



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2022 – 01:11 PM EDT

PDB ID : 3N99  
Title : Crystal structure of TM1086  
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Deposited on : 2010-05-28  
Resolution : 2.38 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](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.

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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	:	2.27
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)	:	2.27

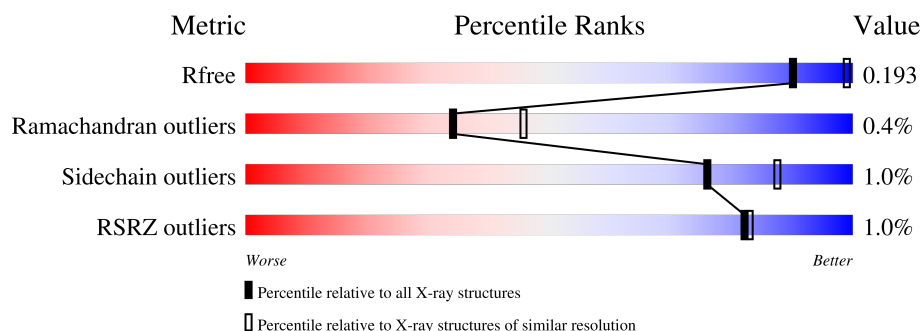
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	290	96%
1	B	290	95%
1	C	290	94%
1	D	290	96%
1	E	290	95%
1	G	290	2%

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Mol	Chain	Length	Quality of chain
1	H	290	<div> <div>2%</div> <div>95%</div> <div>..</div> </div>
1	I	290	<div> <div>%</div> <div>93%</div> <div>..</div> </div>
1	J	290	<div> <div>3%</div> <div>94%</div> <div>..</div> </div>
1	K	290	<div> <div>%</div> <div>95%</div> <div>..</div> </div>
1	L	290	<div> <div>%</div> <div>94%</div> <div>..</div> </div>
1	M	290	<div> <div>95%</div> <div>..</div> </div>
1	N	290	<div> <div>95%</div> <div>..</div> </div>
1	O	290	<div> <div>%</div> <div>95%</div> <div>..</div> </div>
1	P	290	<div> <div>94%</div> <div>..</div> </div>
1	S	290	<div> <div>%</div> <div>95%</div> <div>..</div> </div>
1	T	290	<div> <div>%</div> <div>94%</div> <div>..</div> </div>
1	U	290	<div> <div>2%</div> <div>95%</div> <div>..</div> </div>
1	V	290	<div> <div>%</div> <div>95%</div> <div>..</div> </div>
1	X	290	<div> <div>4%</div> <div>95%</div> <div>..</div> </div>
1	a	290	<div> <div>95%</div> <div>..</div> </div>
1	b	290	<div> <div>95%</div> <div>..</div> </div>
1	c	290	<div> <div>93%</div> <div>..</div> </div>
1	d	290	<div> <div>95%</div> <div>..</div> </div>
1	e	290	<div> <div>%</div> <div>96%</div> <div>..</div> </div>
1	g	290	<div> <div>%</div> <div>96%</div> <div>..</div> </div>
1	h	290	<div> <div>%</div> <div>95%</div> <div>..</div> </div>
1	i	290	<div> <div>%</div> <div>95%</div> <div>..</div> </div>
1	j	290	<div> <div>3%</div> <div>96%</div> <div>..</div> </div>
1	k	290	<div> <div>%</div> <div>94%</div> <div>..</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 68631 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 uncharacterized protein TM1086.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	2	0
			2113	1329	370	400	14			
1	B	282	Total	C	N	O	S	0	4	0
			2121	1336	373	398	14			
1	C	282	Total	C	N	O	S	0	3	0
			2123	1335	374	401	13			
1	D	282	Total	C	N	O	S	0	1	0
			2104	1323	370	398	13			
1	E	282	Total	C	N	O	S	0	1	0
			2108	1325	370	400	13			
1	G	286	Total	C	N	O	S	0	2	0
			2151	1351	382	404	14			
1	H	281	Total	C	N	O	S	0	2	0
			2107	1325	369	399	14			
1	I	281	Total	C	N	O	S	0	3	0
			2121	1333	373	402	13			
1	J	281	Total	C	N	O	S	0	2	0
			2112	1328	372	399	13			
1	K	281	Total	C	N	O	S	0	3	0
			2115	1330	372	399	14			
1	L	282	Total	C	N	O	S	0	2	0
			2111	1327	370	400	14			
1	M	282	Total	C	N	O	S	0	4	0
			2123	1335	373	402	13			
1	N	282	Total	C	N	O	S	0	2	0
			2119	1331	374	401	13			
1	O	282	Total	C	N	O	S	0	1	0
			2108	1325	370	400	13			
1	P	282	Total	C	N	O	S	0	3	0
			2120	1334	373	400	13			
1	S	281	Total	C	N	O	S	0	2	0
			2106	1324	369	399	14			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	282	Total	C	N	O	S	0	2	0
			2116	1332	370	400	14			
1	U	281	Total	C	N	O	S	0	1	0
			2107	1324	370	400	13			
1	V	282	Total	C	N	O	S	0	1	0
			2111	1328	370	400	13			
1	X	281	Total	C	N	O	S	0	1	0
			2101	1322	366	399	14			
1	a	282	Total	C	N	O	S	0	4	0
			2123	1336	373	401	13			
1	b	282	Total	C	N	O	S	0	2	0
			2116	1330	373	400	13			
1	c	282	Total	C	N	O	S	0	1	0
			2111	1326	371	401	13			
1	d	282	Total	C	N	O	S	0	2	0
			2116	1330	373	400	13			
1	e	283	Total	C	N	O	S	0	2	0
			2123	1335	374	401	13			
1	g	287	Total	C	N	O	S	0	3	0
			2166	1361	386	405	14			
1	h	281	Total	C	N	O	S	0	0	0
			2096	1318	366	399	13			
1	i	282	Total	C	N	O	S	0	1	0
			2108	1325	370	400	13			
1	j	282	Total	C	N	O	S	0	2	0
			2116	1330	373	400	13			
1	k	282	Total	C	N	O	S	0	2	0
			2119	1333	373	400	13			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	expression tag	UNP Q9X0H2
A	-6	HIS	-	expression tag	UNP Q9X0H2
A	-5	HIS	-	expression tag	UNP Q9X0H2
A	-4	HIS	-	expression tag	UNP Q9X0H2
A	-3	HIS	-	expression tag	UNP Q9X0H2
A	-2	HIS	-	expression tag	UNP Q9X0H2
A	-1	GLY	-	expression tag	UNP Q9X0H2
A	0	HIS	-	expression tag	UNP Q9X0H2
B	-7	HIS	-	expression tag	UNP Q9X0H2
B	-6	HIS	-	expression tag	UNP Q9X0H2
B	-5	HIS	-	expression tag	UNP Q9X0H2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP Q9X0H2
B	-3	HIS	-	expression tag	UNP Q9X0H2
B	-2	HIS	-	expression tag	UNP Q9X0H2
B	-1	GLY	-	expression tag	UNP Q9X0H2
B	0	HIS	-	expression tag	UNP Q9X0H2
C	-7	HIS	-	expression tag	UNP Q9X0H2
C	-6	HIS	-	expression tag	UNP Q9X0H2
C	-5	HIS	-	expression tag	UNP Q9X0H2
C	-4	HIS	-	expression tag	UNP Q9X0H2
C	-3	HIS	-	expression tag	UNP Q9X0H2
C	-2	HIS	-	expression tag	UNP Q9X0H2
C	-1	GLY	-	expression tag	UNP Q9X0H2
C	0	HIS	-	expression tag	UNP Q9X0H2
D	-7	HIS	-	expression tag	UNP Q9X0H2
D	-6	HIS	-	expression tag	UNP Q9X0H2
D	-5	HIS	-	expression tag	UNP Q9X0H2
D	-4	HIS	-	expression tag	UNP Q9X0H2
D	-3	HIS	-	expression tag	UNP Q9X0H2
D	-2	HIS	-	expression tag	UNP Q9X0H2
D	-1	GLY	-	expression tag	UNP Q9X0H2
D	0	HIS	-	expression tag	UNP Q9X0H2
E	-7	HIS	-	expression tag	UNP Q9X0H2
E	-6	HIS	-	expression tag	UNP Q9X0H2
E	-5	HIS	-	expression tag	UNP Q9X0H2
E	-4	HIS	-	expression tag	UNP Q9X0H2
E	-3	HIS	-	expression tag	UNP Q9X0H2
E	-2	HIS	-	expression tag	UNP Q9X0H2
E	-1	GLY	-	expression tag	UNP Q9X0H2
E	0	HIS	-	expression tag	UNP Q9X0H2
G	-7	HIS	-	expression tag	UNP Q9X0H2
G	-6	HIS	-	expression tag	UNP Q9X0H2
G	-5	HIS	-	expression tag	UNP Q9X0H2
G	-4	HIS	-	expression tag	UNP Q9X0H2
G	-3	HIS	-	expression tag	UNP Q9X0H2
G	-2	HIS	-	expression tag	UNP Q9X0H2
G	-1	GLY	-	expression tag	UNP Q9X0H2
G	0	HIS	-	expression tag	UNP Q9X0H2
H	-7	HIS	-	expression tag	UNP Q9X0H2
H	-6	HIS	-	expression tag	UNP Q9X0H2
H	-5	HIS	-	expression tag	UNP Q9X0H2
H	-4	HIS	-	expression tag	UNP Q9X0H2
H	-3	HIS	-	expression tag	UNP Q9X0H2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	HIS	-	expression tag	UNP Q9X0H2
H	-1	GLY	-	expression tag	UNP Q9X0H2
H	0	HIS	-	expression tag	UNP Q9X0H2
I	-7	HIS	-	expression tag	UNP Q9X0H2
I	-6	HIS	-	expression tag	UNP Q9X0H2
I	-5	HIS	-	expression tag	UNP Q9X0H2
I	-4	HIS	-	expression tag	UNP Q9X0H2
I	-3	HIS	-	expression tag	UNP Q9X0H2
I	-2	HIS	-	expression tag	UNP Q9X0H2
I	-1	GLY	-	expression tag	UNP Q9X0H2
I	0	HIS	-	expression tag	UNP Q9X0H2
J	-7	HIS	-	expression tag	UNP Q9X0H2
J	-6	HIS	-	expression tag	UNP Q9X0H2
J	-5	HIS	-	expression tag	UNP Q9X0H2
J	-4	HIS	-	expression tag	UNP Q9X0H2
J	-3	HIS	-	expression tag	UNP Q9X0H2
J	-2	HIS	-	expression tag	UNP Q9X0H2
J	-1	GLY	-	expression tag	UNP Q9X0H2
J	0	HIS	-	expression tag	UNP Q9X0H2
K	-7	HIS	-	expression tag	UNP Q9X0H2
K	-6	HIS	-	expression tag	UNP Q9X0H2
K	-5	HIS	-	expression tag	UNP Q9X0H2
K	-4	HIS	-	expression tag	UNP Q9X0H2
K	-3	HIS	-	expression tag	UNP Q9X0H2
K	-2	HIS	-	expression tag	UNP Q9X0H2
K	-1	GLY	-	expression tag	UNP Q9X0H2
K	0	HIS	-	expression tag	UNP Q9X0H2
L	-7	HIS	-	expression tag	UNP Q9X0H2
L	-6	HIS	-	expression tag	UNP Q9X0H2
L	-5	HIS	-	expression tag	UNP Q9X0H2
L	-4	HIS	-	expression tag	UNP Q9X0H2
L	-3	HIS	-	expression tag	UNP Q9X0H2
L	-2	HIS	-	expression tag	UNP Q9X0H2
L	-1	GLY	-	expression tag	UNP Q9X0H2
L	0	HIS	-	expression tag	UNP Q9X0H2
M	-7	HIS	-	expression tag	UNP Q9X0H2
M	-6	HIS	-	expression tag	UNP Q9X0H2
M	-5	HIS	-	expression tag	UNP Q9X0H2
M	-4	HIS	-	expression tag	UNP Q9X0H2
M	-3	HIS	-	expression tag	UNP Q9X0H2
M	-2	HIS	-	expression tag	UNP Q9X0H2
M	-1	GLY	-	expression tag	UNP Q9X0H2

