



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 11:59 PM UTC

PDB ID : 3N99 / pdb_00003n99
Title : Crystal structure of TM1086
Authors : Chruszcz, M.; Domagalski, M.J.; Wang, S.; Evdokimova, E.; Kudritska, M.; Savchenko, A.; Edwards, A.; Joachimiak, A.; Minor, W.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2010-05-28
Resolution : 2.38 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

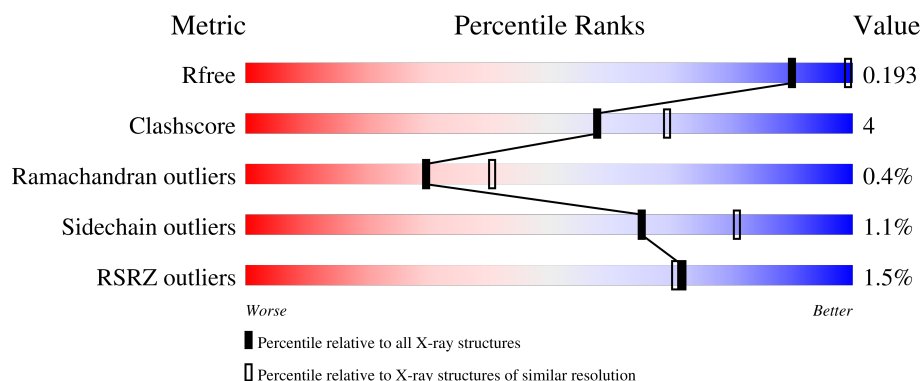
1 Overall quality at a glance

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.



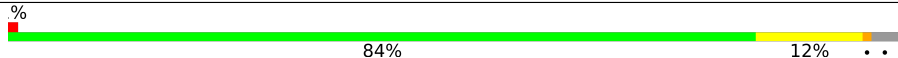
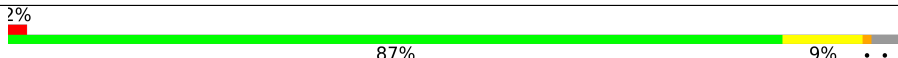
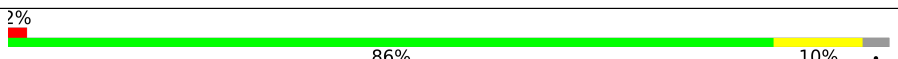
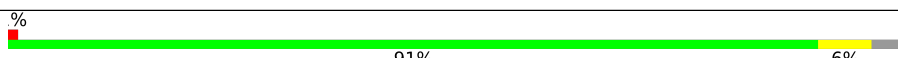
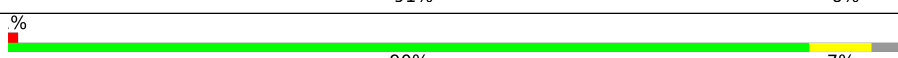
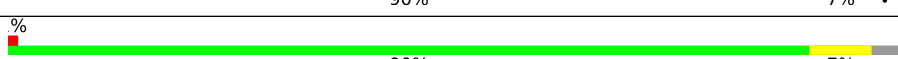
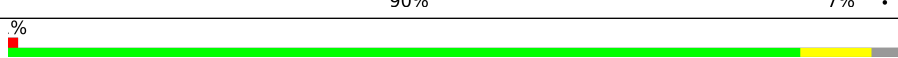
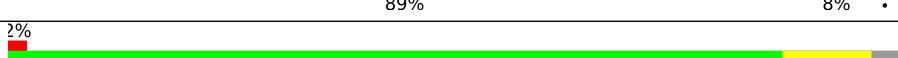
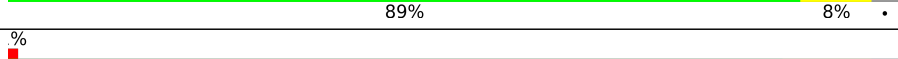
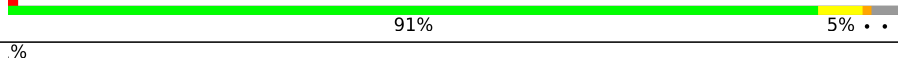
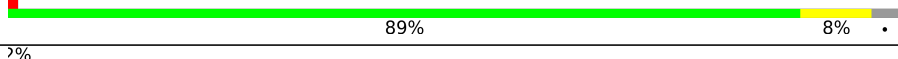
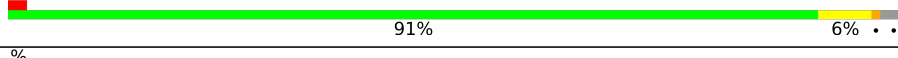
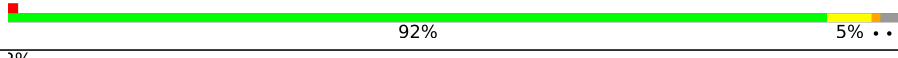
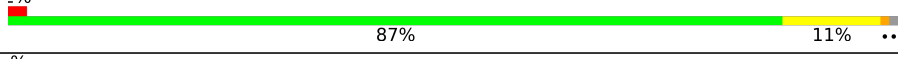
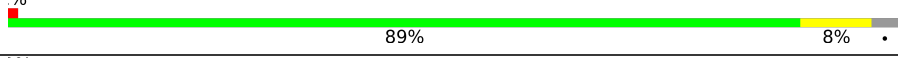
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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 ≥ 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	% 88% 8% ..
1	B	290	% 88% 9% .
1	C	290	% 86% 11% .
1	D	290	% 88% 9% ..
1	E	290	% 89% 8% .

