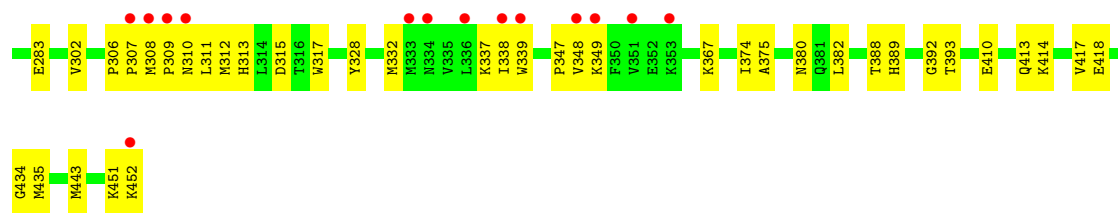


• Molecule 1: Arginine deiminase

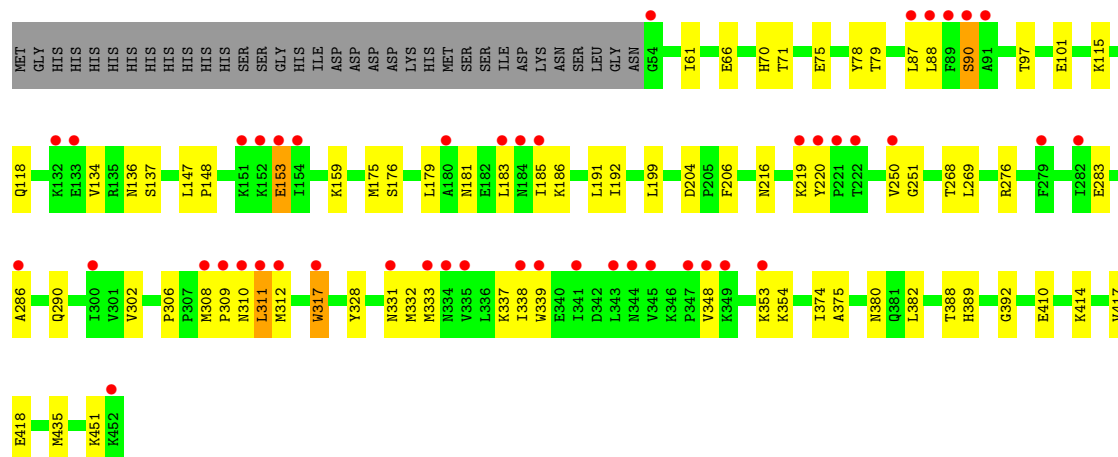
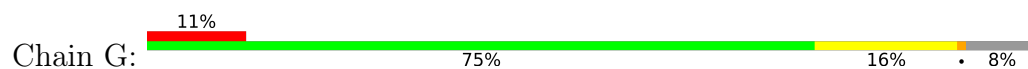


• Molecule 1: Arginine deiminase

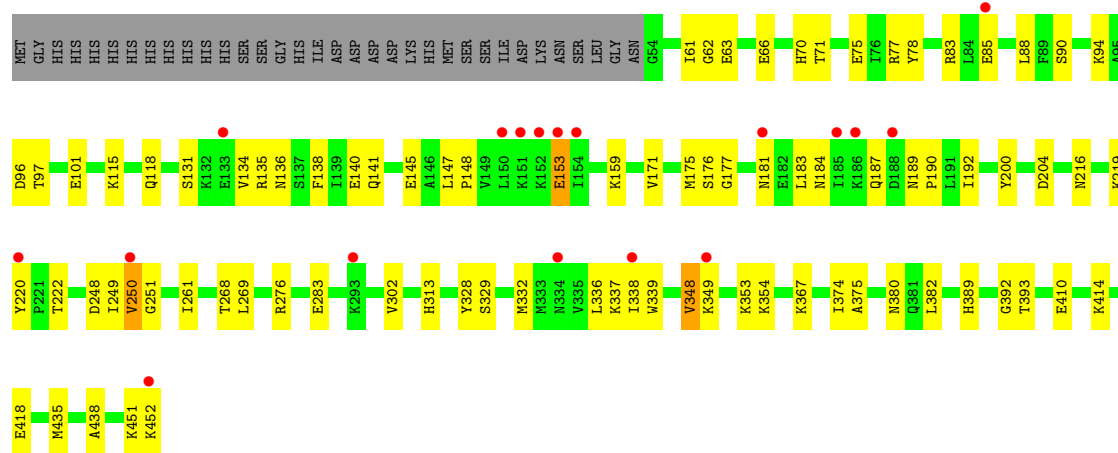
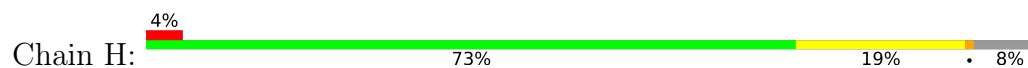