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Chain	Residue	Modelled	Actual	Comment	Reference
M	0	HIS	-	expression tag	UNP Q9X0H2
N	-7	HIS	-	expression tag	UNP Q9X0H2
N	-6	HIS	-	expression tag	UNP Q9X0H2
N	-5	HIS	-	expression tag	UNP Q9X0H2
N	-4	HIS	-	expression tag	UNP Q9X0H2
N	-3	HIS	-	expression tag	UNP Q9X0H2
N	-2	HIS	-	expression tag	UNP Q9X0H2
N	-1	GLY	-	expression tag	UNP Q9X0H2
N	0	HIS	-	expression tag	UNP Q9X0H2
O	-7	HIS	-	expression tag	UNP Q9X0H2
O	-6	HIS	-	expression tag	UNP Q9X0H2
O	-5	HIS	-	expression tag	UNP Q9X0H2
O	-4	HIS	-	expression tag	UNP Q9X0H2
O	-3	HIS	-	expression tag	UNP Q9X0H2
O	-2	HIS	-	expression tag	UNP Q9X0H2
O	-1	GLY	-	expression tag	UNP Q9X0H2
O	0	HIS	-	expression tag	UNP Q9X0H2
P	-7	HIS	-	expression tag	UNP Q9X0H2
P	-6	HIS	-	expression tag	UNP Q9X0H2
P	-5	HIS	-	expression tag	UNP Q9X0H2
P	-4	HIS	-	expression tag	UNP Q9X0H2
P	-3	HIS	-	expression tag	UNP Q9X0H2
P	-2	HIS	-	expression tag	UNP Q9X0H2
P	-1	GLY	-	expression tag	UNP Q9X0H2
P	0	HIS	-	expression tag	UNP Q9X0H2
S	-7	HIS	-	expression tag	UNP Q9X0H2
S	-6	HIS	-	expression tag	UNP Q9X0H2
S	-5	HIS	-	expression tag	UNP Q9X0H2
S	-4	HIS	-	expression tag	UNP Q9X0H2
S	-3	HIS	-	expression tag	UNP Q9X0H2
S	-2	HIS	-	expression tag	UNP Q9X0H2
S	-1	GLY	-	expression tag	UNP Q9X0H2
S	0	HIS	-	expression tag	UNP Q9X0H2
T	-7	HIS	-	expression tag	UNP Q9X0H2
T	-6	HIS	-	expression tag	UNP Q9X0H2
T	-5	HIS	-	expression tag	UNP Q9X0H2
T	-4	HIS	-	expression tag	UNP Q9X0H2
T	-3	HIS	-	expression tag	UNP Q9X0H2
T	-2	HIS	-	expression tag	UNP Q9X0H2
T	-1	GLY	-	expression tag	UNP Q9X0H2
T	0	HIS	-	expression tag	UNP Q9X0H2
U	-7	HIS	-	expression tag	UNP Q9X0H2

