



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2021 – 02:11 PM EDT

PDB ID : 7LBA
Title : E. coli Agmatinase
Authors : Chitrakar, I.; Ahmed, S.F.; Torelli, A.T.; French, J.B.
Deposited on : 2021-01-07
Resolution : 2.20 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	:	2.17.1
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)	:	2.17.1

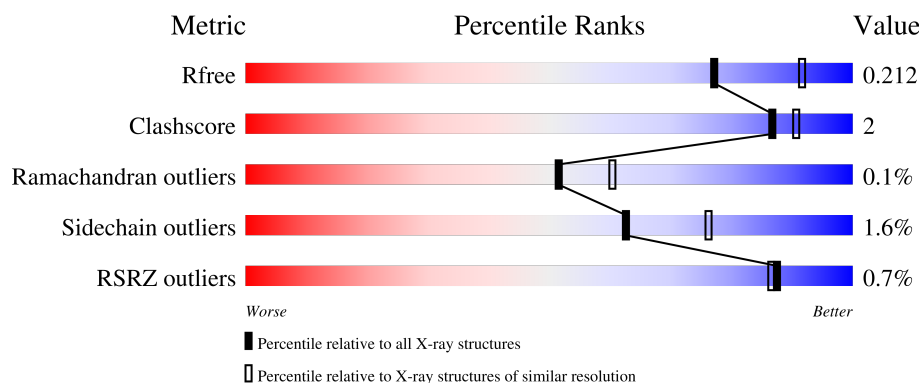
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	329	 88% 7%
1	B	329	 88% 6% 6%
1	C	329	 85% 7% 7%
1	D	329	 87% 5% 8%
1	E	329	 85% 8% 6%

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Mol	Chain	Length	Quality of chain
1	F	329	 85%7%8%
1	G	329	 85%7%7%
1	H	329	 85%7%8%
1	I	329	 86%7%7%
1	J	329	 88%.8%
1	K	329	 86%8%6%
1	L	329	 87%5%8%
1	M	329	 %87%5%8%
1	N	329	 %84%8%8%
1	O	329	 %84%9%7%
1	P	329	 2%85%7%8%
1	Q	329	 3%84%9%8%
1	R	329	 2%85%6%9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 43547 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 Agmatinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2347	1485	406	442	14			
1	B	310	Total	C	N	O	S	0	0	0
			2399	1520	414	450	15			
1	C	305	Total	C	N	O	S	0	0	0
			2350	1487	406	442	15			
1	D	303	Total	C	N	O	S	0	0	0
			2337	1479	403	440	15			
1	E	309	Total	C	N	O	S	0	0	0
			2391	1516	412	448	15			
1	F	302	Total	C	N	O	S	0	0	0
			2329	1474	402	439	14			
1	G	305	Total	C	N	O	S	0	0	0
			2347	1485	406	442	14			
1	H	303	Total	C	N	O	S	0	0	0
			2337	1479	403	440	15			
1	I	305	Total	C	N	O	S	0	0	0
			2350	1487	406	442	15			
1	J	303	Total	C	N	O	S	0	0	0
			2337	1479	403	440	15			
1	K	310	Total	C	N	O	S	0	0	0
			2399	1520	414	450	15			
1	L	302	Total	C	N	O	S	0	0	0
			2329	1474	402	439	14			
1	M	304	Total	C	N	O	S	0	0	0
			2342	1482	405	441	14			
1	N	303	Total	C	N	O	S	0	0	0
			2337	1479	403	440	15			
1	O	305	Total	C	N	O	S	0	0	0
			2350	1487	406	442	15			
1	P	303	Total	C	N	O	S	0	0	0
			2333	1476	402	440	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	303	Total	C	N	O	S	0	0	0
			2337	1479	403	440	15			
1	R	301	Total	C	N	O	S	0	0	0
			2320	1468	400	438	14			

There are 414 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP S0XV43
A	-21	GLY	-	expression tag	UNP S0XV43
A	-20	SER	-	expression tag	UNP S0XV43
A	-19	ASP	-	expression tag	UNP S0XV43
A	-18	LYS	-	expression tag	UNP S0XV43
A	-17	ILE	-	expression tag	UNP S0XV43
A	-16	HIS	-	expression tag	UNP S0XV43
A	-15	HIS	-	expression tag	UNP S0XV43
A	-14	HIS	-	expression tag	UNP S0XV43
A	-13	HIS	-	expression tag	UNP S0XV43
A	-12	HIS	-	expression tag	UNP S0XV43
A	-11	HIS	-	expression tag	UNP S0XV43
A	-10	SER	-	expression tag	UNP S0XV43
A	-9	SER	-	expression tag	UNP S0XV43
A	-8	GLY	-	expression tag	UNP S0XV43
A	-7	GLU	-	expression tag	UNP S0XV43
A	-6	ASN	-	expression tag	UNP S0XV43
A	-5	LEU	-	expression tag	UNP S0XV43
A	-4	TYR	-	expression tag	UNP S0XV43
A	-3	PHE	-	expression tag	UNP S0XV43
A	-2	GLN	-	expression tag	UNP S0XV43
A	-1	GLY	-	expression tag	UNP S0XV43
A	0	HIS	-	expression tag	UNP S0XV43
B	-22	MET	-	initiating methionine	UNP S0XV43
B	-21	GLY	-	expression tag	UNP S0XV43
B	-20	SER	-	expression tag	UNP S0XV43
B	-19	ASP	-	expression tag	UNP S0XV43
B	-18	LYS	-	expression tag	UNP S0XV43
B	-17	ILE	-	expression tag	UNP S0XV43
B	-16	HIS	-	expression tag	UNP S0XV43
B	-15	HIS	-	expression tag	UNP S0XV43
B	-14	HIS	-	expression tag	UNP S0XV43
B	-13	HIS	-	expression tag	UNP S0XV43
B	-12	HIS	-	expression tag	UNP S0XV43

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP S0XV43
B	-10	SER	-	expression tag	UNP S0XV43
B	-9	SER	-	expression tag	UNP S0XV43
B	-8	GLY	-	expression tag	UNP S0XV43
B	-7	GLU	-	expression tag	UNP S0XV43
B	-6	ASN	-	expression tag	UNP S0XV43
B	-5	LEU	-	expression tag	UNP S0XV43
B	-4	TYR	-	expression tag	UNP S0XV43
B	-3	PHE	-	expression tag	UNP S0XV43
B	-2	GLN	-	expression tag	UNP S0XV43
B	-1	GLY	-	expression tag	UNP S0XV43
B	0	HIS	-	expression tag	UNP S0XV43
C	-22	MET	-	initiating methionine	UNP S0XV43
C	-21	GLY	-	expression tag	UNP S0XV43
C	-20	SER	-	expression tag	UNP S0XV43
C	-19	ASP	-	expression tag	UNP S0XV43
C	-18	LYS	-	expression tag	UNP S0XV43
C	-17	ILE	-	expression tag	UNP S0XV43
C	-16	HIS	-	expression tag	UNP S0XV43
C	-15	HIS	-	expression tag	UNP S0XV43
C	-14	HIS	-	expression tag	UNP S0XV43
C	-13	HIS	-	expression tag	UNP S0XV43
C	-12	HIS	-	expression tag	UNP S0XV43
C	-11	HIS	-	expression tag	UNP S0XV43
C	-10	SER	-	expression tag	UNP S0XV43
C	-9	SER	-	expression tag	UNP S0XV43
C	-8	GLY	-	expression tag	UNP S0XV43
C	-7	GLU	-	expression tag	UNP S0XV43
C	-6	ASN	-	expression tag	UNP S0XV43
C	-5	LEU	-	expression tag	UNP S0XV43
C	-4	TYR	-	expression tag	UNP S0XV43
C	-3	PHE	-	expression tag	UNP S0XV43
C	-2	GLN	-	expression tag	UNP S0XV43
C	-1	GLY	-	expression tag	UNP S0XV43
C	0	HIS	-	expression tag	UNP S0XV43
D	-22	MET	-	initiating methionine	UNP S0XV43
D	-21	GLY	-	expression tag	UNP S0XV43
D	-20	SER	-	expression tag	UNP S0XV43
D	-19	ASP	-	expression tag	UNP S0XV43
D	-18	LYS	-	expression tag	UNP S0XV43
D	-17	ILE	-	expression tag	UNP S0XV43
D	-16	HIS	-	expression tag	UNP S0XV43