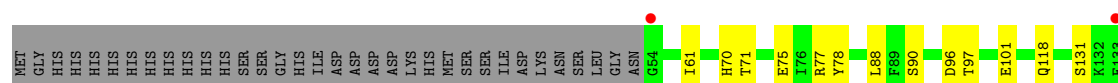
• Molecule 1: Arginine deiminase

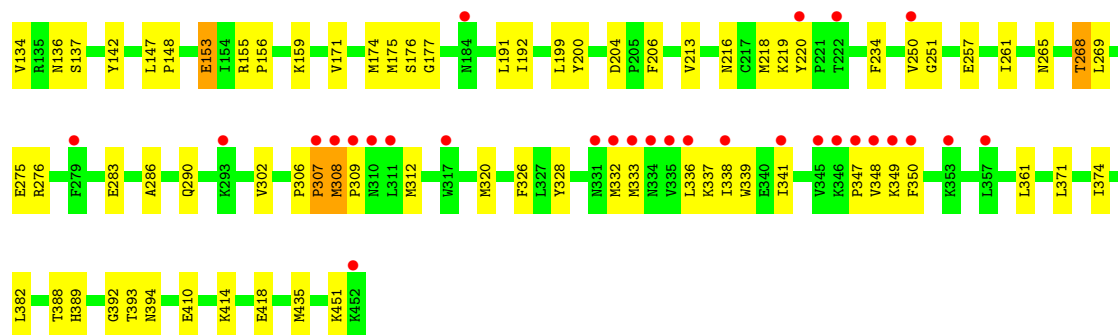


• Molecule 1: Arginine deiminase

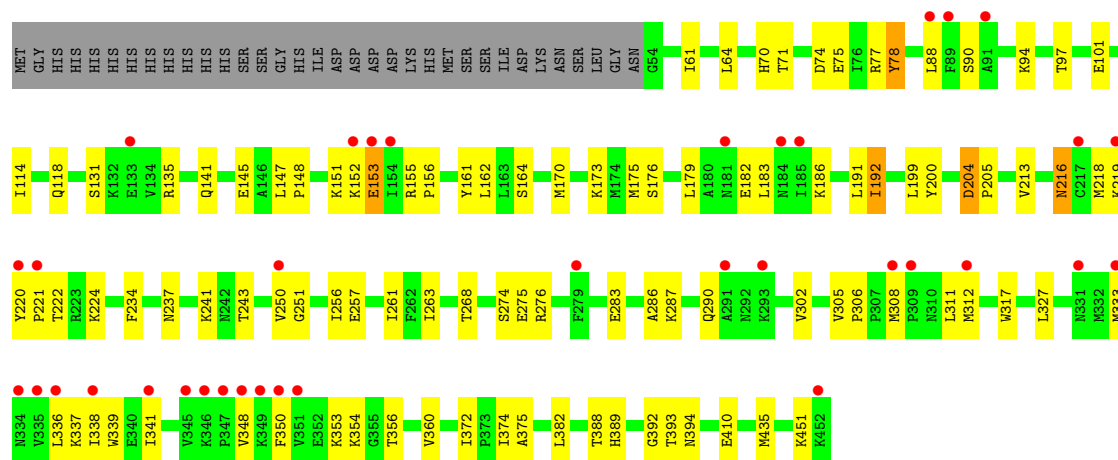


• Molecule 1: Arginine deiminase

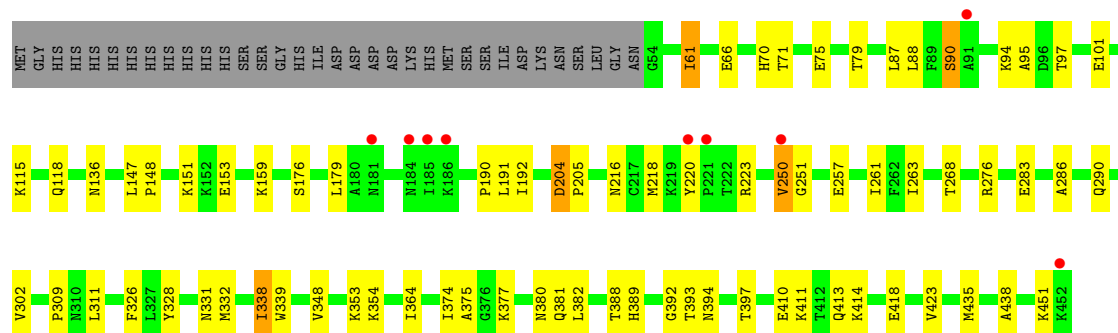
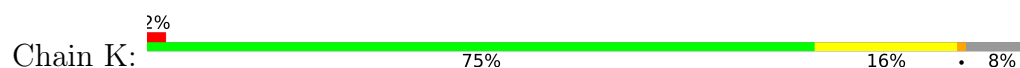




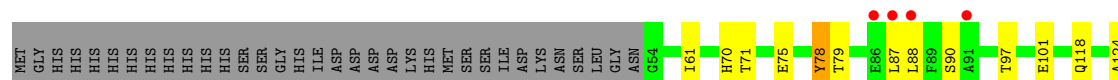
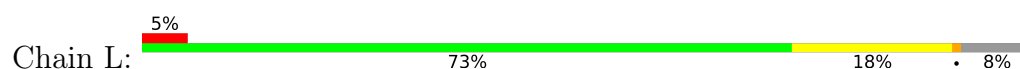
• Molecule 1: Arginine deiminase

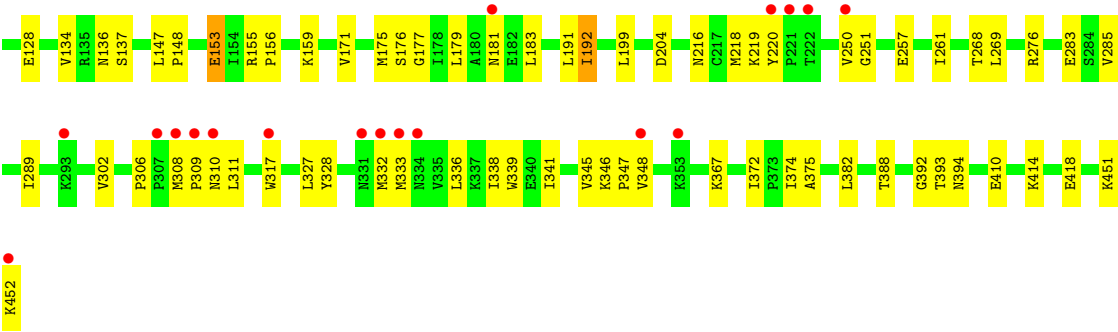


• Molecule 1: Arginine deiminase



• 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 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
$\langle I/\sigma(I) \rangle$ 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)	0.34 , 36.9	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

5.1 Standard geometry

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.