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Chain	Residue	Modelled	Actual	Comment	Reference
U	-6	HIS	-	expression tag	UNP Q9X0H2
U	-5	HIS	-	expression tag	UNP Q9X0H2
U	-4	HIS	-	expression tag	UNP Q9X0H2
U	-3	HIS	-	expression tag	UNP Q9X0H2
U	-2	HIS	-	expression tag	UNP Q9X0H2
U	-1	GLY	-	expression tag	UNP Q9X0H2
U	0	HIS	-	expression tag	UNP Q9X0H2
V	-7	HIS	-	expression tag	UNP Q9X0H2
V	-6	HIS	-	expression tag	UNP Q9X0H2
V	-5	HIS	-	expression tag	UNP Q9X0H2
V	-4	HIS	-	expression tag	UNP Q9X0H2
V	-3	HIS	-	expression tag	UNP Q9X0H2
V	-2	HIS	-	expression tag	UNP Q9X0H2
V	-1	GLY	-	expression tag	UNP Q9X0H2
V	0	HIS	-	expression tag	UNP Q9X0H2
X	-7	HIS	-	expression tag	UNP Q9X0H2
X	-6	HIS	-	expression tag	UNP Q9X0H2
X	-5	HIS	-	expression tag	UNP Q9X0H2
X	-4	HIS	-	expression tag	UNP Q9X0H2
X	-3	HIS	-	expression tag	UNP Q9X0H2
X	-2	HIS	-	expression tag	UNP Q9X0H2
X	-1	GLY	-	expression tag	UNP Q9X0H2
X	0	HIS	-	expression tag	UNP Q9X0H2
a	-7	HIS	-	expression tag	UNP Q9X0H2
a	-6	HIS	-	expression tag	UNP Q9X0H2
a	-5	HIS	-	expression tag	UNP Q9X0H2
a	-4	HIS	-	expression tag	UNP Q9X0H2
a	-3	HIS	-	expression tag	UNP Q9X0H2
a	-2	HIS	-	expression tag	UNP Q9X0H2
a	-1	GLY	-	expression tag	UNP Q9X0H2
a	0	HIS	-	expression tag	UNP Q9X0H2
b	-7	HIS	-	expression tag	UNP Q9X0H2
b	-6	HIS	-	expression tag	UNP Q9X0H2
b	-5	HIS	-	expression tag	UNP Q9X0H2
b	-4	HIS	-	expression tag	UNP Q9X0H2
b	-3	HIS	-	expression tag	UNP Q9X0H2
b	-2	HIS	-	expression tag	UNP Q9X0H2
b	-1	GLY	-	expression tag	UNP Q9X0H2
b	0	HIS	-	expression tag	UNP Q9X0H2
c	-7	HIS	-	expression tag	UNP Q9X0H2
c	-6	HIS	-	expression tag	UNP Q9X0H2
c	-5	HIS	-	expression tag	UNP Q9X0H2

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Chain	Residue	Modelled	Actual	Comment	Reference
c	-4	HIS	-	expression tag	UNP Q9X0H2
c	-3	HIS	-	expression tag	UNP Q9X0H2
c	-2	HIS	-	expression tag	UNP Q9X0H2
c	-1	GLY	-	expression tag	UNP Q9X0H2
c	0	HIS	-	expression tag	UNP Q9X0H2
d	-7	HIS	-	expression tag	UNP Q9X0H2
d	-6	HIS	-	expression tag	UNP Q9X0H2
d	-5	HIS	-	expression tag	UNP Q9X0H2
d	-4	HIS	-	expression tag	UNP Q9X0H2
d	-3	HIS	-	expression tag	UNP Q9X0H2
d	-2	HIS	-	expression tag	UNP Q9X0H2
d	-1	GLY	-	expression tag	UNP Q9X0H2
d	0	HIS	-	expression tag	UNP Q9X0H2
e	-7	HIS	-	expression tag	UNP Q9X0H2
e	-6	HIS	-	expression tag	UNP Q9X0H2
e	-5	HIS	-	expression tag	UNP Q9X0H2
e	-4	HIS	-	expression tag	UNP Q9X0H2
e	-3	HIS	-	expression tag	UNP Q9X0H2
e	-2	HIS	-	expression tag	UNP Q9X0H2
e	-1	GLY	-	expression tag	UNP Q9X0H2
e	0	HIS	-	expression tag	UNP Q9X0H2
g	-7	HIS	-	expression tag	UNP Q9X0H2
g	-6	HIS	-	expression tag	UNP Q9X0H2
g	-5	HIS	-	expression tag	UNP Q9X0H2
g	-4	HIS	-	expression tag	UNP Q9X0H2
g	-3	HIS	-	expression tag	UNP Q9X0H2
g	-2	HIS	-	expression tag	UNP Q9X0H2
g	-1	GLY	-	expression tag	UNP Q9X0H2
g	0	HIS	-	expression tag	UNP Q9X0H2
h	-7	HIS	-	expression tag	UNP Q9X0H2
h	-6	HIS	-	expression tag	UNP Q9X0H2
h	-5	HIS	-	expression tag	UNP Q9X0H2
h	-4	HIS	-	expression tag	UNP Q9X0H2
h	-3	HIS	-	expression tag	UNP Q9X0H2
h	-2	HIS	-	expression tag	UNP Q9X0H2
h	-1	GLY	-	expression tag	UNP Q9X0H2
h	0	HIS	-	expression tag	UNP Q9X0H2
i	-7	HIS	-	expression tag	UNP Q9X0H2
i	-6	HIS	-	expression tag	UNP Q9X0H2
i	-5	HIS	-	expression tag	UNP Q9X0H2
i	-4	HIS	-	expression tag	UNP Q9X0H2
i	-3	HIS	-	expression tag	UNP Q9X0H2

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Chain	Residue	Modelled	Actual	Comment	Reference
i	-2	HIS	-	expression tag	UNP Q9X0H2
i	-1	GLY	-	expression tag	UNP Q9X0H2
i	0	HIS	-	expression tag	UNP Q9X0H2
j	-7	HIS	-	expression tag	UNP Q9X0H2
j	-6	HIS	-	expression tag	UNP Q9X0H2
j	-5	HIS	-	expression tag	UNP Q9X0H2
j	-4	HIS	-	expression tag	UNP Q9X0H2
j	-3	HIS	-	expression tag	UNP Q9X0H2
j	-2	HIS	-	expression tag	UNP Q9X0H2
j	-1	GLY	-	expression tag	UNP Q9X0H2
j	0	HIS	-	expression tag	UNP Q9X0H2
k	-7	HIS	-	expression tag	UNP Q9X0H2
k	-6	HIS	-	expression tag	UNP Q9X0H2
k	-5	HIS	-	expression tag	UNP Q9X0H2
k	-4	HIS	-	expression tag	UNP Q9X0H2
k	-3	HIS	-	expression tag	UNP Q9X0H2
k	-2	HIS	-	expression tag	UNP Q9X0H2
k	-1	GLY	-	expression tag	UNP Q9X0H2
k	0	HIS	-	expression tag	UNP Q9X0H2