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	HIS	-	expression tag	UNP S0XV43
D	-14	HIS	-	expression tag	UNP S0XV43
D	-13	HIS	-	expression tag	UNP S0XV43
D	-12	HIS	-	expression tag	UNP S0XV43
D	-11	HIS	-	expression tag	UNP S0XV43
D	-10	SER	-	expression tag	UNP S0XV43
D	-9	SER	-	expression tag	UNP S0XV43
D	-8	GLY	-	expression tag	UNP S0XV43
D	-7	GLU	-	expression tag	UNP S0XV43
D	-6	ASN	-	expression tag	UNP S0XV43
D	-5	LEU	-	expression tag	UNP S0XV43
D	-4	TYR	-	expression tag	UNP S0XV43
D	-3	PHE	-	expression tag	UNP S0XV43
D	-2	GLN	-	expression tag	UNP S0XV43
D	-1	GLY	-	expression tag	UNP S0XV43
D	0	HIS	-	expression tag	UNP S0XV43
E	-22	MET	-	initiating methionine	UNP S0XV43
E	-21	GLY	-	expression tag	UNP S0XV43
E	-20	SER	-	expression tag	UNP S0XV43
E	-19	ASP	-	expression tag	UNP S0XV43
E	-18	LYS	-	expression tag	UNP S0XV43
E	-17	ILE	-	expression tag	UNP S0XV43
E	-16	HIS	-	expression tag	UNP S0XV43
E	-15	HIS	-	expression tag	UNP S0XV43
E	-14	HIS	-	expression tag	UNP S0XV43
E	-13	HIS	-	expression tag	UNP S0XV43
E	-12	HIS	-	expression tag	UNP S0XV43
E	-11	HIS	-	expression tag	UNP S0XV43
E	-10	SER	-	expression tag	UNP S0XV43
E	-9	SER	-	expression tag	UNP S0XV43
E	-8	GLY	-	expression tag	UNP S0XV43
E	-7	GLU	-	expression tag	UNP S0XV43
E	-6	ASN	-	expression tag	UNP S0XV43
E	-5	LEU	-	expression tag	UNP S0XV43
E	-4	TYR	-	expression tag	UNP S0XV43
E	-3	PHE	-	expression tag	UNP S0XV43
E	-2	GLN	-	expression tag	UNP S0XV43
E	-1	GLY	-	expression tag	UNP S0XV43
E	0	HIS	-	expression tag	UNP S0XV43
F	-22	MET	-	initiating methionine	UNP S0XV43
F	-21	GLY	-	expression tag	UNP S0XV43
F	-20	SER	-	expression tag	UNP S0XV43

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	ASP	-	expression tag	UNP S0XV43
F	-18	LYS	-	expression tag	UNP S0XV43
F	-17	ILE	-	expression tag	UNP S0XV43
F	-16	HIS	-	expression tag	UNP S0XV43
F	-15	HIS	-	expression tag	UNP S0XV43
F	-14	HIS	-	expression tag	UNP S0XV43
F	-13	HIS	-	expression tag	UNP S0XV43
F	-12	HIS	-	expression tag	UNP S0XV43
F	-11	HIS	-	expression tag	UNP S0XV43
F	-10	SER	-	expression tag	UNP S0XV43
F	-9	SER	-	expression tag	UNP S0XV43
F	-8	GLY	-	expression tag	UNP S0XV43
F	-7	GLU	-	expression tag	UNP S0XV43
F	-6	ASN	-	expression tag	UNP S0XV43
F	-5	LEU	-	expression tag	UNP S0XV43
F	-4	TYR	-	expression tag	UNP S0XV43
F	-3	PHE	-	expression tag	UNP S0XV43
F	-2	GLN	-	expression tag	UNP S0XV43
F	-1	GLY	-	expression tag	UNP S0XV43
F	0	HIS	-	expression tag	UNP S0XV43
G	-22	MET	-	initiating methionine	UNP S0XV43
G	-21	GLY	-	expression tag	UNP S0XV43
G	-20	SER	-	expression tag	UNP S0XV43
G	-19	ASP	-	expression tag	UNP S0XV43
G	-18	LYS	-	expression tag	UNP S0XV43
G	-17	ILE	-	expression tag	UNP S0XV43
G	-16	HIS	-	expression tag	UNP S0XV43
G	-15	HIS	-	expression tag	UNP S0XV43
G	-14	HIS	-	expression tag	UNP S0XV43
G	-13	HIS	-	expression tag	UNP S0XV43
G	-12	HIS	-	expression tag	UNP S0XV43
G	-11	HIS	-	expression tag	UNP S0XV43
G	-10	SER	-	expression tag	UNP S0XV43
G	-9	SER	-	expression tag	UNP S0XV43
G	-8	GLY	-	expression tag	UNP S0XV43
G	-7	GLU	-	expression tag	UNP S0XV43
G	-6	ASN	-	expression tag	UNP S0XV43
G	-5	LEU	-	expression tag	UNP S0XV43
G	-4	TYR	-	expression tag	UNP S0XV43
G	-3	PHE	-	expression tag	UNP S0XV43
G	-2	GLN	-	expression tag	UNP S0XV43
G	-1	GLY	-	expression tag	UNP S0XV43

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP S0XV43
H	-22	MET	-	initiating methionine	UNP S0XV43
H	-21	GLY	-	expression tag	UNP S0XV43
H	-20	SER	-	expression tag	UNP S0XV43
H	-19	ASP	-	expression tag	UNP S0XV43
H	-18	LYS	-	expression tag	UNP S0XV43
H	-17	ILE	-	expression tag	UNP S0XV43
H	-16	HIS	-	expression tag	UNP S0XV43
H	-15	HIS	-	expression tag	UNP S0XV43
H	-14	HIS	-	expression tag	UNP S0XV43
H	-13	HIS	-	expression tag	UNP S0XV43
H	-12	HIS	-	expression tag	UNP S0XV43
H	-11	HIS	-	expression tag	UNP S0XV43
H	-10	SER	-	expression tag	UNP S0XV43
H	-9	SER	-	expression tag	UNP S0XV43
H	-8	GLY	-	expression tag	UNP S0XV43
H	-7	GLU	-	expression tag	UNP S0XV43
H	-6	ASN	-	expression tag	UNP S0XV43
H	-5	LEU	-	expression tag	UNP S0XV43
H	-4	TYR	-	expression tag	UNP S0XV43
H	-3	PHE	-	expression tag	UNP S0XV43
H	-2	GLN	-	expression tag	UNP S0XV43
H	-1	GLY	-	expression tag	UNP S0XV43
H	0	HIS	-	expression tag	UNP S0XV43
I	-22	MET	-	initiating methionine	UNP S0XV43
I	-21	GLY	-	expression tag	UNP S0XV43
I	-20	SER	-	expression tag	UNP S0XV43
I	-19	ASP	-	expression tag	UNP S0XV43
I	-18	LYS	-	expression tag	UNP S0XV43
I	-17	ILE	-	expression tag	UNP S0XV43
I	-16	HIS	-	expression tag	UNP S0XV43
I	-15	HIS	-	expression tag	UNP S0XV43
I	-14	HIS	-	expression tag	UNP S0XV43
I	-13	HIS	-	expression tag	UNP S0XV43
I	-12	HIS	-	expression tag	UNP S0XV43
I	-11	HIS	-	expression tag	UNP S0XV43
I	-10	SER	-	expression tag	UNP S0XV43
I	-9	SER	-	expression tag	UNP S0XV43
I	-8	GLY	-	expression tag	UNP S0XV43
I	-7	GLU	-	expression tag	UNP S0XV43
I	-6	ASN	-	expression tag	UNP S0XV43
I	-5	LEU	-	expression tag	UNP S0XV43