All (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
1	L	451	LYS	N-CA-C	-8.73	102.37	113.72
1	L	90	SER	N-CA-C	8.59	123.88	113.23
1	B	90	SER	N-CA-C	8.54	123.47	112.89
1	C	90	SER	N-CA-C	8.45	123.37	112.89
1	A	90	SER	N-CA-C	8.44	123.35	112.89
1	J	90	SER	N-CA-C	8.43	123.34	112.89
1	D	90	SER	N-CA-C	8.39	123.29	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	90	SER	N-CA-C	8.31	123.19	112.89
1	E	90	SER	N-CA-C	8.29	123.18	112.89
1	H	90	SER	N-CA-C	8.28	123.16	112.89
1	I	90	SER	N-CA-C	8.12	122.46	112.23
1	C	216	ASN	N-CA-C	7.84	120.88	110.53
1	D	451	LYS	N-CA-C	-7.64	103.06	113.30
1	G	451	LYS	N-CA-C	-7.62	102.18	113.61
1	B	216	ASN	N-CA-C	7.57	120.53	110.53
1	F	216	ASN	N-CA-C	7.53	120.59	110.35
1	B	451	LYS	N-CA-C	-7.50	102.36	113.61
1	E	216	ASN	N-CA-C	7.49	121.05	110.50
1	D	216	ASN	N-CA-C	7.38	120.91	110.50
1	G	216	ASN	N-CA-C	7.34	120.34	110.35
1	H	451	LYS	N-CA-C	-7.32	103.50	113.30
1	F	410	GLU	N-CA-C	7.30	119.24	111.28
1	J	451	LYS	N-CA-C	-7.30	102.67	113.61
1	A	451	LYS	N-CA-C	-7.26	102.72	113.61
1	K	451	LYS	N-CA-C	-7.20	103.66	113.30
1	E	451	LYS	N-CA-C	-7.17	102.85	113.61
1	K	216	ASN	N-CA-C	7.16	120.59	110.50
1	F	451	LYS	N-CA-C	-7.16	102.88	113.61
1	D	192	ILE	N-CA-C	-7.06	104.09	111.58
1	L	216	ASN	N-CA-C	7.05	120.44	110.50
1	J	216	ASN	N-CA-C	7.02	119.80	110.53
1	H	216	ASN	N-CA-C	7.02	120.40	110.50
1	A	216	ASN	N-CA-C	6.95	120.29	110.50
1	K	410	GLU	N-CA-C	6.92	118.82	111.28
1	E	394	ASN	N-CA-C	6.91	121.40	110.70
1	C	451	LYS	N-CA-C	-6.88	103.29	113.61
1	I	451	LYS	N-CA-C	-6.86	103.33	113.61
1	F	261	ILE	N-CA-C	6.84	117.98	107.99
1	K	192	ILE	N-CA-C	-6.83	104.19	110.82
1	A	61	ILE	N-CA-C	6.71	120.24	113.47
1	E	61	ILE	N-CA-C	6.69	120.23	113.47
1	D	394	ASN	N-CA-C	6.67	121.04	110.70
1	I	216	ASN	N-CA-C	6.63	119.29	110.53
1	C	61	ILE	N-CA-C	6.52	120.06	113.47
1	G	61	ILE	N-CA-C	6.52	120.06	113.47
1	L	410	GLU	N-CA-C	6.49	118.35	111.28
1	G	410	GLU	N-CA-C	6.48	118.00	111.07
1	L	61	ILE	N-CA-C	6.46	119.86	113.53
1	D	410	GLU	N-CA-C	6.45	118.31	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	268	THR	N-CA-C	6.45	118.92	108.41
1	I	61	ILE	N-CA-C	6.42	119.95	113.47
1	E	410	GLU	N-CA-C	6.41	118.26	111.28
1	A	410	GLU	N-CA-C	6.38	118.23	111.28
1	C	388	THR	N-CA-C	-6.34	103.89	111.69
1	J	61	ILE	N-CA-C	6.32	119.85	113.47
1	F	61	ILE	N-CA-C	6.32	119.85	113.47
1	D	61	ILE	N-CA-C	6.31	119.85	113.47
1	C	410	GLU	N-CA-C	6.31	118.16	111.28
1	I	410	GLU	N-CA-C	6.30	118.14	111.28
1	J	394	ASN	N-CA-C	6.24	120.38	110.70
1	D	261	ILE	N-CA-C	6.23	117.09	107.99
1	C	192	ILE	N-CA-C	-6.17	105.04	111.58
1	A	261	ILE	N-CA-C	6.17	116.99	107.99
1	L	261	ILE	N-CA-C	6.13	116.95	107.99
1	B	61	ILE	N-CA-C	6.10	119.63	113.47
1	K	261	ILE	N-CA-C	6.07	116.84	107.99
1	D	268	THR	N-CA-C	6.05	118.81	109.07
1	H	392	GLY	N-CA-C	6.04	121.31	113.27
1	C	94	LYS	N-CA-C	-6.03	96.65	107.98
1	A	392	GLY	N-CA-C	6.00	121.10	113.24
1	A	388	THR	N-CA-C	-5.99	104.33	111.69
1	B	192	ILE	N-CA-C	-5.93	105.29	111.58
1	B	410	GLU	N-CA-C	5.93	117.75	111.28
1	H	410	GLU	N-CA-C	5.93	117.74	111.28
1	K	392	GLY	N-CA-C	5.88	120.94	113.24
1	E	204	ASP	N-CA-C	5.87	122.78	109.81
1	B	78	TYR	N-CA-C	5.82	119.15	112.57
1	K	204	ASP	N-CA-C	5.78	122.58	109.81
1	A	204	ASP	N-CA-C	5.76	122.54	109.81
1	L	204	ASP	N-CA-C	5.76	122.54	109.81
1	J	410	GLU	N-CA-C	5.75	117.55	111.28
1	A	438	ALA	N-CA-C	5.73	117.98	111.11