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Cl 3 3	0	0
2	B	3	Total Cl 3 3	0	0
2	C	3	Total Cl 3 3	0	0
2	D	3	Total Cl 3 3	0	0
2	E	2	Total Cl 2 2	0	0
2	G	3	Total Cl 3 3	0	0
2	H	3	Total Cl 3 3	0	0
2	I	3	Total Cl 3 3	0	0
2	J	2	Total Cl 2 2	0	0
2	K	2	Total Cl 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	3	Total 3	Cl 3	0	0
2	M	3	Total 3	Cl 3	0	0
2	N	3	Total 3	Cl 3	0	0
2	O	3	Total 3	Cl 3	0	0
2	P	2	Total 2	Cl 2	0	0
2	S	3	Total 3	Cl 3	0	0
2	T	3	Total 3	Cl 3	0	0
2	U	3	Total 3	Cl 3	0	0
2	V	3	Total 3	Cl 3	0	0
2	X	3	Total 3	Cl 3	0	0
2	a	3	Total 3	Cl 3	0	0
2	b	3	Total 3	Cl 3	0	0
2	c	3	Total 3	Cl 3	0	0
2	d	3	Total 3	Cl 3	0	0
2	e	3	Total 3	Cl 3	0	0
2	g	2	Total 2	Cl 2	0	0
2	h	3	Total 3	Cl 3	0	0
2	i	3	Total 3	Cl 3	0	0
2	j	3	Total 3	Cl 3	0	0
2	k	4	Total 4	Cl 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	175	Total O 175 175	0	0
3	B	182	Total O 182 182	0	0
3	C	185	Total O 185 185	0	0
3	D	190	Total O 190 190	0	0
3	E	192	Total O 192 192	0	0
3	G	145	Total O 145 145	0	0
3	H	153	Total O 153 153	0	0
3	I	164	Total O 164 164	0	0
3	J	135	Total O 135 135	0	0
3	K	156	Total O 156 156	0	0
3	L	179	Total O 179 179	0	0
3	M	176	Total O 176 176	0	0
3	N	174	Total O 174 174	0	0
3	O	183	Total O 183 183	0	0
3	P	170	Total O 170 170	0	0
3	S	166	Total O 166 166	0	0
3	T	158	Total O 158 158	0	0
3	U	147	Total O 147 147	0	0
3	V	148	Total O 148 148	0	0
3	X	155	Total O 155 155	0	0
3	a	194	Total O 194 194	0	0
3	b	195	Total O 195 195	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	c	196	Total 196	O 196	0	0
3	d	179	Total 179	O 179	0	0
3	e	183	Total 183	O 183	0	0
3	g	152	Total 152	O 152	0	0
3	h	158	Total 158	O 158	0	0
3	i	139	Total 139	O 139	0	0
3	j	151	Total 151	O 151	0	0
3	k	174	Total 174	O 174	0	0



- Molecule 1: uncharacterized protein TM1086



- Chain B:  95% 5%



- Chain C:  94% . .



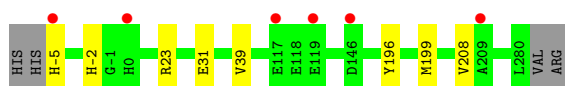
- Chain D:  96%



- Chain E:  95% . .



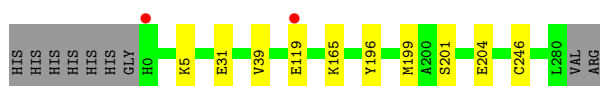
- Chain G:  2% 96%



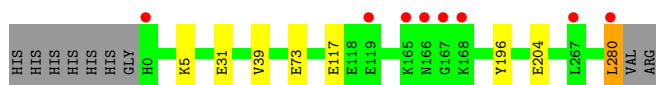
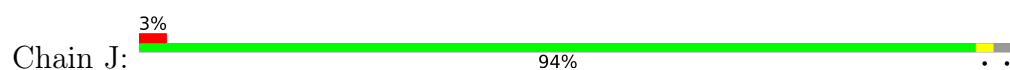
- Molecule 1: uncharacterized protein TM1086



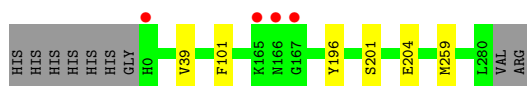
- Molecule 1: uncharacterized protein TM1086



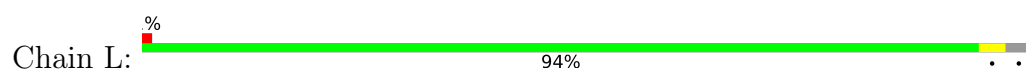
- Molecule 1: uncharacterized protein TM1086



- Molecule 1: uncharacterized protein TM1086



- Molecule 1: uncharacterized protein TM1086



- Molecule 1: uncharacterized protein TM1086



- Molecule 1: uncharacterized protein TM1086



Chain N:  95%



• Molecule 1: uncharacterized protein TM1086

Chain O:  95%



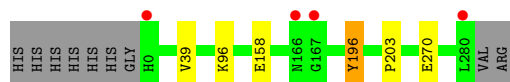
• Molecule 1: uncharacterized protein TM1086

Chain P:  94%



• Molecule 1: uncharacterized protein TM1086

Chain S:  95%



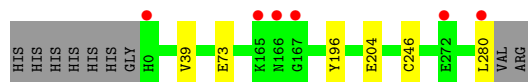
• Molecule 1: uncharacterized protein TM1086

Chain T:  94%



• Molecule 1: uncharacterized protein TM1086

Chain U:  95%

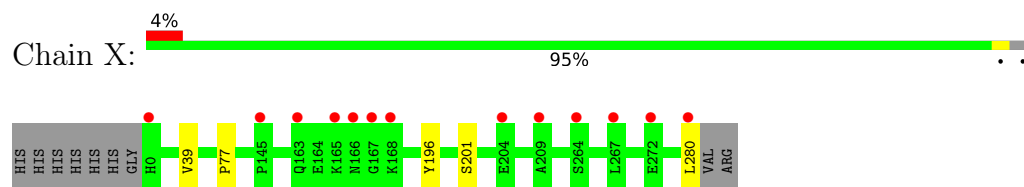


• Molecule 1: uncharacterized protein TM1086

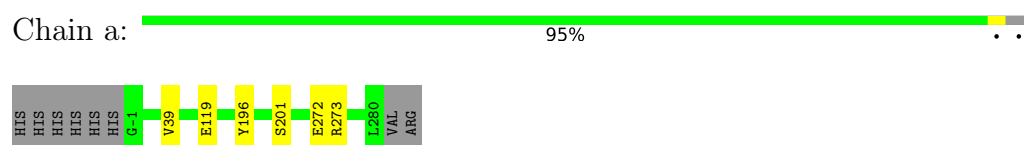
Chain V:  95%



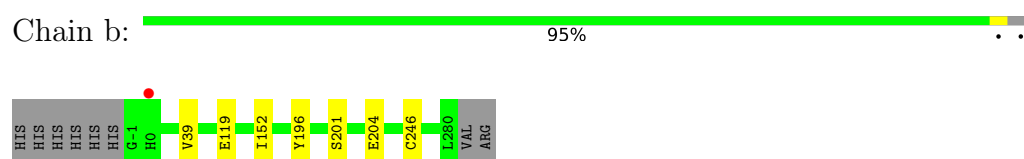
- Molecule 1: uncharacterized protein TM1086



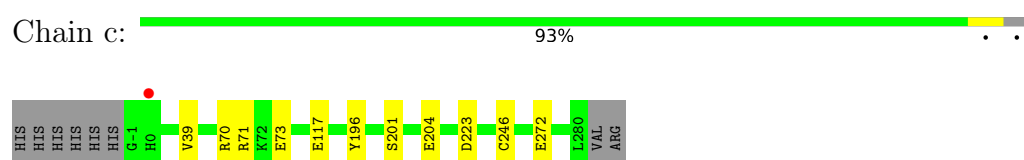
- Molecule 1: uncharacterized protein TM1086



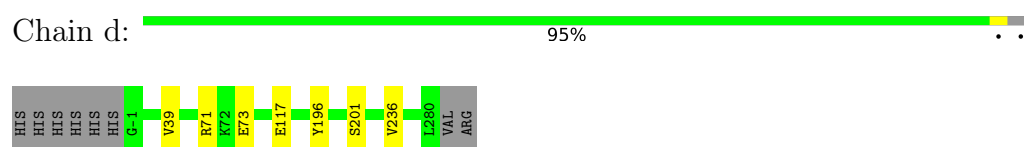
- Molecule 1: uncharacterized protein TM1086



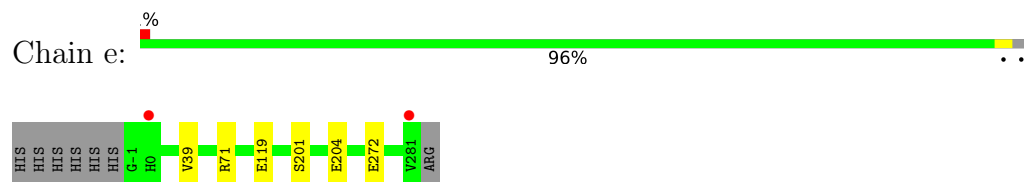
- Molecule 1: uncharacterized protein TM1086