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-4	TYR	-	expression tag	UNP S0XV43
I	-3	PHE	-	expression tag	UNP S0XV43
I	-2	GLN	-	expression tag	UNP S0XV43
I	-1	GLY	-	expression tag	UNP S0XV43
I	0	HIS	-	expression tag	UNP S0XV43
J	-22	MET	-	initiating methionine	UNP S0XV43
J	-21	GLY	-	expression tag	UNP S0XV43
J	-20	SER	-	expression tag	UNP S0XV43
J	-19	ASP	-	expression tag	UNP S0XV43
J	-18	LYS	-	expression tag	UNP S0XV43
J	-17	ILE	-	expression tag	UNP S0XV43
J	-16	HIS	-	expression tag	UNP S0XV43
J	-15	HIS	-	expression tag	UNP S0XV43
J	-14	HIS	-	expression tag	UNP S0XV43
J	-13	HIS	-	expression tag	UNP S0XV43
J	-12	HIS	-	expression tag	UNP S0XV43
J	-11	HIS	-	expression tag	UNP S0XV43
J	-10	SER	-	expression tag	UNP S0XV43
J	-9	SER	-	expression tag	UNP S0XV43
J	-8	GLY	-	expression tag	UNP S0XV43
J	-7	GLU	-	expression tag	UNP S0XV43
J	-6	ASN	-	expression tag	UNP S0XV43
J	-5	LEU	-	expression tag	UNP S0XV43
J	-4	TYR	-	expression tag	UNP S0XV43
J	-3	PHE	-	expression tag	UNP S0XV43
J	-2	GLN	-	expression tag	UNP S0XV43
J	-1	GLY	-	expression tag	UNP S0XV43
J	0	HIS	-	expression tag	UNP S0XV43
K	-22	MET	-	initiating methionine	UNP S0XV43
K	-21	GLY	-	expression tag	UNP S0XV43
K	-20	SER	-	expression tag	UNP S0XV43
K	-19	ASP	-	expression tag	UNP S0XV43
K	-18	LYS	-	expression tag	UNP S0XV43
K	-17	ILE	-	expression tag	UNP S0XV43
K	-16	HIS	-	expression tag	UNP S0XV43
K	-15	HIS	-	expression tag	UNP S0XV43
K	-14	HIS	-	expression tag	UNP S0XV43
K	-13	HIS	-	expression tag	UNP S0XV43
K	-12	HIS	-	expression tag	UNP S0XV43
K	-11	HIS	-	expression tag	UNP S0XV43
K	-10	SER	-	expression tag	UNP S0XV43
K	-9	SER	-	expression tag	UNP S0XV43

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-8	GLY	-	expression tag	UNP S0XV43
K	-7	GLU	-	expression tag	UNP S0XV43
K	-6	ASN	-	expression tag	UNP S0XV43
K	-5	LEU	-	expression tag	UNP S0XV43
K	-4	TYR	-	expression tag	UNP S0XV43
K	-3	PHE	-	expression tag	UNP S0XV43
K	-2	GLN	-	expression tag	UNP S0XV43
K	-1	GLY	-	expression tag	UNP S0XV43
K	0	HIS	-	expression tag	UNP S0XV43
L	-22	MET	-	initiating methionine	UNP S0XV43
L	-21	GLY	-	expression tag	UNP S0XV43
L	-20	SER	-	expression tag	UNP S0XV43
L	-19	ASP	-	expression tag	UNP S0XV43
L	-18	LYS	-	expression tag	UNP S0XV43
L	-17	ILE	-	expression tag	UNP S0XV43
L	-16	HIS	-	expression tag	UNP S0XV43
L	-15	HIS	-	expression tag	UNP S0XV43
L	-14	HIS	-	expression tag	UNP S0XV43
L	-13	HIS	-	expression tag	UNP S0XV43
L	-12	HIS	-	expression tag	UNP S0XV43
L	-11	HIS	-	expression tag	UNP S0XV43
L	-10	SER	-	expression tag	UNP S0XV43
L	-9	SER	-	expression tag	UNP S0XV43
L	-8	GLY	-	expression tag	UNP S0XV43
L	-7	GLU	-	expression tag	UNP S0XV43
L	-6	ASN	-	expression tag	UNP S0XV43
L	-5	LEU	-	expression tag	UNP S0XV43
L	-4	TYR	-	expression tag	UNP S0XV43
L	-3	PHE	-	expression tag	UNP S0XV43
L	-2	GLN	-	expression tag	UNP S0XV43
L	-1	GLY	-	expression tag	UNP S0XV43
L	0	HIS	-	expression tag	UNP S0XV43
M	-22	MET	-	initiating methionine	UNP S0XV43
M	-21	GLY	-	expression tag	UNP S0XV43
M	-20	SER	-	expression tag	UNP S0XV43
M	-19	ASP	-	expression tag	UNP S0XV43
M	-18	LYS	-	expression tag	UNP S0XV43
M	-17	ILE	-	expression tag	UNP S0XV43
M	-16	HIS	-	expression tag	UNP S0XV43
M	-15	HIS	-	expression tag	UNP S0XV43
M	-14	HIS	-	expression tag	UNP S0XV43
M	-13	HIS	-	expression tag	UNP S0XV43

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-12	HIS	-	expression tag	UNP S0XV43
M	-11	HIS	-	expression tag	UNP S0XV43
M	-10	SER	-	expression tag	UNP S0XV43
M	-9	SER	-	expression tag	UNP S0XV43
M	-8	GLY	-	expression tag	UNP S0XV43
M	-7	GLU	-	expression tag	UNP S0XV43
M	-6	ASN	-	expression tag	UNP S0XV43
M	-5	LEU	-	expression tag	UNP S0XV43
M	-4	TYR	-	expression tag	UNP S0XV43
M	-3	PHE	-	expression tag	UNP S0XV43
M	-2	GLN	-	expression tag	UNP S0XV43
M	-1	GLY	-	expression tag	UNP S0XV43
M	0	HIS	-	expression tag	UNP S0XV43
N	-22	MET	-	initiating methionine	UNP S0XV43
N	-21	GLY	-	expression tag	UNP S0XV43
N	-20	SER	-	expression tag	UNP S0XV43
N	-19	ASP	-	expression tag	UNP S0XV43
N	-18	LYS	-	expression tag	UNP S0XV43
N	-17	ILE	-	expression tag	UNP S0XV43
N	-16	HIS	-	expression tag	UNP S0XV43
N	-15	HIS	-	expression tag	UNP S0XV43
N	-14	HIS	-	expression tag	UNP S0XV43
N	-13	HIS	-	expression tag	UNP S0XV43
N	-12	HIS	-	expression tag	UNP S0XV43
N	-11	HIS	-	expression tag	UNP S0XV43
N	-10	SER	-	expression tag	UNP S0XV43
N	-9	SER	-	expression tag	UNP S0XV43
N	-8	GLY	-	expression tag	UNP S0XV43
N	-7	GLU	-	expression tag	UNP S0XV43
N	-6	ASN	-	expression tag	UNP S0XV43
N	-5	LEU	-	expression tag	UNP S0XV43
N	-4	TYR	-	expression tag	UNP S0XV43
N	-3	PHE	-	expression tag	UNP S0XV43
N	-2	GLN	-	expression tag	UNP S0XV43
N	-1	GLY	-	expression tag	UNP S0XV43
N	0	HIS	-	expression tag	UNP S0XV43
O	-22	MET	-	initiating methionine	UNP S0XV43
O	-21	GLY	-	expression tag	UNP S0XV43
O	-20	SER	-	expression tag	UNP S0XV43
O	-19	ASP	-	expression tag	UNP S0XV43
O	-18	LYS	-	expression tag	UNP S0XV43
O	-17	ILE	-	expression tag	UNP S0XV43

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-16	HIS	-	expression tag	UNP S0XV43
O	-15	HIS	-	expression tag	UNP S0XV43
O	-14	HIS	-	expression tag	UNP S0XV43
O	-13	HIS	-	expression tag	UNP S0XV43
O	-12	HIS	-	expression tag	UNP S0XV43
O	-11	HIS	-	expression tag	UNP S0XV43
O	-10	SER	-	expression tag	UNP S0XV43
O	-9	SER	-	expression tag	UNP S0XV43
O	-8	GLY	-	expression tag	UNP S0XV43
O	-7	GLU	-	expression tag	UNP S0XV43
O	-6	ASN	-	expression tag	UNP S0XV43
O	-5	LEU	-	expression tag	UNP S0XV43
O	-4	TYR	-	expression tag	UNP S0XV43
O	-3	PHE	-	expression tag	UNP S0XV43
O	-2	GLN	-	expression tag	UNP S0XV43
O	-1	GLY	-	expression tag	UNP S0XV43
O	0	HIS	-	expression tag	UNP S0XV43
P	-22	MET	-	initiating methionine	UNP S0XV43
P	-21	GLY	-	expression tag	UNP S0XV43
P	-20	SER	-	expression tag	UNP S0XV43
P	-19	ASP	-	expression tag	UNP S0XV43
P	-18	LYS	-	expression tag	UNP S0XV43
P	-17	ILE	-	expression tag	UNP S0XV43
P	-16	HIS	-	expression tag	UNP S0XV43
P	-15	HIS	-	expression tag	UNP S0XV43
P	-14	HIS	-	expression tag	UNP S0XV43
P	-13	HIS	-	expression tag	UNP S0XV43
P	-12	HIS	-	expression tag	UNP S0XV43
P	-11	HIS	-	expression tag	UNP S0XV43
P	-10	SER	-	expression tag	UNP S0XV43
P	-9	SER	-	expression tag	UNP S0XV43
P	-8	GLY	-	expression tag	UNP S0XV43
P	-7	GLU	-	expression tag	UNP S0XV43
P	-6	ASN	-	expression tag	UNP S0XV43
P	-5	LEU	-	expression tag	UNP S0XV43
P	-4	TYR	-	expression tag	UNP S0XV43
P	-3	PHE	-	expression tag	UNP S0XV43
P	-2	GLN	-	expression tag	UNP S0XV43
P	-1	GLY	-	expression tag	UNP S0XV43
P	0	HIS	-	expression tag	UNP S0XV43
Q	-22	MET	-	initiating methionine	UNP S0XV43
Q	-21	GLY	-	expression tag	UNP S0XV43