1	L	177	GLY	N-CA-C	-5.71	105.42	112.33
1	L	388	THR	N-CA-C	-5.71	104.67	111.69
1	H	204	ASP	N-CA-C	5.67	122.35	109.81
1	D	388	THR	N-CA-C	-5.66	104.72	111.69
1	C	438	ALA	N-CA-C	5.64	118.16	111.33
1	J	388	THR	N-CA-C	-5.64	104.75	111.69
1	J	78	TYR	N-CA-C	5.62	118.92	112.57
1	D	204	ASP	N-CA-C	5.60	122.18	109.81
1	H	177	GLY	N-CA-C	-5.59	105.57	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	61	ILE	N-CA-C	5.58	119.11	113.47
1	A	268	THR	N-CA-C	5.58	117.99	108.90
1	L	392	GLY	N-CA-C	5.56	120.53	113.24
1	I	261	ILE	N-CA-C	5.56	116.10	107.99
1	K	388	THR	N-CA-C	-5.56	104.85	111.69
1	J	261	ILE	N-CA-C	5.55	116.10	107.99
1	B	261	ILE	N-CA-C	5.55	116.09	107.99
1	B	94	LYS	N-CA-C	-5.53	97.58	107.98
1	H	268	THR	N-CA-C	5.53	117.91	108.90
1	C	204	ASP	N-CA-C	5.51	122.00	109.81
1	B	204	ASP	N-CA-C	5.50	121.97	109.81
1	B	438	ALA	N-CA-C	5.48	117.68	111.11
1	K	61	ILE	N-CA-C	5.48	118.90	113.53
1	F	204	ASP	N-CA-C	5.47	121.89	109.81
1	C	268	THR	N-CA-C	5.46	117.79	108.90
1	E	261	ILE	N-CA-C	5.45	115.94	107.99
1	L	268	THR	N-CA-C	5.44	117.84	109.07
1	G	268	THR	N-CA-C	5.43	117.82	109.07
1	K	95	ALA	N-CA-C	5.43	120.27	111.37
1	L	192	ILE	N-CA-C	-5.43	105.08	111.00
1	K	268	THR	N-CA-C	5.41	117.71	108.90
1	J	392	GLY	N-CA-C	5.40	120.45	113.27
1	H	94	LYS	N-CA-C	-5.38	97.87	107.98
1	K	394	ASN	N-CA-C	5.36	122.23	110.80
1	B	388	THR	N-CA-C	-5.36	105.09	111.69
1	C	78	TYR	N-CA-C	5.34	118.81	112.72
1	I	388	THR	N-CA-C	-5.34	105.12	111.69
1	E	388	THR	N-CA-C	-5.33	105.14	111.69
1	I	191	LEU	N-CA-C	5.33	117.64	109.07
1	F	268	THR	N-CA-C	5.31	117.62	109.07
1	F	388	THR	N-CA-C	-5.30	105.17	111.69
1	I	268	THR	N-CA-C	5.30	117.60	109.07
1	C	394	ASN	N-CA-C	5.30	122.08	110.80
1	I	177	GLY	N-CA-C	-5.30	105.92	112.33
1	I	204	ASP	N-CA-C	5.29	121.50	109.81
1	C	261	ILE	N-CA-C	5.28	115.70	107.99
1	F	392	GLY	N-CA-C	5.28	120.16	113.24
1	I	392	GLY	N-CA-C	5.28	120.29	113.27
1	H	438	ALA	N-CA-C	5.27	117.70	111.33
1	D	403	VAL	N-CA-C	5.26	117.20	108.99
1	I	192	ILE	N-CA-C	-5.25	105.28	111.00
1	D	95	ALA	N-CA-C	5.25	119.97	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	78	TYR	N-CA-C	5.23	118.69	112.72
1	D	94	LYS	N-CA-C	-5.21	98.18	107.98
1	J	94	LYS	N-CA-C	-5.21	98.18	107.98
1	K	94	LYS	N-CA-C	-5.21	98.19	107.98
1	J	192	ILE	N-CA-C	-5.20	105.34	111.00
1	B	268	THR	N-CA-C	5.17	117.33	108.90
1	B	394	ASN	N-CA-C	5.17	121.81	110.80
1	G	392	GLY	N-CA-C	5.17	120.61	113.99
1	G	388	THR	N-CA-C	-5.17	105.33	111.69
1	K	364	ILE	CB-CA-C	-5.16	106.54	111.44
1	C	250	VAL	N-CA-C	5.15	120.05	109.34
1	D	250	VAL	N-CA-C	5.15	120.04	109.34
1	E	438	ALA	N-CA-C	5.13	117.54	111.33
1	F	94	LYS	N-CA-C	-5.12	98.36	107.98
1	G	204	ASP	N-CA-C	5.10	121.08	109.81
1	A	77	ARG	N-CA-C	-5.10	107.10	113.72
1	C	95	ALA	N-CA-C	5.09	119.72	111.37
1	H	261	ILE	N-CA-C	5.08	115.62	108.36
1	I	394	ASN	N-CA-C	5.08	121.61	110.80
1	A	250	VAL	N-CA-C	5.07	119.88	109.34
1	J	204	ASP	N-CA-C	5.06	120.98	109.81
1	E	78	TYR	N-CA-C	5.05	118.48	112.72
1	F	78	TYR	N-CA-C	5.05	118.48	112.72
1	E	177	GLY	N-CA-C	-5.05	105.34	112.81
1	C	167	THR	N-CA-C	5.03	119.63	111.37
1	D	438	ALA	N-CA-C	5.03	117.41	111.33
1	J	268	THR	N-CA-C	5.03	117.16	109.07
1	F	250	VAL	N-CA-C	5.02	119.79	109.34
1	K	438	ALA	N-CA-C	5.02	117.14	111.11
1	A	191	LEU	N-CA-C	5.02	117.15	109.07
1	L	394	ASN	N-CA-C	5.01	121.47	110.80
1	B	392	GLY	N-CA-C	5.01	120.40	113.99