- Molecule 1: uncharacterized protein TM1086



- Molecule 1: uncharacterized protein TM1086



- Molecule 1: uncharacterized protein TM1086





- Molecule 1: uncharacterized protein TM1086



- Molecule 1: uncharacterized protein TM1086



- Molecule 1: uncharacterized protein TM1086



- Molecule 1: uncharacterized protein TM1086



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	289.84Å 299.52Å 316.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.38 37.32 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.38) 99.1 (37.32-2.38)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.67 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.151 , 0.191 0.155 , 0.193	Depositor DCC
$R_{free}$ test set	26930 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	68631	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 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	0.95	1/2155 (0.0%)	0.84	2/2912 (0.1%)
1	B	0.92	3/2169 (0.1%)	0.83	0/2931
1	C	0.94	1/2165 (0.0%)	0.89	5/2926 (0.2%)
1	D	0.98	3/2143 (0.1%)	0.85	0/2897
1	E	0.96	2/2147 (0.1%)	0.85	0/2902
1	G	0.95	1/2197 (0.0%)	0.83	0/2970
1	H	0.91	3/2149 (0.1%)	0.84	1/2905 (0.0%)
1	I	0.92	4/2163 (0.2%)	0.84	2/2923 (0.1%)
1	J	0.96	4/2154 (0.2%)	0.84	1/2911 (0.0%)
1	K	0.91	2/2160 (0.1%)	0.83	1/2919 (0.0%)
1	L	0.95	3/2153 (0.1%)	0.85	2/2910 (0.1%)
1	M	0.95	2/2171 (0.1%)	0.84	1/2934 (0.0%)
1	N	0.91	4/2158 (0.2%)	0.84	1/2916 (0.0%)
1	O	0.96	3/2147 (0.1%)	0.85	0/2902
1	P	0.96	3/2165 (0.1%)	0.87	2/2926 (0.1%)
1	S	0.91	2/2148 (0.1%)	0.82	2/2903 (0.1%)
1	T	0.91	5/2158 (0.2%)	0.83	2/2917 (0.1%)
1	U	0.91	3/2143 (0.1%)	0.84	1/2897 (0.0%)
1	V	0.94	3/2150 (0.1%)	0.83	0/2907
1	X	0.93	0/2140	0.84	0/2893
1	a	0.94	2/2171 (0.1%)	0.82	0/2934
1	b	0.93	3/2158 (0.1%)	0.84	0/2916
1	c	0.97	5/2147 (0.2%)	0.84	3/2902 (0.1%)
1	d	0.91	3/2158 (0.1%)	0.84	1/2916 (0.0%)
1	e	0.90	3/2165 (0.1%)	0.84	1/2926 (0.0%)
1	g	0.93	3/2215 (0.1%)	0.85	2/2994 (0.1%)
1	h	0.92	2/2132 (0.1%)	0.83	2/2883 (0.1%)
1	i	0.95	4/2147 (0.2%)	0.84	0/2902
1	j	0.97	2/2158 (0.1%)	0.83	1/2916 (0.0%)
1	k	0.97	4/2161 (0.2%)	0.84	0/2921
All	All	0.94	83/64747 (0.1%)	0.84	33/87511 (0.0%)

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	j	117	GLU	CG-CD	5.99	1.60	1.51
1	b	204	GLU	CG-CD	5.93	1.60	1.51
1	C	73	GLU	CG-CD	5.92	1.60	1.51
1	c	117	GLU	CG-CD	5.90	1.60	1.51
1	I	204	GLU	CG-CD	5.89	1.60	1.51
1	P	73	GLU	CG-CD	5.89	1.60	1.51
1	e	204	GLU	CG-CD	5.88	1.60	1.51
1	L	272	GLU	CG-CD	5.85	1.60	1.51
1	T	204	GLU	CG-CD	5.84	1.60	1.51
1	H	73	GLU	CG-CD	5.83	1.60	1.51
1	L	204	GLU	CG-CD	5.83	1.60	1.51
1	V	31	GLU	CG-CD	5.82	1.60	1.51
1	J	117	GLU	CG-CD	5.79	1.60	1.51
1	g	73	GLU	CG-CD	5.79	1.60	1.51
1	D	119	GLU	CG-CD	5.77	1.60	1.51
1	D	73	GLU	CG-CD	5.73	1.60	1.51
1	j	73	GLU	CG-CD	5.73	1.60	1.51
1	b	246	CYS	CB-SG	5.72	1.92	1.82
1	c	73	GLU	CG-CD	5.72	1.60	1.51
1	d	73	GLU	CG-CD	5.71	1.60	1.51
1	d	236	VAL	CB-CG1	-5.71	1.40	1.52
1	c	272	GLU	CG-CD	5.69	1.60	1.51
1	G	31	GLU	CG-CD	5.68	1.60	1.51
1	P	31	GLU	CG-CD	5.68	1.60	1.51
1	i	117	GLU	CG-CD	5.66	1.60	1.51
1	i	204	GLU	CG-CD	5.66	1.60	1.51
1	D	31	GLU	CG-CD	5.63	1.60	1.51
1	I	119	GLU	CG-CD	5.62	1.60	1.51
1	d	117	GLU	CG-CD	5.62	1.60	1.51
1	B	272	GLU	CG-CD	5.61	1.60	1.51
1	I	246	CYS	CB-SG	5.61	1.91	1.82
1	i	73	GLU	CG-CD	5.60	1.60	1.51
1	e	119	GLU	CG-CD	5.56	1.60	1.51
1	i	270	GLU	CD-OE1	5.56	1.31	1.25
1	k	31	GLU	CG-CD	5.56	1.60	1.51
1	K	204	GLU	CG-CD	5.54	1.60	1.51
1	N	73	GLU	CG-CD	5.53	1.60	1.51
1	N	117	GLU	CG-CD	5.53	1.60	1.51
1	I	31	GLU	CG-CD	5.52	1.60	1.51
1	U	204	GLU	CG-CD	5.50	1.60	1.51
1	N	119	GLU	CG-CD	5.48	1.60	1.51
1	A	73	GLU	CG-CD	5.47	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	k	117	GLU	CG-CD	5.47	1.60	1.51
1	J	31	GLU	CG-CD	5.46	1.60	1.51
1	k	204	GLU	CG-CD	5.45	1.60	1.51
1	h	204	GLU	CG-CD	5.45	1.60	1.51
1	E	204	GLU	CG-CD	5.44	1.60	1.51
1	B	73	GLU	CG-CD	5.43	1.60	1.51
1	H	117	GLU	CG-CD	5.43	1.60	1.51
1	J	204	GLU	CG-CD	5.42	1.60	1.51
1	a	119	GLU	CG-CD	5.41	1.60	1.51
1	M	73	GLU	CG-CD	5.41	1.60	1.51
1	M	119	GLU	CG-CD	5.40	1.60	1.51
1	c	204	GLU	CG-CD	5.39	1.60	1.51
1	T	101	PHE	CD2-CE2	5.35	1.50	1.39
1	O	246	CYS	CB-SG	5.34	1.91	1.82
1	T	117	GLU	CG-CD	5.33	1.59	1.51
1	U	73	GLU	CG-CD	5.32	1.59	1.51
1	P	204	GLU	CG-CD	5.32	1.59	1.51
1	e	272	GLU	CG-CD	5.32	1.59	1.51
1	k	119	GLU	CG-CD	5.32	1.59	1.51
1	H	204	GLU	CG-CD	5.31	1.59	1.51
1	J	73	GLU	CG-CD	5.27	1.59	1.51
1	K	101	PHE	CD1-CE1	5.27	1.49	1.39
1	T	73	GLU	CG-CD	5.26	1.59	1.51
1	g	119	GLU	CG-CD	5.26	1.59	1.51
1	B	34	VAL	CB-CG1	5.24	1.63	1.52
1	V	204	GLU	CG-CD	5.24	1.59	1.51
1	L	73	GLU	CG-CD	5.23	1.59	1.51
1	b	119	GLU	CG-CD	5.17	1.59	1.51
1	N	272	GLU	CG-CD	5.16	1.59	1.51
1	U	246	CYS	CB-SG	5.15	1.91	1.82
1	a	272	GLU	CG-CD	5.13	1.59	1.51
1	S	158	GLU	CG-CD	5.12	1.59	1.51
1	E	272	GLU	CB-CG	5.10	1.61	1.52
1	g	117	GLU	CG-CD	5.08	1.59	1.51
1	V	119	GLU	CG-CD	5.06	1.59	1.51
1	T	119	GLU	CG-CD	5.05	1.59	1.51
1	O	73	GLU	CG-CD	5.05	1.59	1.51
1	S	270	GLU	CG-CD	5.04	1.59	1.51
1	c	246	CYS	CB-SG	5.04	1.90	1.82
1	h	119	GLU	CG-CD	5.04	1.59	1.51
1	O	119	GLU	CG-CD	5.01	1.59	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	155	ASP	CB-CG-OD1	5.99	123.69	118.30
1	c	71	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	N	155	ASP	CB-CG-OD1	5.86	123.57	118.30
1	K	259	MET	CG-SD-CE	-5.79	90.94	100.20
1	T	71	ARG	NE-CZ-NH2	5.75	123.18	120.30
1	A	10[A]	ARG	NE-CZ-NH1	-5.73	117.43	120.30
1	A	10[B]	ARG	NE-CZ-NH1	-5.73	117.43	120.30
1	M	259	MET	CG-SD-CE	-5.61	91.23	100.20
1	C	273	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	U	280	LEU	CA-CB-CG	5.52	127.99	115.30
1	j	280	LEU	CA-CB-CG	5.51	127.96	115.30
1	I	199	MET	CG-SD-CE	-5.43	91.51	100.20
1	d	71	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	P	71	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	T	181	MET	CG-SD-CE	5.30	108.67	100.20
1	C	210	ASP	CB-CG-OD1	5.27	123.05	118.30
1	H	59	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	h	280	LEU	CA-CB-CG	5.21	127.28	115.30
1	P	6	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	c	223	ASP	CB-CG-OD1	5.18	122.96	118.30
1	e	71	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	S	96	LYS	CD-CE-NZ	-5.14	99.89	111.70
1	c	70	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	C	232[A]	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	C	232[B]	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	L	195	ASP	CB-CG-OD1	5.12	122.91	118.30
1	L	199	MET	CG-SD-CE	-5.11	92.02	100.20
1	J	280	LEU	CA-CB-CG	5.08	126.98	115.30
1	I	165	LYS	CB-CA-C	-5.08	100.25	110.40
1	g	10[A]	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	g	10[B]	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	S	196	TYR	CA-CB-CG	5.05	123.00	113.40
1	h	71	ARG	NE-CZ-NH2	5.03	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.