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-20	SER	-	expression tag	UNP S0XV43
Q	-19	ASP	-	expression tag	UNP S0XV43
Q	-18	LYS	-	expression tag	UNP S0XV43
Q	-17	ILE	-	expression tag	UNP S0XV43
Q	-16	HIS	-	expression tag	UNP S0XV43
Q	-15	HIS	-	expression tag	UNP S0XV43
Q	-14	HIS	-	expression tag	UNP S0XV43
Q	-13	HIS	-	expression tag	UNP S0XV43
Q	-12	HIS	-	expression tag	UNP S0XV43
Q	-11	HIS	-	expression tag	UNP S0XV43
Q	-10	SER	-	expression tag	UNP S0XV43
Q	-9	SER	-	expression tag	UNP S0XV43
Q	-8	GLY	-	expression tag	UNP S0XV43
Q	-7	GLU	-	expression tag	UNP S0XV43
Q	-6	ASN	-	expression tag	UNP S0XV43
Q	-5	LEU	-	expression tag	UNP S0XV43
Q	-4	TYR	-	expression tag	UNP S0XV43
Q	-3	PHE	-	expression tag	UNP S0XV43
Q	-2	GLN	-	expression tag	UNP S0XV43
Q	-1	GLY	-	expression tag	UNP S0XV43
Q	0	HIS	-	expression tag	UNP S0XV43
R	-22	MET	-	initiating methionine	UNP S0XV43
R	-21	GLY	-	expression tag	UNP S0XV43
R	-20	SER	-	expression tag	UNP S0XV43
R	-19	ASP	-	expression tag	UNP S0XV43
R	-18	LYS	-	expression tag	UNP S0XV43
R	-17	ILE	-	expression tag	UNP S0XV43
R	-16	HIS	-	expression tag	UNP S0XV43
R	-15	HIS	-	expression tag	UNP S0XV43
R	-14	HIS	-	expression tag	UNP S0XV43
R	-13	HIS	-	expression tag	UNP S0XV43
R	-12	HIS	-	expression tag	UNP S0XV43
R	-11	HIS	-	expression tag	UNP S0XV43
R	-10	SER	-	expression tag	UNP S0XV43
R	-9	SER	-	expression tag	UNP S0XV43
R	-8	GLY	-	expression tag	UNP S0XV43
R	-7	GLU	-	expression tag	UNP S0XV43
R	-6	ASN	-	expression tag	UNP S0XV43
R	-5	LEU	-	expression tag	UNP S0XV43
R	-4	TYR	-	expression tag	UNP S0XV43
R	-3	PHE	-	expression tag	UNP S0XV43
R	-2	GLN	-	expression tag	UNP S0XV43

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-1	GLY	-	expression tag	UNP S0XV43
R	0	HIS	-	expression tag	UNP S0XV43

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mn 2 2	0	0
2	B	2	Total Mn 2 2	0	0
2	C	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0
2	E	2	Total Mn 2 2	0	0
2	F	2	Total Mn 2 2	0	0
2	G	2	Total Mn 2 2	0	0
2	H	2	Total Mn 2 2	0	0
2	I	2	Total Mn 2 2	0	0
2	J	2	Total Mn 2 2	0	0
2	K	2	Total Mn 2 2	0	0
2	L	2	Total Mn 2 2	0	0
2	M	1	Total Mn 1 1	0	0
2	P	1	Total Mn 1 1	0	0
2	Q	1	Total Mn 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	110	Total O 110 110	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	97	Total 97	O 97	0	0
3	C	110	Total 110	O 110	0	0
3	D	106	Total 106	O 106	0	0
3	E	98	Total 98	O 98	0	0
3	F	87	Total 87	O 87	0	0
3	G	92	Total 92	O 92	0	0
3	H	91	Total 91	O 91	0	0
3	I	108	Total 108	O 108	0	0
3	J	107	Total 107	O 107	0	0
3	K	108	Total 108	O 108	0	0
3	L	102	Total 102	O 102	0	0
3	M	5	Total 5	O 5	0	0
3	N	3	Total 3	O 3	0	0
3	O	1	Total 1	O 1	0	0
3	P	8	Total 8	O 8	0	0
3	Q	12	Total 12	O 12	0	0
3	R	4	Total 4	O 4	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Agmatinase

Chain A: 



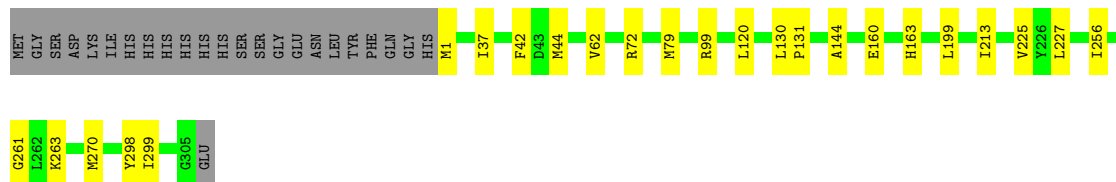
- Molecule 1: Agmatinase

Chain B: 



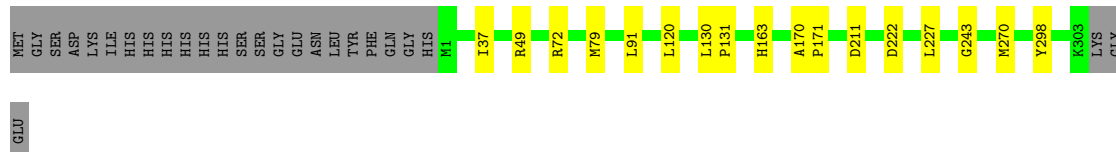
- Molecule 1: Agmatinase

Chain C: 




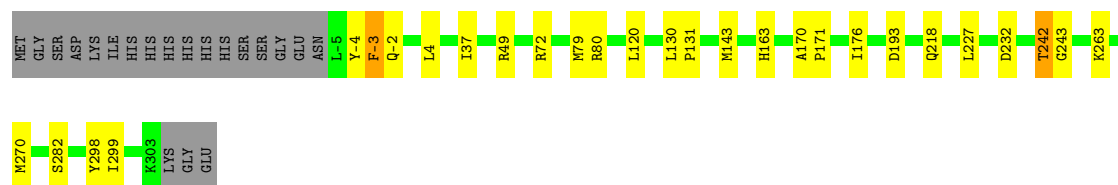
- Molecule 1: Agmatinase

Chain D: 



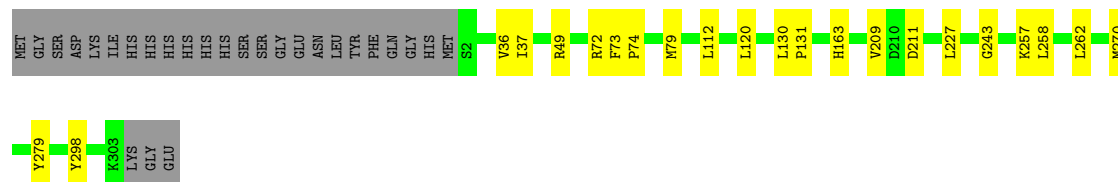
- Molecule 1: Agmatinase

Chain E: 