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.

All (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
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:HD12	1:D:311:LEU:H	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: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
1:H:71:THR:N	1:H:118:GLN:HE22	1.82	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:184:ASN:HB2	1:I:333:MET:HE2	1.67	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:K:328:TYR:HB2	1:K:332:MET:HE1	1.69	0.73
1:G:71:THR:N	1:G:118:GLN:HE22	1.85	0.72
1:K:218:MET:HE3	1:K:223:ARG:HB3	1.71	0.72
1:K:353:LYS:HG2	1:K:354:LYS:H	1.55	0.72
1:G:389:HIS:CE1	1:G:435:MET:HE1	2.25	0.71
1:H:184:ASN:CB	1:I:333:MET:HE2	2.21	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:D:353:LYS:HG2	1:D:354:LYS:N	2.02	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:153:GLU:CD	1:J:153:GLU:H	2.03	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:J:306:PRO:HB2	1:J:308:MET:CE	2.20	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:88:LEU:HD11	1:H:220:TYR:HB2	1.80	0.64
1:H:136:ASN:HD21	1:H:159:LYS:NZ	1.96	0.64
1:J:338:ILE:HG22	1:J:339:TRP:N	2.11	0.64
1:C:283:GLU:HG3	1:C:348:VAL:HG11	1.78	0.64
1:F:389:HIS:CE1	1:F:435:MET:HE1	2.32	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:54:GLY:N	3:A:660:HOH:O	2.31	0.63
1:A:374:ILE:HD11	1:A:393:THR:HG22	1.80	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:308:MET:HE1	1:J:333:MET:HE3	1.82	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:308:MET:HE3	1:L:309:PRO:HD2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:78:TYR:HA	1:J:382:LEU:HD21	1.84	0.60
1:J:338:ILE:N	1:J:338:ILE:HD12	2.17	0.60
1:J:341:ILE:HD11	1:J:350:PHE:CE1	2.37	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: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:H:184:ASN:ND2	1:I:333:MET:HE2	2.18	0.59
1:J:71:THR:N	1:J:118:GLN:NE2	2.44	0.59
1:K:136:ASN:HD21	1:K:159:LYS:HZ3	1.49	0.58
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:H:184:ASN:HB2	1:I:333:MET:CE	2.32	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:308:MET:C	1:E:153:GLU:HG3	2.28	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:H:136:ASN:HD21	1:H:159:LYS:HZ1	1.52	0.58
1:L:310:ASN:C	1:L:311:LEU:HD12	2.29	0.57
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:276:ARG:NH2	1:I:312:MET:HE3	2.19	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:F:308:MET:HE2	1:F:311:LEU:HD22	1.86	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:H:389:HIS:CE1	1:H:435:MET:HE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:J:311:LEU:O	1:J:312:MET:HE2	2.07	0.54
1:K:302:VAL:HB	1:K:339:TRP:HB2	1.89	0.54
1:B:389:HIS:CE1	1:B:435:MET:HE1	2.42	0.54
1:C:337:LYS:C	1:C:338:ILE:HD12	2.32	0.54
1:F:70:HIS:HA	1:F:118:GLN:NE2	2.22	0.54
1:I:389:HIS:CE1	1:I:435:MET:HE1	2.42	0.54
1:J:71:THR:N	1:J:118:GLN:HE22	2.02	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:J:374:ILE:HD11	1:J:393:THR:HG22	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:136:ASN:HD21	1:E:159:LYS:HZ3	1.56	0.53
1:F:374:ILE:O	1:F:375:ALA:HB3	2.08	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:F:207:ALA:HA	1:F:443:MET:HE3	1.90	0.53
1:E:389:HIS:CE1	1:E:435:MET:HE1	2.44	0.52
1:C:136:ASN:HD21	1:C:159:LYS:HZ3	1.57	0.52
1:I:97:THR:O	1:I:101:GLU:HG3	2.09	0.52
1:B:70:HIS:HA	1:B:118:GLN:NE2	2.25	0.52
1:B:151:LYS:HE3	3:E:682:HOH:O	2.09	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:G:276:ARG:NH2	1:G:312:MET:HE3	2.23	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:C:389:HIS:CE1	1:C:435:MET:HE1	2.46	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:A:136:ASN:HD21	1:A:159:LYS:HZ3	1.58	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:F:153:GLU:H	1:F:153:GLU:CD	2.19	0.51
1:I:219:LYS:HD2	1:I:276:ARG:NE	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:312:MET:HA	1:D:312:MET:HE2	1.92	0.51
1:J:70:HIS:HA	1:J:118:GLN:HE21	1.76	0.51
1:J:70:HIS:CD2	1:J:199:LEU:HB3	2.46	0.51
1:F:118:GLN:HG3	3:F:605:HOH:O	2.11	0.50
1:I:308:MET:HE3	1:I:308:MET:HA	1.93	0.50
1:A:70:HIS:HA	1:A:118:GLN:NE2	2.26	0.50
1:D:317:TRP:HE3	1:D:332:MET:HB2	1.76	0.50
1:F:276:ARG:NH2	1:F:312:MET:HE3	2.27	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
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:I:153:GLU:CD	1:I:153:GLU:H	2.20	0.50
1:J:336:LEU:N	1:J:336:LEU:HD12	2.26	0.50
1:A:337:LYS:C	1:A:338:ILE:HD12	2.36	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:F:250:VAL:HG13	1:F:251:GLY:N	2.26	0.49
1:H:184:ASN:HD22	1:I:333:MET:HE2	1.77	0.49
1:K:147:LEU:HA	1:K:148:PRO:C	2.37	0.49
1:B:302:VAL:HB	1:B:339:TRP:HB2	1.94	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:B:337:LYS:C	1:B:338:ILE:HD12	2.38	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:K:328:TYR:HD1	1:K:332:MET:HE3	1.77	0.49
1:L:136:ASN:HD21	1:L:159:LYS:HZ3	1.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:311:LEU:N	1:G:311:LEU:HD12	2.28	0.49
1:L:88:LEU:HD11	1:L:220:TYR:CB	2.41	0.48
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: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:C:328:TYR:HB2	1:C:332:MET:HE3	1.96	0.48
1:D:136:ASN:HD21	1:D:159:LYS:HZ3	1.60	0.48
1:D:250:VAL:HG13	1:D:251:GLY:N	2.28	0.48
1:F:147:LEU:HA	1:F:148:PRO:C	2.38	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
1:A:328:TYR:HB2	1:A:332:MET:HE3	1.96	0.48
1:D:367:LYS:HZ1	1:D:452:LYS:HE3	1.78	0.48
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:L:218:MET:HE2	1:L:218:MET:HA	1.96	0.48
1:B:346:LYS:HA	1:B:347:PRO:C	2.39	0.48
1:G:380:ASN:HB2	1:H:190:PRO:HB3	1.95	0.48
1:H:328:TYR:HB2	1:H:332:MET:HE3	1.95	0.48
1:I:328:TYR:HB2	1:I:332:MET:HE3	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:GLU:CD	1:D:153:GLU:H	2.21	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:C:147:LEU:HA	1:C:148:PRO:C	2.39	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:J:389:HIS:CE1	1:J:435:MET:HE1	2.49	0.47
1:A:313:HIS:HB2	1:A:315:ASP:OD1	2.14	0.47
1:B:147:LEU:HA	1:B:148:PRO:C	2.39	0.47
1:F:313:HIS:HB2	1:F:315:ASP:OD1	2.15	0.47
1:F:328:TYR:HB2	1:F:332:MET:HE3	1.95	0.47
1:A:309:PRO:N	1:E:153:GLU:HG3	2.30	0.47
1:B:153:GLU:CD	1:B:153:GLU:H	2.23	0.47
1:E:374:ILE:O	1:E:375:ALA:HB3	2.14	0.47
1:G:175:MET:HB3	1:G:199:LEU:CD1	2.45	0.47
1:G:328:TYR:HB2	1:G:332:MET:HE3	1.97	0.47
1:I:136:ASN:HD21	1:I:159:LYS:HZ3	1.62	0.47
1:J:337:LYS:C	1:J:338:ILE:HD12	2.40	0.47
1:K:136:ASN:HD21	1:K:159:LYS:HZ1	1.62	0.47
1:K:374:ILE:HD11	1:K:393:THR:HG22	1.97	0.47
1:L:153:GLU:CD	1:L:153:GLU:H	2.22	0.47
1:C:70:HIS:HA	1:C:118:GLN:HE21	1.80	0.47
1:I:337:LYS:C	1:I:338:ILE:HD12	2.40	0.47
1:J:356:THR:O	1:J:360:VAL:HG23	2.14	0.47
1:K:389:HIS:CE1	1:K:435:MET:HE1	2.49	0.47
1:D:389:HIS:CE1	1:D:435:MET:HE1	2.50	0.47
1:B:88:LEU:HD11	1:B:220:TYR:CB	2.45	0.46