## 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	282/290 (97%)	272 (96%)	9 (3%)	1 (0%)	34	46
1	B	284/290 (98%)	274 (96%)	9 (3%)	1 (0%)	34	46
1	C	283/290 (98%)	273 (96%)	9 (3%)	1 (0%)	34	46
1	D	281/290 (97%)	270 (96%)	10 (4%)	1 (0%)	34	46
1	E	281/290 (97%)	271 (96%)	9 (3%)	1 (0%)	34	46
1	G	286/290 (99%)	277 (97%)	8 (3%)	1 (0%)	41	53
1	H	281/290 (97%)	271 (96%)	9 (3%)	1 (0%)	34	46
1	I	282/290 (97%)	272 (96%)	9 (3%)	1 (0%)	34	46
1	J	281/290 (97%)	269 (96%)	11 (4%)	1 (0%)	34	46
1	K	282/290 (97%)	270 (96%)	11 (4%)	1 (0%)	34	46
1	L	282/290 (97%)	271 (96%)	10 (4%)	1 (0%)	34	46
1	M	284/290 (98%)	275 (97%)	8 (3%)	1 (0%)	34	46
1	N	282/290 (97%)	273 (97%)	8 (3%)	1 (0%)	34	46
1	O	281/290 (97%)	273 (97%)	7 (2%)	1 (0%)	34	46
1	P	283/290 (98%)	275 (97%)	7 (2%)	1 (0%)	34	46
1	S	281/290 (97%)	269 (96%)	11 (4%)	1 (0%)	34	46
1	T	282/290 (97%)	271 (96%)	10 (4%)	1 (0%)	34	46
1	U	280/290 (97%)	268 (96%)	11 (4%)	1 (0%)	34	46
1	V	281/290 (97%)	272 (97%)	8 (3%)	1 (0%)	34	46
1	X	280/290 (97%)	271 (97%)	8 (3%)	1 (0%)	34	46
1	a	284/290 (98%)	275 (97%)	8 (3%)	1 (0%)	34	46
1	b	282/290 (97%)	272 (96%)	9 (3%)	1 (0%)	34	46
1	c	281/290 (97%)	271 (96%)	9 (3%)	1 (0%)	34	46
1	d	282/290 (97%)	271 (96%)	10 (4%)	1 (0%)	34	46
1	e	283/290 (98%)	272 (96%)	10 (4%)	1 (0%)	34	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	g	288/290 (99%)	277 (96%)	9 (3%)	2 (1%)	22	30
1	h	279/290 (96%)	266 (95%)	12 (4%)	1 (0%)	34	46
1	i	281/290 (97%)	269 (96%)	11 (4%)	1 (0%)	34	46
1	j	282/290 (97%)	271 (96%)	10 (4%)	1 (0%)	34	46
1	k	282/290 (97%)	272 (96%)	9 (3%)	1 (0%)	34	46
All	All	8463/8700 (97%)	8153 (96%)	279 (3%)	31 (0%)	34	46

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	g	205	ASP
1	B	39	VAL
1	C	39	VAL
1	G	39	VAL
1	H	39	VAL
1	I	39	VAL
1	J	39	VAL
1	K	39	VAL
1	N	39	VAL
1	O	39	VAL
1	P	39	VAL
1	S	39	VAL
1	T	39	VAL
1	U	39	VAL
1	V	39	VAL
1	X	39	VAL
1	a	39	VAL
1	c	39	VAL
1	e	39	VAL
1	h	39	VAL
1	i	39	VAL
1	k	39	VAL
1	A	39	VAL
1	D	39	VAL
1	E	39	VAL
1	L	39	VAL
1	M	39	VAL
1	b	39	VAL
1	d	39	VAL
1	g	39	VAL

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Mol	Chain	Res	Type
1	j	39	VAL

