



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 11, 2023 – 05:18 AM 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

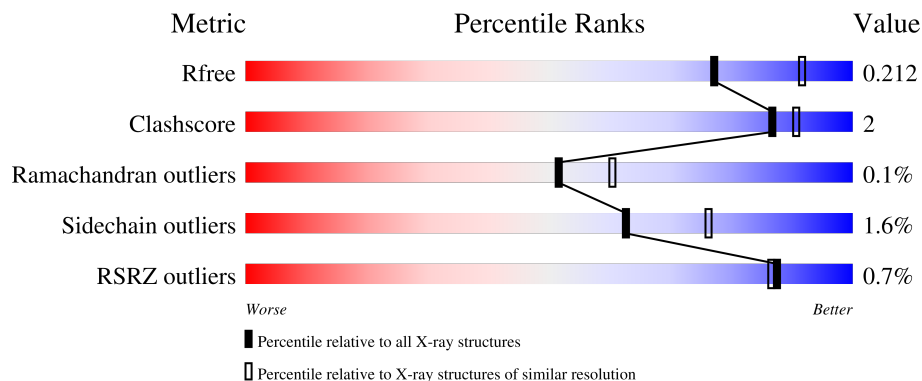
# 1 Overall quality at a glance

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

Mol	Chain	Length	Quality of chain
1	A	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% 7% 8%
1	K	329	 86% 8% 6%
1	L	329	 87% 5% 8%
1	M	329	 87% 5% 8% 2%
1	N	329	 84% 8% 8% 3%
1	O	329	 84% 9% 7% 2%
1	P	329	 85% 7% 8% 2%
1	Q	329	 84% 9% 8% 3%
1	R	329	 85% 6% 9% 2%

## 2 Entry composition [i](#)

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

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

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



### 3 Residue-property plots


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: 




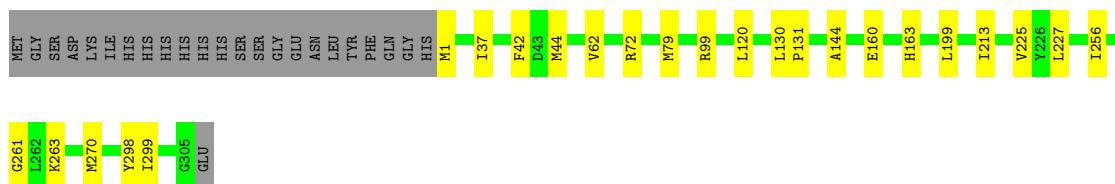
- Molecule 1: Agmatinase

Chain B: 




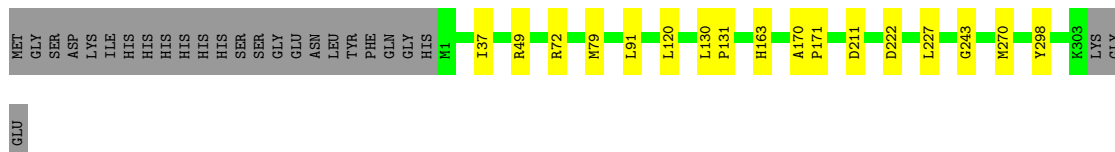
- Molecule 1: Agmatinase

Chain C: 




- Molecule 1: Agmatinase

Chain D: 

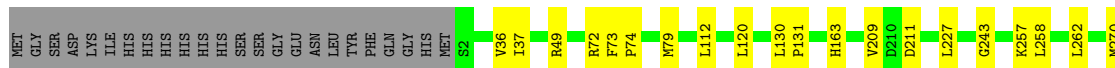
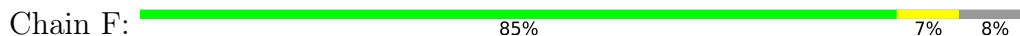


- Molecule 1: Agmatinase

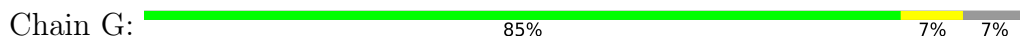
Chain E: 



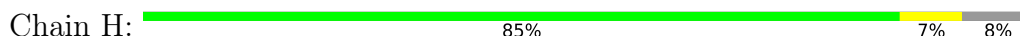
• Molecule 1: Agmatinase



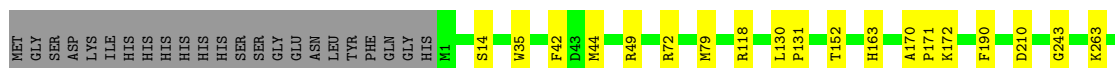
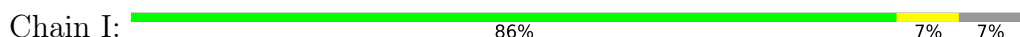
• Molecule 1: Agmatinase