1:B:361:LEU:HD12	1:B:371:LEU:HD21	1.96	0.46
1:E:147:LEU:HA	1:E:148:PRO:C	2.40	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:B:306:PRO:HB2	1:B:308:MET:HE2	1.97	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:J:213:VAL:HG11	1:J:234:PHE:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:ILE:CG2	1:C:339:TRP:N	2.78	0.46
1:G:250:VAL:HG13	1:G:251:GLY:N	2.30	0.46
1:J:222:THR:HB	3:J:642:HOH:O	2.16	0.46
1:A:147:LEU:HA	1:A:148:PRO:C	2.40	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:70:HIS:HA	1:I:118:GLN:NE2	2.30	0.46
1:I:320:MET:HG3	1:I:326:PHE:CE2	2.51	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:G:147:LEU:HA	1:G:148:PRO:C	2.41	0.46
1:K:136:ASN:ND2	1:K:159:LYS:NZ	2.62	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:B:140:GLU:OE2	1:B:159:LYS:NZ	2.49	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:O	1:C:348:VAL:HG13	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:H:184:ASN:CG	1:I:333:MET:HE2	2.42	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:L:328:TYR:HB2	1:L:332:MET:HE3	1.99	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:G:136:ASN:HD21	1:G:159:LYS:HZ3	1.63	0.45
1:I:336:LEU:HB3	1:I:338:ILE:CD1	2.46	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:A:183:LEU:HD12	1:A:192:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:328:TYR:HB2	1:B:332:MET:HE3	1.98	0.44
1:I:218:MET:HE2	1:I:218:MET:HA	1.99	0.44
1:K:263:ILE:HD12	1:K:263:ILE:N	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:J:305:VAL:HG13	1:J:311:LEU:HD21	1.98	0.44
1:B:136:ASN:HD21	1:B:159:LYS:HZ1	1.64	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:G:206:PHE:CD1	1:G:206:PHE:C	2.96	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:I:147:LEU:HA	1:I:148:PRO:C	2.42	0.44
1:J:213:VAL:HG13	1:J:243:THR:HG21	2.00	0.44
1:D:337:LYS:C	1:D:338:ILE:HD12	2.42	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:250:VAL:HG13	1:C:251:GLY:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:190:PRO:HG3	1:L:382:LEU:HB2	2.00	0.44
1:L:179:LEU:HD23	1:L:191:LEU:HD23	2.00	0.44
1:C:88:LEU:HD11	1:C:220:TYR:CB	2.47	0.44
1:A:389:HIS:CE1	1:A:435:MET:HE1	2.53	0.44
1:D:218:MET:HE2	1:D:218:MET:HA	2.00	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:E:153:GLU:CD	1:E:153:GLU:H	2.26	0.43
1:E:218:MET:HE2	1:E:218:MET:HA	2.00	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:L:136:ASN:HD21	1:L:159:LYS:HZ1	1.66	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:E:312:MET:HE2	1:E:313:HIS:NE2	2.33	0.43
1:J:336:LEU:CB	1:J:338:ILE:HD11	2.48	0.43
1:B:207:ALA:HA	1:B:443:MET:HE3	2.00	0.43
1:D:306:PRO:HG2	1:D:317:TRP:CZ2	2.52	0.43
1:H:85:GLU:HB2	3:H:716:HOH:O	2.19	0.43
1:H:250:VAL:HG13	1:H:251:GLY:N	2.33	0.43
1:J:64:LEU:HD23	1:J:114:ILE:HD13	2.01	0.43
1:L:147:LEU:HA	1:L:148:PRO:C	2.42	0.43
1:L:345:VAL:HG12	1:L:346:LYS:N	2.32	0.43
1:E:183:LEU:O	1:E:184:ASN:HB2	2.18	0.43
1:H:337:LYS:C	1:H:338:ILE:HD12	2.43	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:O	1:B:275:GLU:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:147:LEU:HA	1:H:148:PRO:C	2.44	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: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:88:LEU:HD11	1:H:220:TYR:CB	2.48	0.43
1:H:414:LYS:O	1:H:418:GLU:HG3	2.19	0.43
1:C:136:ASN:HD21	1:C:159:LYS:HZ1	1.62	0.42
1:C:220:TYR:HA	1:C:221:PRO:HD3	1.95	0.42
1:E:276:ARG:HG3	1:E:313:HIS:CE1	2.54	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:C:173:LYS:NZ	1:C:182:GLU:OE2	2.49	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:F:337:LYS:C	1:F:338:ILE:HD12	2.44	0.42
1:F:338:ILE:HG23	1:F:339:TRP:N	2.34	0.42
1:J:216:ASN:HB3	1:J:256:ILE:O	2.20	0.42
1:J:237:ASN:O	1:J:241:LYS:HB2	2.19	0.42
1:B:276:ARG:HG3	1:B:276:ARG:HH11	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:F:136:ASN:HD21	1:F:159:LYS:HZ1	1.68	0.42
1:J:257:GLU:HG3	1:J:276:ARG:HB3	2.02	0.42
1:D:310:ASN:HD22	1:D:311:LEU:CD1	2.33	0.42
1:H:77:ARG:NH2	1:H:96:ASP:OD1	2.53	0.42
1:H:248:ASP:OD1	1:H:249:ILE:N	2.50	0.42
1:K:326:PHE:CD1	1:K:326:PHE:N	2.88	0.42
1:J:152:LYS:HG3	1:J:153:GLU:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:C:276:ARG:HG3	1.85	0.41
1:D:147:LEU:HA	1:D:148:PRO:C	2.44	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
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: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:F:308:MET:HE2	1:F:311:LEU:CD2	2.49	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:E:190:PRO:HB3	1:F:380:ASN:HB2	2.02	0.41
1:J:147:LEU:HA	1:J:148:PRO:C	2.45	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: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:H:62:GLY:O	1:H:63:GLU:C	2.64	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:206:PHE:CD1	1:B:206:PHE:C	2.98	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: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:173:LYS:NZ	1:D:182:GLU:OE2	2.43	0.41
1:G:153:GLU:CD	1:G:153:GLU:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:LYS:HZ1	1:C:452:LYS:HE3	1.84	0.41
1:D:171:VAL:O	1:D:175:MET:HG3	2.21	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:I:142:TYR:CG	1:I:174:MET:HE3	2.55	0.41
1:K:61:ILE:HG22	1:K:397:THR:HG21	2.03	0.41
1:K:179:LEU:HD23	1:K:191:LEU:HD23	2.02	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:70:HIS:HB3	1:H:200:TYR:HA	2.03	0.41
1:H:135:ARG:O	1:H:138:PHE:HB3	2.21	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
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:F:206:PHE:CD1	1:F:206:PHE:C	2.98	0.40
1:H:153:GLU:CD	1:H:153:GLU:H	2.29	0.40
1:I:206:PHE:CD1	1:I:206:PHE:C	2.99	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:J:374:ILE:O	1:J:375:ALA:HB3	2.20	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:D:328:TYR:HB2	1:D:332:MET:HE3	2.02	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:G:337:LYS:C	1:G:338:ILE:HD12	2.47	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:70:HIS:HB3	1:B:200:TYR:HA	2.04	0.40
1:B:353:LYS:HD3	1:B:354:LYS:N	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:283:GLU:HG3	1:G:348:VAL:CG1	2.43	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: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%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	GLU
1	A	269	LEU
1	A	348	VAL
1	B	153	GLU
1	B	269	LEU
1	B	317	TRP
1	B	349	LYS
1	C	153	GLU
1	C	269	LEU
1	C	312	MET
1	D	218	MET
1	D	269	LEU
1	D	310	ASN
1	D	417	VAL
1	E	153	GLU
1	E	217	CYS
1	E	218	MET
1	E	269	LEU
1	F	153	GLU
1	F	269	LEU
1	F	317	TRP
1	G	153	GLU
1	G	269	LEU
1	G	317	TRP
1	G	417	VAL
1	H	153	GLU
1	H	269	LEU
1	H	348	VAL
1	I	153	GLU
1	I	269	LEU
1	I	308	MET
1	J	153	GLU
1	J	317	TRP
1	K	153	GLU
1	K	338	ILE
1	L	153	GLU
1	L	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	118	GLN