### 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	231/237 (98%)	230 (100%)	1 (0%)	91	96
1	B	232/237 (98%)	230 (99%)	2 (1%)	78	89
1	C	232/237 (98%)	230 (99%)	2 (1%)	78	89
1	D	229/237 (97%)	229 (100%)	0	100	100
1	E	230/237 (97%)	227 (99%)	3 (1%)	69	82
1	G	235/237 (99%)	229 (97%)	6 (3%)	46	64
1	H	231/237 (98%)	230 (100%)	1 (0%)	91	96
1	I	232/237 (98%)	229 (99%)	3 (1%)	69	82
1	J	231/237 (98%)	228 (99%)	3 (1%)	69	82
1	K	232/237 (98%)	230 (99%)	2 (1%)	78	89
1	L	231/237 (98%)	228 (99%)	3 (1%)	69	82
1	M	233/237 (98%)	231 (99%)	2 (1%)	78	89
1	N	231/237 (98%)	230 (100%)	1 (0%)	91	96
1	O	230/237 (97%)	228 (99%)	2 (1%)	78	89
1	P	232/237 (98%)	229 (99%)	3 (1%)	69	82
1	S	230/237 (97%)	228 (99%)	2 (1%)	78	89
1	T	232/237 (98%)	230 (99%)	2 (1%)	78	89
1	U	230/237 (97%)	229 (100%)	1 (0%)	91	96
1	V	231/237 (98%)	229 (99%)	2 (1%)	78	89
1	X	230/237 (97%)	226 (98%)	4 (2%)	60	76
1	a	233/237 (98%)	230 (99%)	3 (1%)	69	82
1	b	231/237 (98%)	228 (99%)	3 (1%)	69	82
1	c	230/237 (97%)	228 (99%)	2 (1%)	78	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	d	231/237 (98%)	229 (99%)	2 (1%)	78	89
1	e	232/237 (98%)	231 (100%)	1 (0%)	91	96
1	g	237/237 (100%)	233 (98%)	4 (2%)	60	76
1	h	229/237 (97%)	228 (100%)	1 (0%)	91	96
1	i	230/237 (97%)	229 (100%)	1 (0%)	91	96
1	j	231/237 (98%)	230 (100%)	1 (0%)	91	96
1	k	232/237 (98%)	229 (99%)	3 (1%)	69	82
All	All	6941/7110 (98%)	6875 (99%)	66 (1%)	76	87

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	TYR
1	B	196	TYR
1	B	201	SER
1	C	196	TYR
1	C	265	LYS
1	E	189	SER
1	E	196	TYR
1	E	201	SER
1	G	-5	HIS
1	G	-2	HIS
1	G	23	ARG
1	G	196	TYR
1	G	199	MET
1	G	208	VAL
1	H	201	SER
1	I	5	LYS
1	I	196	TYR
1	I	201	SER
1	J	5	LYS
1	J	196	TYR
1	J	280	LEU
1	K	196	TYR
1	K	201	SER
1	L	196	TYR
1	L	201	SER
1	L	279	TYR
1	M	196	TYR
1	M	201	SER

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Mol	Chain	Res	Type
1	N	196	TYR
1	O	196	TYR
1	O	201	SER
1	P	189	SER
1	P	196	TYR
1	P	201	SER
1	S	196	TYR
1	S	203	PRO
1	T	196	TYR
1	T	201	SER
1	U	196	TYR
1	V	48	LYS
1	V	196	TYR
1	X	77	PRO
1	X	196	TYR
1	X	201	SER
1	X	280	LEU
1	a	196	TYR
1	a	201	SER
1	a	273	ARG
1	b	152	ILE
1	b	196	TYR
1	b	201	SER
1	c	196	TYR
1	c	201	SER
1	d	196	TYR
1	d	201	SER
1	e	201	SER
1	g	-5	HIS
1	g	-2	HIS
1	g	196	TYR
1	g	201	SER
1	h	152	ILE
1	i	201	SER
1	j	279	TYR
1	k	196	TYR
1	k	201	SER
1	k	244	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	163	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 [i](#)