- Molecule 1: Agmatinase

Chain F: 85% 7% 8%



- Molecule 1: Agmatinase

Chain G: 85% 7% 7%



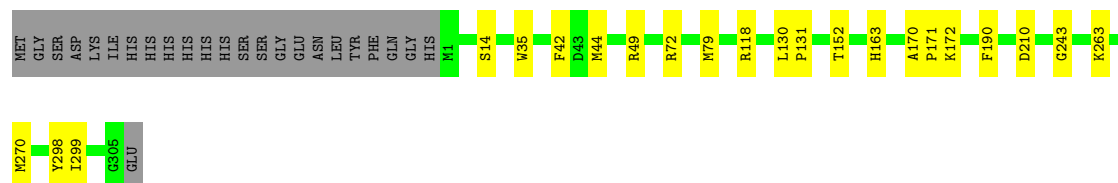
- Molecule 1: Agmatinase

Chain H: 85% 7% 8%



- Molecule 1: Agmatinase

Chain I: 86% 7% 7%



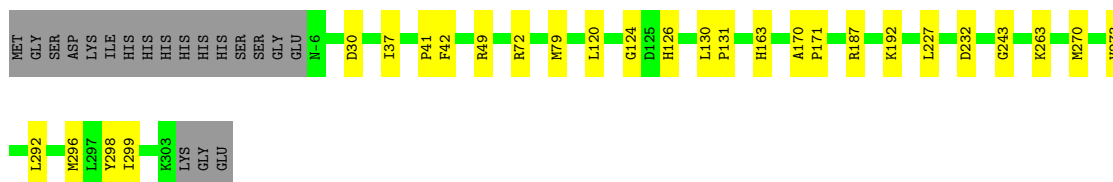
- Molecule 1: Agmatinase

Chain J: 88% 0% 8%



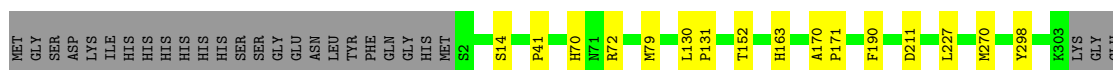
• Molecule 1: Agmatinase

Chain K: 86% 8% 6%



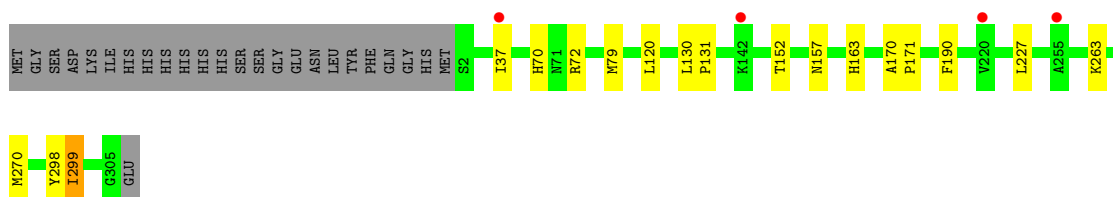
• Molecule 1: Agmatinase

Chain L: 87% 5% 8%



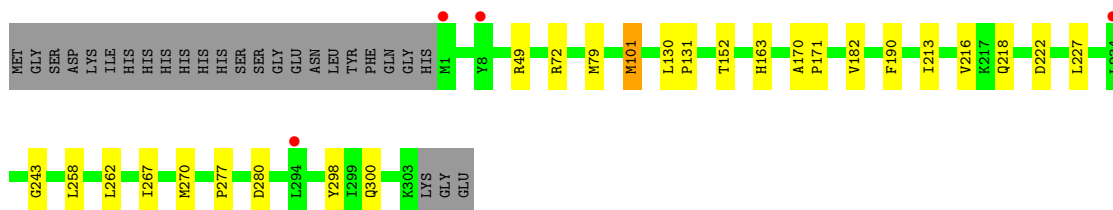
• Molecule 1: Agmatinase

Chain M: 87% 5% 8%



• Molecule 1: Agmatinase

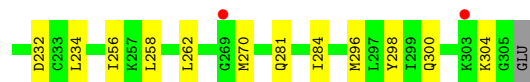
Chain N: 84% 8% 8%



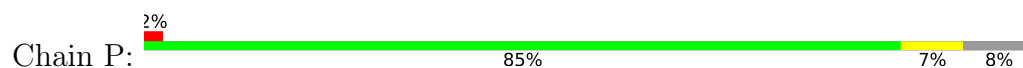
• Molecule 1: Agmatinase

Chain O: 84% 9% 7%

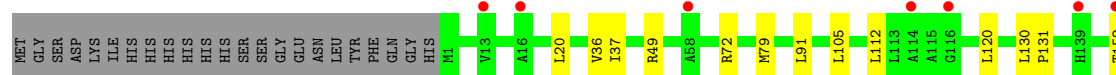
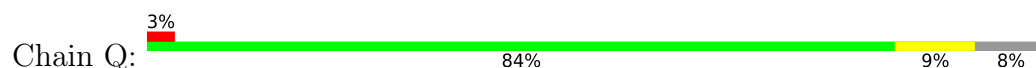




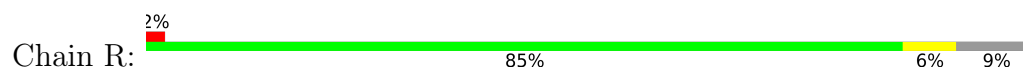
• Molecule 1: Agmatinase



• Molecule 1: Agmatinase



• Molecule 1: Agmatinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	139.81Å 139.81Å 222.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	82.02 – 2.20 82.02 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (82.02-2.20) 99.9 (82.02-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.179 , 0.213 0.179 , 0.212	Depositor DCC
R_{free} test set	12405 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 9.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.477 for -h,-k,l 0.245 for h,-h-k,-l 0.246 for -k,-h,-l	Xtriage
Reported twinning fraction	0.418 for H, K, L 0.087 for K, H, -L 0.403 for -h,-k,l 0.092 for -K, -H, -L	Depositor
Outliers	0 of 247335 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	43547	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.2641e-03.*

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: MN

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	0.66	0/2401	0.72	0/3259
1	B	0.65	0/2456	0.71	0/3334
1	C	0.65	0/2404	0.71	0/3262
1	D	0.65	0/2391	0.71	0/3246
1	E	0.65	0/2448	0.71	0/3323
1	F	0.65	0/2383	0.71	0/3236
1	G	0.65	0/2401	0.72	0/3259
1	H	0.66	0/2391	0.71	0/3246
1	I	0.65	0/2404	0.71	0/3262
1	J	0.65	0/2391	0.71	0/3246
1	K	0.65	0/2456	0.71	0/3334
1	L	0.65	0/2383	0.72	0/3236
1	M	0.66	0/2396	0.71	0/3252
1	N	0.66	0/2391	0.72	0/3246
1	O	0.66	0/2404	0.72	0/3262
1	P	0.66	0/2387	0.72	0/3242
1	Q	0.66	0/2391	0.72	0/3246
1	R	0.66	0/2374	0.71	0/3225
All	All	0.66	0/43252	0.71	0/58716

There are no bond length outliers.

There are no bond angle outliers.

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	2347	0	2271	5	0
1	B	2399	0	2318	8	0
1	C	2350	0	2281	9	0
1	D	2337	0	2265	7	0
1	E	2391	0	2312	14	0
1	F	2329	0	2253	10	0
1	G	2347	0	2271	11	0
1	H	2337	0	2265	12	0
1	I	2350	0	2281	9	0
1	J	2337	0	2265	5	0
1	K	2399	0	2318	13	0
1	L	2329	0	2253	8	0
1	M	2342	0	2269	9	0
1	N	2337	0	2265	14	0
1	O	2350	0	2281	12	0
1	P	2333	0	2254	10	0
1	Q	2337	0	2265	15	0
1	R	2320	0	2240	9	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
3	A	110	0	0	0	0
3	B	97	0	0	0	0
3	C	110	0	0	0	0
3	D	106	0	0	0	0
3	E	98	0	0	0	0
3	F	87	0	0	0	0
3	G	92	0	0	0	0
3	H	91	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	108	0	0	0	0
3	J	107	0	0	0	0
3	K	108	0	0	0	0
3	L	102	0	0	0	0
3	M	5	0	0	0	0
3	N	3	0	0	0	0
3	O	1	0	0	0	0
3	P	8	0	0	0	0
3	Q	12	0	0	0	0
3	R	4	0	0	0	0
All	All	43547	0	40927	172	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 2.