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Mol	Chain	Res	Type
1	A	136	ASN
1	A	181	ASN
1	A	288	ASN
1	A	381	GLN
1	B	56	ASN
1	B	110	GLN
1	B	118	GLN
1	B	136	ASN
1	B	181	ASN
1	B	242	ASN
1	B	273	ASN
1	B	288	ASN
1	B	389	HIS
1	C	118	GLN
1	C	136	ASN
1	C	169	GLN
1	C	181	ASN
1	C	216	ASN
1	C	242	ASN
1	C	253	ASN
1	C	273	ASN
1	C	288	ASN
1	C	304	ASN
1	C	310	ASN
1	C	381	GLN
1	D	118	GLN
1	D	136	ASN
1	D	181	ASN
1	D	198	ASN
1	D	288	ASN
1	D	310	ASN
1	D	331	ASN
1	D	413	GLN
1	E	118	GLN
1	E	136	ASN
1	E	169	GLN
1	E	181	ASN
1	E	198	ASN
1	E	216	ASN
1	E	242	ASN
1	E	273	ASN
1	E	288	ASN

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Mol	Chain	Res	Type
1	E	304	ASN
1	E	310	ASN
1	F	118	GLN
1	F	136	ASN
1	F	181	ASN
1	F	273	ASN
1	F	288	ASN
1	F	304	ASN
1	F	310	ASN
1	F	331	ASN
1	G	110	GLN
1	G	118	GLN
1	G	136	ASN
1	G	181	ASN
1	G	198	ASN
1	G	273	ASN
1	G	288	ASN
1	G	304	ASN
1	H	112	ASN
1	H	118	GLN
1	H	136	ASN
1	H	181	ASN
1	H	184	ASN
1	H	187	GLN
1	H	242	ASN
1	H	288	ASN
1	H	313	HIS
1	H	331	ASN
1	H	389	HIS
1	I	56	ASN
1	I	118	GLN
1	I	136	ASN
1	I	181	ASN
1	I	273	ASN
1	I	288	ASN
1	I	304	ASN
1	I	331	ASN
1	I	389	HIS
1	J	110	GLN
1	J	118	GLN
1	J	136	ASN
1	J	198	ASN

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Mol	Chain	Res	Type
1	J	273	ASN
1	J	288	ASN
1	J	304	ASN
1	J	331	ASN
1	J	389	HIS
1	K	110	GLN
1	K	118	GLN
1	K	136	ASN
1	K	181	ASN
1	K	253	ASN
1	K	273	ASN
1	K	288	ASN
1	K	381	GLN
1	K	413	GLN
1	L	118	GLN
1	L	136	ASN
1	L	181	ASN
1	L	198	ASN
1	L	273	ASN
1	L	288	ASN
1	L	290	GLN
1	L	304	ASN
1	L	331	ASN
1	L	413	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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%)	-0.40	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