Of 86 ligands modelled in this entry, 86 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, 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	282/290 (97%)	-0.56	0 100 100	19, 29, 47, 57	0
1	B	282/290 (97%)	-0.58	0 100 100	18, 28, 46, 57	0
1	C	282/290 (97%)	-0.59	0 100 100	16, 26, 42, 55	0
1	D	282/290 (97%)	-0.55	0 100 100	18, 28, 44, 55	0
1	E	282/290 (97%)	-0.54	1 (0%) 92 93	18, 27, 45, 56	0
1	G	286/290 (98%)	-0.44	6 (2%) 63 65	23, 33, 56, 64	0
1	H	281/290 (96%)	-0.35	5 (1%) 68 70	22, 31, 55, 68	0
1	I	281/290 (96%)	-0.45	2 (0%) 87 88	19, 29, 46, 58	0
1	J	281/290 (96%)	-0.37	8 (2%) 53 55	25, 35, 58, 74	0
1	K	281/290 (96%)	-0.44	4 (1%) 75 77	23, 32, 57, 69	0
1	L	282/290 (97%)	-0.57	2 (0%) 87 88	18, 27, 45, 56	0
1	M	282/290 (97%)	-0.60	0 100 100	18, 28, 44, 57	0
1	N	282/290 (97%)	-0.58	1 (0%) 92 93	18, 28, 46, 56	0
1	O	282/290 (97%)	-0.61	2 (0%) 87 88	18, 27, 45, 57	0
1	P	282/290 (97%)	-0.58	1 (0%) 92 93	18, 27, 44, 55	0
1	S	281/290 (96%)	-0.37	4 (1%) 75 77	23, 33, 56, 70	0
1	T	282/290 (97%)	-0.38	2 (0%) 87 88	23, 32, 54, 63	0
1	U	281/290 (96%)	-0.35	6 (2%) 63 65	24, 33, 57, 70	0
1	V	282/290 (97%)	-0.47	4 (1%) 75 77	22, 31, 53, 62	0
1	X	281/290 (96%)	-0.41	13 (4%) 32 35	21, 27, 45, 62	0
1	a	282/290 (97%)	-0.64	0 100 100	17, 27, 45, 56	0
1	b	282/290 (97%)	-0.56	1 (0%) 92 93	16, 25, 42, 56	0
1	c	282/290 (97%)	-0.50	1 (0%) 92 93	19, 27, 45, 58	0
1	d	282/290 (97%)	-0.55	0 100 100	19, 28, 45, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	e	283/290 (97%)	-0.45	2 (0%) 87 88	20, 29, 47, 58	0
1	g	287/290 (98%)	-0.29	4 (1%) 75 77	23, 34, 57, 66	0
1	h	281/290 (96%)	-0.36	3 (1%) 80 81	23, 33, 56, 69	0
1	i	282/290 (97%)	-0.38	4 (1%) 75 77	22, 33, 56, 68	0
1	j	282/290 (97%)	-0.34	8 (2%) 53 55	22, 32, 58, 71	0
1	k	282/290 (97%)	-0.49	2 (0%) 87 88	18, 29, 47, 57	0
All	All	8462/8700 (97%)	-0.48	86 (1%) 82 83	16, 30, 50, 74	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	281	VAL	6.9
1	g	281	VAL	6.3
1	T	281	VAL	5.7
1	e	281	VAL	5.4
1	j	167	GLY	4.8
1	X	166	ASN	4.7
1	J	167	GLY	4.7
1	j	166	ASN	4.6
1	U	0	HIS	4.3
1	j	0	HIS	4.2
1	J	0	HIS	4.2
1	S	166	ASN	4.2
1	U	166	ASN	4.2
1	j	-1	GLY	4.1
1	h	0	HIS	3.9
1	J	166	ASN	3.9
1	i	0	HIS	3.9
1	X	280	LEU	3.8
1	J	165	LYS	3.7
1	X	165	LYS	3.6
1	S	0	HIS	3.6
1	H	0	HIS	3.6
1	X	0	HIS	3.6
1	S	167	GLY	3.6
1	K	0	HIS	3.5
1	X	167	GLY	3.4
1	i	166	ASN	3.3
1	K	167	GLY	3.2
1	V	0	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	k	0	HIS	3.1
1	L	280	LEU	3.0
1	i	167	GLY	3.0
1	H	166	ASN	2.9
1	h	167	GLY	2.9
1	J	280	LEU	2.9
1	c	0	HIS	2.9
1	i	-1	GLY	2.9
1	H	167	GLY	2.8
1	J	168	LYS	2.8
1	T	0	HIS	2.8
1	G	-5	HIS	2.8
1	X	168	LYS	2.7
1	U	167	GLY	2.7
1	j	165	LYS	2.7
1	j	280	LEU	2.7
1	k	281	VAL	2.6
1	K	166	ASN	2.6
1	V	119	GLU	2.5
1	X	272	GLU	2.5
1	U	280	LEU	2.5
1	X	267	LEU	2.5
1	G	209	ALA	2.5
1	X	264	SER	2.5
1	I	0	HIS	2.5
1	I	119	GLU	2.5
1	S	280	LEU	2.5
1	h	166	ASN	2.4
1	g	204	GLU	2.4
1	e	0	HIS	2.4
1	g	-5	HIS	2.4
1	G	119	GLU	2.4
1	H	165	LYS	2.3
1	j	168	LYS	2.3
1	U	272	GLU	2.3
1	g	145	PRO	2.3
1	N	204	GLU	2.3
1	O	0	HIS	2.2
1	U	165	LYS	2.2
1	K	165	LYS	2.2
1	J	119	GLU	2.2
1	J	267	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	V	145	PRO	2.1
1	X	145	PRO	2.1
1	G	146	ASP	2.1
1	E	280	LEU	2.1
1	X	204	GLU	2.1
1	O	-1	GLY	2.1
1	X	163	GLN	2.0
1	j	272	GLU	2.0
1	H	209	ALA	2.0
1	G	117	GLU	2.0
1	G	0	HIS	2.0
1	L	207	GLY	2.0
1	P	0	HIS	2.0
1	b	0	HIS	2.0
1	X	209	ALA	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 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	CL	k	284	1/1	0.93	0.20	63,63,63,63	0
2	CL	j	283	1/1	0.94	0.06	43,43,43,43	0
2	CL	i	285	1/1	0.94	0.06	42,42,42,42	0
2	CL	N	285	1/1	0.95	0.05	41,41,41,41	0
2	CL	P	284	1/1	0.95	0.15	44,44,44,44	0
2	CL	U	284	1/1	0.95	0.17	58,58,58,58	0
2	CL	U	285	1/1	0.95	0.07	37,37,37,37	0
2	CL	V	285	1/1	0.95	0.13	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	h	283	1/1	0.95	0.07	48,48,48,48	0
2	CL	A	285	1/1	0.95	0.14	45,45,45,45	0
2	CL	D	283	1/1	0.95	0.08	42,42,42,42	0
2	CL	H	285	1/1	0.95	0.15	51,51,51,51	0
2	CL	S	285	1/1	0.96	0.15	52,52,52,52	0
2	CL	T	283	1/1	0.96	0.10	44,44,44,44	0
2	CL	C	284	1/1	0.96	0.15	45,45,45,45	0
2	CL	J	283	1/1	0.96	0.05	47,47,47,47	0
2	CL	M	283	1/1	0.96	0.06	42,42,42,42	0
2	CL	N	284	1/1	0.96	0.09	43,43,43,43	0
2	CL	C	285	1/1	0.96	0.07	37,37,37,37	0
2	CL	O	285	1/1	0.96	0.12	41,41,41,41	0
2	CL	B	283	1/1	0.96	0.06	44,44,44,44	0
2	CL	k	285	1/1	0.96	0.06	40,40,40,40	0
2	CL	A	283	1/1	0.97	0.08	40,40,40,40	0
2	CL	V	283	1/1	0.97	0.07	42,42,42,42	0
2	CL	I	285	1/1	0.97	0.07	38,38,38,38	0
2	CL	X	284	1/1	0.97	0.15	56,56,56,56	0
2	CL	d	283	1/1	0.97	0.11	44,44,44,44	0
2	CL	d	285	1/1	0.97	0.16	41,41,41,41	0
2	CL	g	283	1/1	0.97	0.05	43,43,43,43	0
2	CL	D	285	1/1	0.97	0.18	42,42,42,42	0
2	CL	h	285	1/1	0.97	0.20	47,47,47,47	0
2	CL	S	283	1/1	0.97	0.06	42,42,42,42	0
2	CL	E	284	1/1	0.97	0.13	40,40,40,40	0
2	CL	M	285	1/1	0.97	0.09	42,42,42,42	0
2	CL	G	285	1/1	0.97	0.18	59,59,59,59	0
2	CL	a	283	1/1	0.98	0.08	43,43,43,43	0
2	CL	a	285	1/1	0.98	0.13	43,43,43,43	0
2	CL	b	283	1/1	0.98	0.08	36,36,36,36	0
2	CL	b	285	1/1	0.98	0.15	40,40,40,40	0
2	CL	c	284	1/1	0.98	0.10	39,39,39,39	0
2	CL	c	285	1/1	0.98	0.07	36,36,36,36	0
2	CL	G	283	1/1	0.98	0.07	40,40,40,40	0
2	CL	I	284	1/1	0.98	0.14	48,48,48,48	0
2	CL	e	284	1/1	0.98	0.09	43,43,43,43	0
2	CL	e	285	1/1	0.98	0.13	39,39,39,39	0
2	CL	N	283	1/1	0.98	0.06	34,34,34,34	0
2	CL	B	285	1/1	0.98	0.13	40,40,40,40	0
2	CL	h	284	1/1	0.98	0.05	40,40,40,40	0
2	CL	H	283	1/1	0.98	0.04	46,46,46,46	0
2	CL	i	284	1/1	0.98	0.10	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	O	283	1/1	0.98	0.05	44,44,44,44	0
2	CL	K	284	1/1	0.98	0.19	48,48,48,48	0
2	CL	j	285	1/1	0.98	0.18	57,57,57,57	0
2	CL	L	285	1/1	0.98	0.15	43,43,43,43	0
2	CL	X	285	1/1	0.98	0.09	44,44,44,44	0
2	CL	G	284	1/1	0.99	0.07	33,33,33,33	0
2	CL	a	284	1/1	0.99	0.04	31,31,31,31	0
2	CL	O	284	1/1	0.99	0.05	32,32,32,32	0
2	CL	J	284	1/1	0.99	0.14	38,38,38,38	0
2	CL	b	284	1/1	0.99	0.04	32,32,32,32	0
2	CL	P	283	1/1	0.99	0.04	32,32,32,32	0
2	CL	c	283	1/1	0.99	0.05	32,32,32,32	0
2	CL	K	283	1/1	0.99	0.04	34,34,34,34	0
2	CL	D	284	1/1	0.99	0.04	32,32,32,32	0
2	CL	S	284	1/1	0.99	0.05	39,39,39,39	0
2	CL	d	284	1/1	0.99	0.03	29,29,29,29	0
2	CL	L	283	1/1	0.99	0.11	37,37,37,37	0
2	CL	B	284	1/1	0.99	0.06	33,33,33,33	0
2	CL	T	284	1/1	0.99	0.08	36,36,36,36	0
2	CL	T	285	1/1	0.99	0.18	47,47,47,47	0
2	CL	g	284	1/1	0.99	0.05	37,37,37,37	0
2	CL	U	283	1/1	0.99	0.05	36,36,36,36	0
2	CL	H	284	1/1	0.99	0.05	35,35,35,35	0
2	CL	M	284	1/1	0.99	0.09	32,32,32,32	0
2	CL	i	283	1/1	0.99	0.06	35,35,35,35	0
2	CL	E	283	1/1	0.99	0.06	31,31,31,31	0
2	CL	V	284	1/1	0.99	0.07	41,41,41,41	0
2	CL	I	283	1/1	0.99	0.05	34,34,34,34	0
2	CL	j	284	1/1	0.99	0.07	37,37,37,37	0
2	CL	X	283	1/1	0.99	0.06	39,39,39,39	0
2	CL	k	283	1/1	0.99	0.05	38,38,38,38	0
2	CL	A	284	1/1	0.99	0.04	32,32,32,32	0
2	CL	C	283	1/1	0.99	0.05	29,29,29,29	0
2	CL	k	286	1/1	0.99	0.17	47,47,47,47	0
2	CL	e	283	1/1	1.00	0.05	33,33,33,33	0
2	CL	L	284	1/1	1.00	0.03	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.