All (172) 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:Q:253:ASP:O	1:Q:256:ILE:HG22	1.92	0.70
1:G:82:ARG:HD3	1:G:305:GLY:HA2	1.76	0.67
1:P:227:LEU:O	1:P:270:MET:HA	1.98	0.64
1:R:130:LEU:HB3	1:R:131:PRO:HD3	1.81	0.62
1:O:281:GLN:O	1:O:284:ILE:HD13	2.01	0.61
1:O:172:LYS:O	1:O:173:GLU:HG2	2.00	0.60
1:F:130:LEU:HB3	1:F:131:PRO:HD3	1.85	0.58
1:L:170:ALA:HB3	1:L:171:PRO:HD3	1.85	0.58
1:E:37:ILE:HA	1:E:120:LEU:O	2.05	0.57
1:P:49:ARG:HB2	1:P:243:GLY:HA2	1.87	0.57
1:J:130:LEU:HB3	1:J:131:PRO:HD3	1.88	0.56
1:K:227:LEU:O	1:K:270:MET:HA	2.06	0.56
1:P:130:LEU:HB3	1:P:131:PRO:HD3	1.88	0.56
1:K:263:LYS:HA	1:K:299:ILE:HB	1.88	0.55
1:E:130:LEU:HB3	1:E:131:PRO:HD3	1.89	0.55
1:K:130:LEU:HB3	1:K:131:PRO:HD3	1.89	0.55
1:O:270:MET:SD	1:O:296:MET:HB3	2.46	0.55
1:D:130:LEU:HB3	1:D:131:PRO:HD3	1.89	0.55
1:B:263:LYS:HA	1:B:299:ILE:HB	1.88	0.55
1:M:227:LEU:O	1:M:270:MET:HA	2.08	0.54
1:D:227:LEU:O	1:D:270:MET:HA	2.07	0.54
1:A:37:ILE:HA	1:A:120:LEU:O	2.08	0.53
1:G:41:PRO:HG3	1:I:14:SER:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:LEU:O	1:E:270:MET:HA	2.08	0.53
1:A:130:LEU:HB3	1:A:131:PRO:HD3	1.91	0.53
1:Q:130:LEU:HB3	1:Q:131:PRO:HD3	1.90	0.53
1:L:72:ARG:HB3	1:L:298:TYR:CZ	2.44	0.52
1:G:130:LEU:HB3	1:G:131:PRO:HD3	1.91	0.52
1:M:263:LYS:HA	1:M:299:ILE:HB	1.92	0.52
1:H:130:LEU:HB3	1:H:131:PRO:HD3	1.92	0.51
1:D:49:ARG:HB2	1:D:243:GLY:HA2	1.93	0.51
1:G:227:LEU:O	1:G:270:MET:HA	2.11	0.51
1:K:49:ARG:HB2	1:K:243:GLY:HA2	1.92	0.51
1:E:263:LYS:HA	1:E:299:ILE:HB	1.92	0.51
1:G:170:ALA:HB3	1:G:171:PRO:HD3	1.93	0.51
1:I:130:LEU:HB3	1:I:131:PRO:HD3	1.92	0.51
1:N:267:ILE:O	1:N:300:GLN:NE2	2.44	0.51
1:F:37:ILE:HA	1:F:120:LEU:O	2.12	0.50
1:P:170:ALA:HB3	1:P:171:PRO:HD3	1.92	0.50
1:O:215:GLN:O	1:O:218:GLN:HG3	2.12	0.50
1:F:49:ARG:HB2	1:F:243:GLY:HA2	1.94	0.50
1:N:130:LEU:HB3	1:N:131:PRO:HD3	1.93	0.50
1:G:60:ARG:NE	1:G:87:ASP:OD2	2.42	0.50
1:K:170:ALA:HB3	1:K:171:PRO:HD3	1.93	0.50
1:N:101:MET:SD	1:N:101:MET:C	2.90	0.50
1:G:152:THR:HG21	1:G:190:PHE:HB2	1.94	0.49
1:N:152:THR:HG21	1:N:190:PHE:HB2	1.93	0.49
1:K:37:ILE:HA	1:K:120:LEU:O	2.12	0.49
1:L:130:LEU:HB3	1:L:131:PRO:HD3	1.94	0.49
1:Q:170:ALA:HB3	1:Q:171:PRO:HD3	1.94	0.49
1:R:144:ALA:O	1:R:225:VAL:HA	2.13	0.49
1:B:37:ILE:HA	1:B:120:LEU:O	2.12	0.48
1:M:72:ARG:HB3	1:M:298:TYR:CZ	2.47	0.48
1:J:170:ALA:HB3	1:J:171:PRO:HD3	1.95	0.48
1:B:72:ARG:HB3	1:B:298:TYR:CZ	2.48	0.48
1:E:49:ARG:HB2	1:E:243:GLY:HA2	1.94	0.48
1:K:187:ARG:NH2	1:K:232:ASP:O	2.47	0.48
1:Q:49:ARG:HB2	1:Q:243:GLY:HA2	1.96	0.48
1:R:213:ILE:HD11	1:R:258:LEU:HA	1.94	0.48
1:P:109:ALA:HB1	1:P:119:MET:HE1	1.94	0.48
1:H:14:SER:HB3	1:L:41:PRO:HG3	1.95	0.48
1:H:152:THR:HG21	1:H:190:PHE:HB2	1.96	0.48
1:E:72:ARG:HB3	1:E:298:TYR:CZ	2.49	0.48
1:B:130:LEU:HB3	1:B:131:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:170:ALA:HB3	1:I:171:PRO:HD3	1.96	0.47
1:J:49:ARG:HB2	1:J:243:GLY:HA2	1.96	0.47
1:M:70:HIS:N	1:Q:189:GLU:OE1	2.47	0.47
1:A:152:THR:HG21	1:A:190:PHE:HB2	1.95	0.47
1:E:-4:TYR:O	1:E:-3:PHE:HB2	2.15	0.47
1:H:37:ILE:HA	1:H:120:LEU:O	2.14	0.47
1:H:72:ARG:HB3	1:H:298:TYR:CZ	2.50	0.47
1:N:182:VAL:HG11	1:N:216:VAL:HG23	1.95	0.47
1:H:126:HIS:CG	1:H:273:VAL:HG21	2.50	0.47
1:K:130:LEU:HB3	1:K:131:PRO:CD	2.45	0.47
1:F:72:ARG:HB3	1:F:298:TYR:CZ	2.50	0.47
1:C:37:ILE:HA	1:C:120:LEU:O	2.15	0.47
1:C:130:LEU:HB3	1:C:131:PRO:HD3	1.97	0.47
1:F:227:LEU:O	1:F:270:MET:HA	2.15	0.47
1:D:72:ARG:HB3	1:D:298:TYR:CE2	2.50	0.47
1:B:170:ALA:HB3	1:B:171:PRO:HD3	1.97	0.47
1:G:49:ARG:HB2	1:G:243:GLY:HA2	1.96	0.47
1:N:213:ILE:HD11	1:N:258:LEU:HA	1.96	0.47
1:P:267:ILE:HG21	1:P:270:MET:HE3	1.96	0.47
1:H:170:ALA:HB3	1:H:171:PRO:HD3	1.98	0.46
1:O:37:ILE:HA	1:O:120:LEU:O	2.15	0.46
1:R:72:ARG:HB3	1:R:298:TYR:CZ	2.50	0.46
1:F:209:VAL:HG11	1:F:257:LYS:HB3	1.97	0.46
1:C:263:LYS:HA	1:C:299:ILE:HB	1.97	0.46
1:E:72:ARG:HB3	1:E:298:TYR:CE2	2.50	0.46
1:I:49:ARG:HB2	1:I:243:GLY:HA2	1.97	0.46
1:N:72:ARG:HB3	1:N:298:TYR:CZ	2.51	0.46
1:E:232:ASP:HB3	1:E:242:THR:HG21	1.97	0.46
1:N:227:LEU:O	1:N:270:MET:HA	2.16	0.45
1:O:270:MET:CE	1:O:300:GLN:HE21	2.30	0.45
1:R:263:LYS:HA	1:R:299:ILE:HB	1.98	0.45
1:G:37:ILE:HA	1:G:120:LEU:O	2.15	0.45
1:M:130:LEU:HB3	1:M:131:PRO:HD3	1.98	0.45
1:I:263:LYS:HA	1:I:299:ILE:HB	1.99	0.45
1:Q:20:LEU:CD1	1:Q:294:LEU:HD13	2.47	0.45
1:B:152:THR:HG21	1:B:190:PHE:HB2	1.99	0.45
1:L:227:LEU:O	1:L:270:MET:HA	2.16	0.45
1:N:49:ARG:HB2	1:N:243:GLY:HA2	1.98	0.45
1:O:187:ARG:NH2	1:O:232:ASP:O	2.49	0.45
1:O:130:LEU:HB3	1:O:131:PRO:HD3	1.98	0.45
1:H:49:ARG:HB2	1:H:243:GLY:HA2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:72:ARG:HB3	1:K:298:TYR:CZ	2.51	0.45
1:O:258:LEU:O	1:O:262:LEU:HG	2.17	0.44
1:J:72:ARG:HB3	1:J:298:TYR:CZ	2.52	0.44
1:N:277:PRO:HA	1:N:280:ASP:HB2	1.99	0.44
1:E:-2:GLN:O	1:E:80:ARG:HD2	2.17	0.44
1:M:170:ALA:HB3	1:M:171:PRO:HD3	1.98	0.44
1:I:152:THR:HG21	1:I:190:PHE:HB2	1.99	0.44
1:K:292:LEU:O	1:K:296:MET:HG3	2.18	0.44
1:R:49:ARG:HD2	1:R:279:TYR:CZ	2.53	0.44
1:N:170:ALA:HB3	1:N:171:PRO:HD3	1.99	0.44
1:F:258:LEU:O	1:F:262:LEU:HG	2.18	0.44
1:I:72:ARG:HB3	1:I:298:TYR:CZ	2.53	0.44
1:A:170:ALA:HB3	1:A:171:PRO:HD3	2.00	0.44
1:C:99:ARG:NH2	1:C:160:GLU:OE1	2.51	0.44
1:C:144:ALA:O	1:C:225:VAL:HA	2.18	0.44
1:H:41:PRO:HG3	1:L:14:SER:HB3	1.99	0.44
1:M:130:LEU:HB3	1:M:131:PRO:CD	2.48	0.44
1:G:72:ARG:HB3	1:G:298:TYR:CZ	2.53	0.43
1:H:227:LEU:O	1:H:270:MET:HA	2.17	0.43
1:E:170:ALA:HB3	1:E:171:PRO:HD3	2.00	0.43
1:O:22:LEU:HD22	1:O:85:VAL:HG13	2.01	0.43
1:C:227:LEU:O	1:C:270:MET:HA	2.18	0.43
1:I:35:TRP:CD2	1:I:118:ARG:HB2	2.53	0.43
1:K:42:PHE:O	1:K:124:GLY:HA2	2.18	0.43
1:Q:152:THR:HG21	1:Q:190:PHE:HB2	2.00	0.43
1:D:170:ALA:HB3	1:D:171:PRO:HD3	2.00	0.43
1:H:35:TRP:O	1:H:85:VAL:HA	2.19	0.43
1:E:143:MET:O	1:E:176:ILE:HA	2.18	0.43
1:Q:37:ILE:HA	1:Q:120:LEU:O	2.18	0.43
1:J:14:SER:HB3	1:K:41:PRO:HG3	2.01	0.43
1:Q:105:LEU:HD12	1:Q:131:PRO:HB2	2.01	0.43
1:M:152:THR:HG21	1:M:190:PHE:HB2	2.01	0.43
1:P:213:ILE:HD11	1:P:258:LEU:O	2.19	0.43
1:R:170:ALA:HB3	1:R:171:PRO:HD3	2.00	0.43
1:E:282:SER:OG	1:F:279:TYR:O	2.29	0.42
1:R:37:ILE:HA	1:R:120:LEU:O	2.19	0.42
1:N:258:LEU:O	1:N:262:LEU:HG	2.19	0.42
1:M:37:ILE:HA	1:M:120:LEU:O	2.19	0.42
1:O:72:ARG:HB3	1:O:298:TYR:CZ	2.55	0.42
1:Q:36:VAL:HG11	1:Q:112:LEU:HD22	2.01	0.42
1:N:216:VAL:HG11	1:N:262:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:49:ARG:HB2	1:R:243:GLY:HA2	2.01	0.42
1:P:73:PHE:HA	1:P:74:PRO:HA	1.88	0.42
1:Q:277:PRO:HA	1:Q:280:ASP:HB2	2.00	0.42
1:C:42:PHE:CE1	1:C:44:MET:HB2	2.54	0.42
1:Q:20:LEU:HD12	1:Q:294:LEU:HD13	2.00	0.42
1:C:213:ILE:HD13	1:C:261:GLY:HA3	2.02	0.42
1:G:189:GLU:OE1	1:L:70:HIS:N	2.50	0.42
1:F:73:PHE:HA	1:F:74:PRO:HA	1.89	0.41
1:L:152:THR:HG21	1:L:190:PHE:HB2	2.02	0.41
1:D:37:ILE:HA	1:D:120:LEU:O	2.20	0.41
1:P:37:ILE:HA	1:P:120:LEU:O	2.20	0.41
1:F:36:VAL:HG21	1:F:112:LEU:HD22	2.01	0.41
1:D:91:LEU:HA	1:E:4:LEU:HD23	2.03	0.41
1:P:72:ARG:HB3	1:P:298:TYR:CE2	2.55	0.41
1:K:126:HIS:CG	1:K:273:VAL:HG21	2.56	0.41
1:Q:91:LEU:HD22	1:Q:105:LEU:HD23	2.03	0.41
1:B:213:ILE:HD11	1:B:258:LEU:O	2.20	0.41
1:O:29:TYR:CD2	1:O:112:LEU:HD22	2.56	0.41
1:Q:72:ARG:HB3	1:Q:298:TYR:CZ	2.56	0.41
1:A:227:LEU:O	1:A:270:MET:HA	2.21	0.41
1:I:42:PHE:CE1	1:I:44:MET:HB2	2.55	0.40
1:B:227:LEU:O	1:B:270:MET:HA	2.21	0.40
1:C:72:ARG:HB3	1:C:298:TYR:CE2	2.56	0.40
1:H:42:PHE:CE1	1:H:44:MET:HB2	2.56	0.40
1:Q:258:LEU:O	1:Q:262:LEU:HG	2.21	0.40
1:N:72:ARG:HB3	1:N:298:TYR:CE2	2.57	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	303/329 (92%)	292 (96%)	11 (4%)	0	100	100
1	B	308/329 (94%)	297 (96%)	11 (4%)	0	100	100
1	C	303/329 (92%)	296 (98%)	7 (2%)	0	100	100
1	D	301/329 (92%)	295 (98%)	6 (2%)	0	100	100
1	E	307/329 (93%)	298 (97%)	8 (3%)	1 (0%)	41	46
1	F	300/329 (91%)	292 (97%)	8 (3%)	0	100	100
1	G	303/329 (92%)	288 (95%)	14 (5%)	1 (0%)	41	46
1	H	301/329 (92%)	288 (96%)	13 (4%)	0	100	100
1	I	303/329 (92%)	296 (98%)	7 (2%)	0	100	100
1	J	301/329 (92%)	292 (97%)	9 (3%)	0	100	100
1	K	308/329 (94%)	298 (97%)	10 (3%)	0	100	100
1	L	300/329 (91%)	293 (98%)	7 (2%)	0	100	100
1	M	302/329 (92%)	292 (97%)	9 (3%)	1 (0%)	41	46
1	N	301/329 (92%)	289 (96%)	12 (4%)	0	100	100
1	O	303/329 (92%)	286 (94%)	16 (5%)	1 (0%)	41	46
1	P	301/329 (92%)	284 (94%)	17 (6%)	0	100	100
1	Q	301/329 (92%)	286 (95%)	15 (5%)	0	100	100
1	R	299/329 (91%)	287 (96%)	11 (4%)	1 (0%)	41	46
All	All	5445/5922 (92%)	5249 (96%)	191 (4%)	5 (0%)	51	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	157	ASN
1	G	304	LYS
1	E	-3	PHE
1	M	157	ASN
1	O	174	GLY