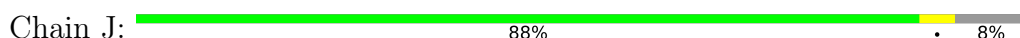
• Molecule 1: Agmatinase



• Molecule 1: Agmatinase

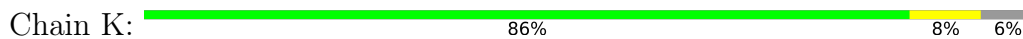


• Molecule 1: Agmatinase

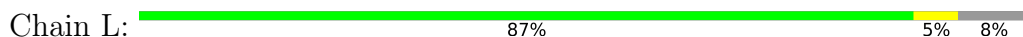




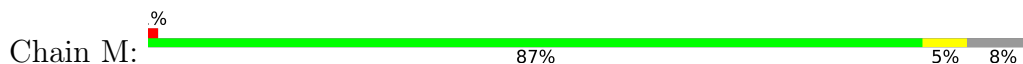
● Molecule 1: Agmatinase



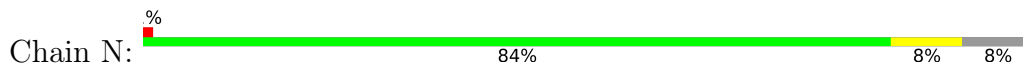
● Molecule 1: Agmatinase



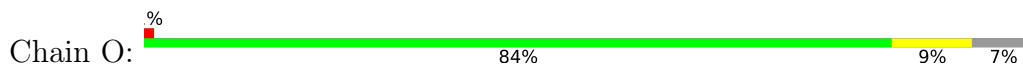
● Molecule 1: Agmatinase

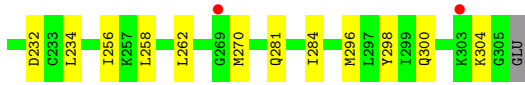


● Molecule 1: Agmatinase

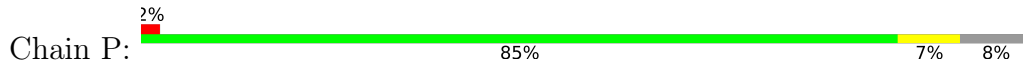


● Molecule 1: Agmatinase

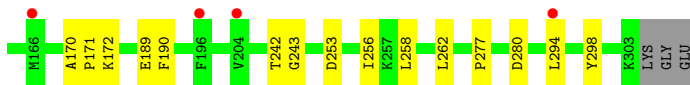
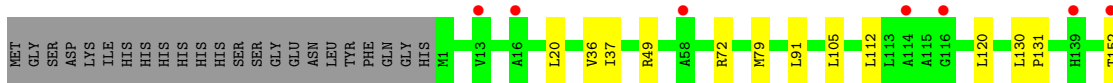
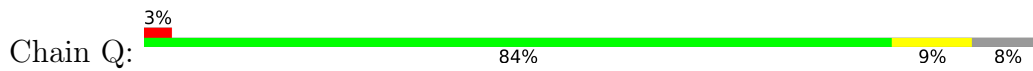




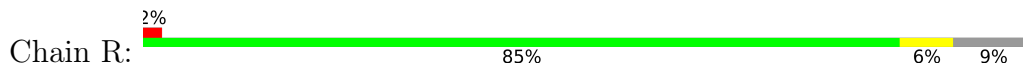
- Molecule 1: Agmatinase



- Molecule 1: Agmatinase



- Molecule 1: Agmatinase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 2.20Å)	Xtrriage
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 <sup>2</sup> )	23.6	Xtrriage
Anisotropy	0.234	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 9.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.477 for -h,-k,l 0.245 for h,-h-k,-l 0.246 for -k,-h,-l	Xtrriage
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	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	43547	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage'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.*

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

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

## 5 Model quality

### 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.

The worst 5 of 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

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	303/329 (92%)	292 (96%)	11 (4%)	0	100   100
1	B	308/329 (94%)	297 (96%)	11 (4%)	0	100   100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	234	LEU
1	O	304	LYS
1	Q	79	MET
1	F	211	ASP
1	F	163	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	61	GLN
1	G	61	GLN
1	O	300	GLN
1	G	218	GLN

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Mol	Chain	Res	Type
1	E	54	HIS

### 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 [i](#)

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9	
1	A	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

The worst 5 of 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

## 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 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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.