All (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
1	D	331	ASN	5.3
1	G	311	LEU	5.1
1	K	452	LYS	5.1
1	C	186	LYS	5.0
1	D	220	TYR	4.7
1	J	220	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	220	TYR	4.6
1	G	91	ALA	4.5
1	L	332	MET	4.5
1	G	185	ILE	4.5
1	L	220	TYR	4.4
1	D	332	MET	4.4
1	G	154	ILE	4.4
1	F	333	MET	4.4
1	J	91	ALA	4.3
1	A	452	LYS	4.3
1	L	91	ALA	4.3
1	C	452	LYS	4.3
1	I	333	MET	4.2
1	B	312	MET	4.2
1	J	333	MET	4.2
1	H	154	ILE	4.1
1	I	250	VAL	4.1
1	G	348	VAL	4.1
1	H	151	LYS	4.1
1	A	184	ASN	4.1
1	B	250	VAL	4.0
1	F	452	LYS	4.0
1	C	185	ILE	4.0
1	G	333	MET	3.9
1	H	185	ILE	3.9
1	G	309	PRO	3.9
1	I	309	PRO	3.9
1	C	220	TYR	3.9
1	L	331	ASN	3.9
1	A	220	TYR	3.8
1	B	91	ALA	3.8
1	E	452	LYS	3.7
1	I	452	LYS	3.7
1	I	332	MET	3.7
1	K	220	TYR	3.7
1	I	347	PRO	3.7
1	J	452	LYS	3.7
1	G	184	ASN	3.6
1	D	309	PRO	3.6
1	J	347	PRO	3.5
1	I	307	PRO	3.5
1	J	338	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	221	PRO	3.4
1	H	452	LYS	3.4
1	I	334	ASN	3.4
1	D	452	LYS	3.4
1	F	220	TYR	3.4
1	G	152	LYS	3.4
1	H	220	TYR	3.4
1	G	222	THR	3.4
1	I	349	LYS	3.4
1	G	221	PRO	3.4
1	F	222	THR	3.4
1	G	151	LYS	3.3
1	G	250	VAL	3.3
1	F	221	PRO	3.3
1	L	317	TRP	3.3
1	J	88	LEU	3.2
1	I	317	TRP	3.2
1	G	88	LEU	3.2
1	G	452	LYS	3.2
1	I	311	LEU	3.2
1	B	338	ILE	3.2
1	K	91	ALA	3.1
1	D	338	ILE	3.1
1	K	221	PRO	3.1
1	H	338	ILE	3.1
1	L	308	MET	3.1
1	L	221	PRO	3.1
1	E	184	ASN	3.1
1	B	347	PRO	3.1
1	I	335	VAL	3.1
1	J	221	PRO	3.0
1	I	220	TYR	3.0
1	G	338	ILE	3.0
1	L	334	ASN	3.0
1	I	345	VAL	3.0
1	G	349	LYS	3.0
1	H	334	ASN	3.0
1	E	334	ASN	3.0
1	I	338	ILE	2.9
1	D	334	ASN	2.9
1	L	88	LEU	2.9
1	E	217	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	153	GLU	2.9
1	E	250	VAL	2.9
1	G	331	ASN	2.9
1	J	350	PHE	2.9
1	I	348	VAL	2.9
1	D	275	GLU	2.9
1	G	353	LYS	2.8
1	H	133	GLU	2.8
1	J	293	LYS	2.8
1	B	221	PRO	2.8
1	G	345	VAL	2.8
1	I	310	ASN	2.8
1	J	309	PRO	2.8
1	H	152	LYS	2.8
1	D	250	VAL	2.8
1	D	345	VAL	2.8
1	J	345	VAL	2.8
1	J	348	VAL	2.8
1	E	275	GLU	2.7
1	F	181	ASN	2.7
1	G	317	TRP	2.7
1	F	88	LEU	2.7
1	G	87	LEU	2.7
1	H	150	LEU	2.7
1	B	452	LYS	2.7
1	G	90	SER	2.7
1	H	153	GLU	2.7
1	H	293	LYS	2.7
1	L	293	LYS	2.7
1	I	346	LYS	2.7
1	B	309	PRO	2.7
1	D	347	PRO	2.7
1	J	336	LEU	2.7
1	C	250	VAL	2.6
1	L	222	THR	2.6
1	G	183	LEU	2.6
1	K	181	ASN	2.6
1	H	250	VAL	2.6
1	E	221	PRO	2.6
1	B	87	LEU	2.6
1	D	129	LEU	2.6
1	J	349	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	309	PRO	2.6
1	I	331	ASN	2.6
1	A	250	VAL	2.6
1	F	338	ILE	2.6
1	D	349	LYS	2.6
1	L	452	LYS	2.6
1	G	133	GLU	2.5
1	G	339	TRP	2.5
1	C	222	THR	2.5
1	G	219	LYS	2.5
1	E	218	MET	2.5
1	J	312	MET	2.5
1	I	184	ASN	2.5
1	G	279	PHE	2.5
1	J	133	GLU	2.5
1	E	349	LYS	2.5
1	F	310	ASN	2.5
1	B	222	THR	2.5
1	E	85	GLU	2.5
1	I	350	PHE	2.5
1	L	86	GLU	2.5
1	J	154	ILE	2.5
1	K	185	ILE	2.5
1	L	250	VAL	2.5
1	D	353	LYS	2.5
1	G	132	LYS	2.5
1	G	310	ASN	2.5
1	G	334	ASN	2.5
1	J	181	ASN	2.5
1	E	222	THR	2.4
1	E	276	ARG	2.4
1	J	185	ILE	2.4
1	I	336	LEU	2.4
1	D	310	ASN	2.4
1	J	152	LYS	2.4
1	B	88	LEU	2.4
1	B	331	ASN	2.4
1	J	184	ASN	2.4
1	B	133	GLU	2.4
1	F	91	ALA	2.4
1	D	88	LEU	2.4
1	J	331	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	286	ALA	2.4
1	G	89	PHE	2.4
1	F	133	GLU	2.4
1	G	344	ASN	2.3
1	J	334	ASN	2.3
1	B	349	LYS	2.3
1	B	353	LYS	2.3
1	E	219	LYS	2.3
1	L	353	LYS	2.3
1	G	308	MET	2.3
1	I	133	GLU	2.3
1	C	184	ASN	2.3
1	C	334	ASN	2.3
1	E	331	ASN	2.3
1	A	353	LYS	2.3
1	I	222	THR	2.3
1	F	348	VAL	2.3
1	J	250	VAL	2.3
1	K	250	VAL	2.3
1	G	343	LEU	2.3
1	L	87	LEU	2.3
1	F	307	PRO	2.3
1	J	341	ILE	2.3
1	G	335	VAL	2.3
1	H	188	ASP	2.3
1	J	291	ALA	2.3
1	D	335	VAL	2.3
1	J	153	GLU	2.2
1	E	353	LYS	2.2
1	F	89	PHE	2.2
1	B	334	ASN	2.2
1	C	181	ASN	2.2
1	G	347	PRO	2.2
1	L	307	PRO	2.2
1	G	300	ILE	2.2
1	I	341	ILE	2.2
1	F	134	VAL	2.2
1	L	348	VAL	2.2
1	F	353	LYS	2.2
1	D	181	ASN	2.2
1	F	351	VAL	2.2
1	F	308	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	181	ASN	2.2
1	J	89	PHE	2.2
1	J	308	MET	2.2
1	K	184	ASN	2.2
1	L	310	ASN	2.2
1	H	186	LYS	2.2
1	H	349	LYS	2.2
1	B	181	ASN	2.1
1	D	308	MET	2.1
1	D	348	VAL	2.1
1	F	188	ASP	2.1
1	J	335	VAL	2.1
1	F	219	LYS	2.1
1	H	85	GLU	2.1
1	I	293	LYS	2.1
1	J	219	LYS	2.1
1	B	251	GLY	2.1
1	B	152	LYS	2.1
1	F	349	LYS	2.1
1	F	339	TRP	2.1
1	J	351	VAL	2.1
1	G	54	GLY	2.1
1	J	217	CYS	2.1
1	D	91	ALA	2.1
1	A	133	GLU	2.1
1	C	187	GLN	2.1
1	I	279	PHE	2.1
1	I	54	GLY	2.1
1	G	180	ALA	2.1
1	G	312	MET	2.1
1	F	336	LEU	2.1
1	I	357	LEU	2.1
1	F	334	ASN	2.1
1	G	282	ILE	2.1
1	J	279	PHE	2.1
1	J	346	LYS	2.0
1	K	186	LYS	2.0
1	F	86	GLU	2.0
1	B	269	LEU	2.0
1	D	132	LYS	2.0
1	I	308	MET	2.0
1	L	181	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	309	PRO	2.0
1	G	341	ILE	2.0
1	D	152	LYS	2.0
1	I	353	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 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, 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($\text{\AA}^2$)	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.