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	245/267 (92%)	241 (98%)	4 (2%)	62	76
1	B	251/267 (94%)	248 (99%)	3 (1%)	71	83
1	C	246/267 (92%)	240 (98%)	6 (2%)	49	62
1	D	245/267 (92%)	241 (98%)	4 (2%)	62	76
1	E	250/267 (94%)	245 (98%)	5 (2%)	55	69
1	F	244/267 (91%)	241 (99%)	3 (1%)	71	83
1	G	245/267 (92%)	242 (99%)	3 (1%)	71	83
1	H	245/267 (92%)	243 (99%)	2 (1%)	81	90
1	I	246/267 (92%)	241 (98%)	5 (2%)	55	69
1	J	245/267 (92%)	241 (98%)	4 (2%)	62	76
1	K	251/267 (94%)	247 (98%)	4 (2%)	62	76
1	L	244/267 (91%)	241 (99%)	3 (1%)	71	83
1	M	245/267 (92%)	242 (99%)	3 (1%)	71	83
1	N	245/267 (92%)	240 (98%)	5 (2%)	55	69
1	O	246/267 (92%)	240 (98%)	6 (2%)	49	62
1	P	244/267 (91%)	239 (98%)	5 (2%)	55	69
1	Q	245/267 (92%)	242 (99%)	3 (1%)	71	83
1	R	243/267 (91%)	240 (99%)	3 (1%)	71	83
All	All	4425/4806 (92%)	4354 (98%)	71 (2%)	62	76

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	MET
1	A	163	HIS
1	A	210	ASP
1	A	218	GLN
1	B	-6	ASN
1	B	79	MET
1	B	163	HIS
1	C	1	MET
1	C	62	VAL
1	C	79	MET
1	C	163	HIS
1	C	199	LEU
1	C	256	ILE
1	D	79	MET

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Mol	Chain	Res	Type
1	D	163	HIS
1	D	211	ASP
1	D	222	ASP
1	E	79	MET
1	E	163	HIS
1	E	193	ASP
1	E	218	GLN
1	E	242	THR
1	F	79	MET
1	F	163	HIS
1	F	211	ASP
1	G	79	MET
1	G	163	HIS
1	G	218	GLN
1	H	79	MET
1	H	163	HIS
1	I	79	MET
1	I	163	HIS
1	I	172	LYS
1	I	210	ASP
1	I	270	MET
1	J	79	MET
1	J	163	HIS
1	J	211	ASP
1	J	222	ASP
1	K	30	ASP
1	K	79	MET
1	K	163	HIS
1	K	192	LYS
1	L	79	MET
1	L	163	HIS
1	L	211	ASP
1	M	79	MET
1	M	163	HIS
1	M	299	ILE
1	N	79	MET
1	N	101	MET
1	N	163	HIS
1	N	218	GLN
1	N	222	ASP
1	O	32	ASP
1	O	79	MET

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Mol	Chain	Res	Type
1	O	163	HIS
1	O	234	LEU
1	O	256	ILE
1	O	304	LYS
1	P	133	LEU
1	P	163	HIS
1	P	211	ASP
1	P	222	ASP
1	P	270	MET
1	Q	79	MET
1	Q	172	LYS
1	Q	242	THR
1	R	79	MET
1	R	130	LEU
1	R	163	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	54	HIS
1	E	-2	GLN
1	E	54	HIS
1	E	61	GLN
1	G	61	GLN
1	G	218	GLN
1	O	300	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 27 ligands modelled in this entry, 27 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	305/329 (92%)	-0.63	0 100 100	13, 19, 25, 31	0
1	B	310/329 (94%)	-0.60	0 100 100	13, 19, 25, 27	0
1	C	305/329 (92%)	-0.57	0 100 100	13, 19, 26, 29	0
1	D	303/329 (92%)	-0.57	0 100 100	13, 20, 26, 30	0
1	E	309/329 (93%)	-0.52	0 100 100	13, 20, 27, 49	0
1	F	302/329 (91%)	-0.56	0 100 100	14, 20, 26, 29	0
1	G	305/329 (92%)	-0.48	0 100 100	15, 23, 28, 34	0
1	H	303/329 (92%)	-0.52	0 100 100	16, 21, 27, 35	0
1	I	305/329 (92%)	-0.56	0 100 100	14, 20, 27, 31	0
1	J	303/329 (92%)	-0.52	0 100 100	15, 22, 29, 35	0
1	K	310/329 (94%)	-0.52	0 100 100	16, 21, 27, 32	0
1	L	302/329 (91%)	-0.52	0 100 100	15, 22, 29, 31	0
1	M	304/329 (92%)	0.36	4 (1%) 77 75	37, 45, 52, 60	0
1	N	303/329 (92%)	0.31	4 (1%) 77 75	35, 44, 53, 61	0
1	O	305/329 (92%)	0.41	4 (1%) 77 75	39, 49, 58, 60	0
1	P	303/329 (92%)	0.34	6 (1%) 65 63	36, 49, 57, 60	0
1	Q	303/329 (92%)	0.45	11 (3%) 42 41	34, 48, 57, 60	0
1	R	301/329 (91%)	0.36	8 (2%) 54 52	37, 47, 61, 65	0
All	All	5481/5922 (92%)	-0.24	37 (0%) 87 86	13, 23, 53, 65	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	114	ALA	4.2
1	Q	16	ALA	3.9
1	O	40	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	N	294	LEU	3.1
1	R	264	ASP	2.8
1	Q	139	HIS	2.8
1	R	299	ILE	2.7
1	M	255	ALA	2.7
1	N	1	MET	2.7
1	P	20	LEU	2.6
1	N	8	TYR	2.6
1	Q	58	ALA	2.6
1	P	105	LEU	2.5
1	Q	294	LEU	2.5
1	R	55	GLY	2.5
1	M	37	ILE	2.5
1	M	142	LYS	2.4
1	R	137	ALA	2.4
1	R	198	VAL	2.4
1	O	269	GLY	2.4
1	P	1	MET	2.4
1	Q	116	GLY	2.4
1	Q	204	VAL	2.3
1	P	30	ASP	2.3
1	M	220	VAL	2.3
1	Q	13	VAL	2.2
1	O	164	GLY	2.2
1	N	234	LEU	2.2
1	P	83	LEU	2.2
1	R	185	GLY	2.1
1	R	168	TYR	2.1
1	R	223	MET	2.1
1	Q	166	MET	2.1
1	P	133	LEU	2.1
1	Q	196	PHE	2.0
1	Q	152	THR	2.0
1	O	303	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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	MN	M	401	1/1	0.24	0.17	108,108,108,108	0
2	MN	Q	401	1/1	0.86	0.06	101,101,101,101	0
2	MN	P	401	1/1	0.93	0.11	102,102,102,102	0
2	MN	L	401	1/1	0.95	0.03	40,40,40,40	0
2	MN	C	402	1/1	0.96	0.16	62,62,62,62	0
2	MN	B	402	1/1	0.97	0.04	52,52,52,52	0
2	MN	J	402	1/1	0.97	0.05	44,44,44,44	0
2	MN	J	401	1/1	0.98	0.06	40,40,40,40	0
2	MN	A	401	1/1	0.98	0.04	32,32,32,32	0
2	MN	H	402	1/1	0.98	0.03	39,39,39,39	0
2	MN	F	402	1/1	0.99	0.04	32,32,32,32	0
2	MN	G	401	1/1	0.99	0.03	31,31,31,31	0
2	MN	G	402	1/1	0.99	0.05	27,27,27,27	0
2	MN	H	401	1/1	0.99	0.04	32,32,32,32	0
2	MN	A	402	1/1	0.99	0.07	38,38,38,38	0
2	MN	I	401	1/1	0.99	0.04	31,31,31,31	0
2	MN	I	402	1/1	0.99	0.07	43,43,43,43	0
2	MN	C	401	1/1	0.99	0.03	35,35,35,35	0
2	MN	B	401	1/1	0.99	0.03	29,29,29,29	0
2	MN	K	401	1/1	0.99	0.03	29,29,29,29	0
2	MN	D	401	1/1	0.99	0.04	26,26,26,26	0
2	MN	L	402	1/1	0.99	0.06	31,31,31,31	0
2	MN	E	401	1/1	0.99	0.05	32,32,32,32	0
2	MN	E	402	1/1	0.99	0.09	39,39,39,39	0
2	MN	F	401	1/1	0.99	0.05	27,27,27,27	0
2	MN	K	402	1/1	1.00	0.05	33,33,33,33	0
2	MN	D	402	1/1	1.00	0.04	86,86,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.