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Mol	Chain	Length	Quality of chain
1	G	290	
1	H	290	
1	I	290	
1	J	290	
1	K	290	
1	L	290	
1	M	290	
1	N	290	
1	O	290	
1	P	290	
1	S	290	
1	T	290	
1	U	290	
1	V	290	
1	X	290	
1	a	290	
1	b	290	
1	c	290	
1	d	290	
1	e	290	
1	g	290	
1	h	290	
1	i	290	
1	j	290	
1	k	290	

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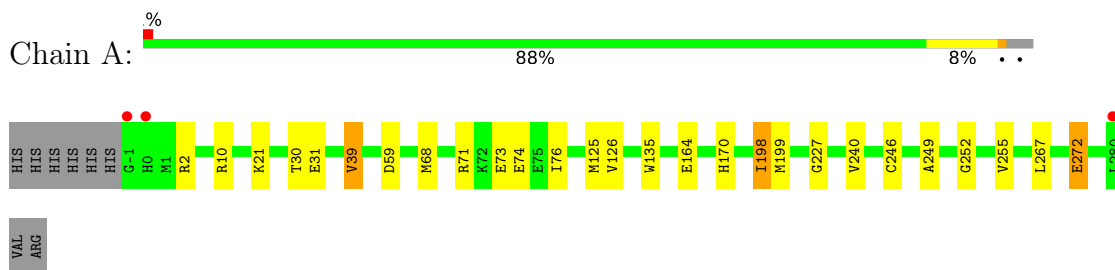
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	c	196	Total 196	O 196	0	0
3	d	179	Total 179	O 179	0	0
3	e	183	Total 183	O 183	0	0
3	g	152	Total 152	O 152	0	0
3	h	158	Total 158	O 158	0	0
3	i	139	Total 139	O 139	0	0
3	j	151	Total 151	O 151	0	0
3	k	174	Total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

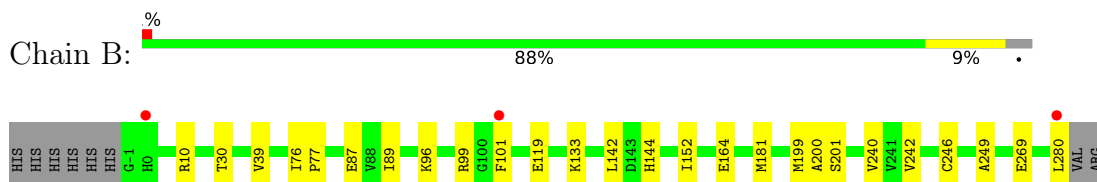
3 Residue-property plots [i](#)

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.

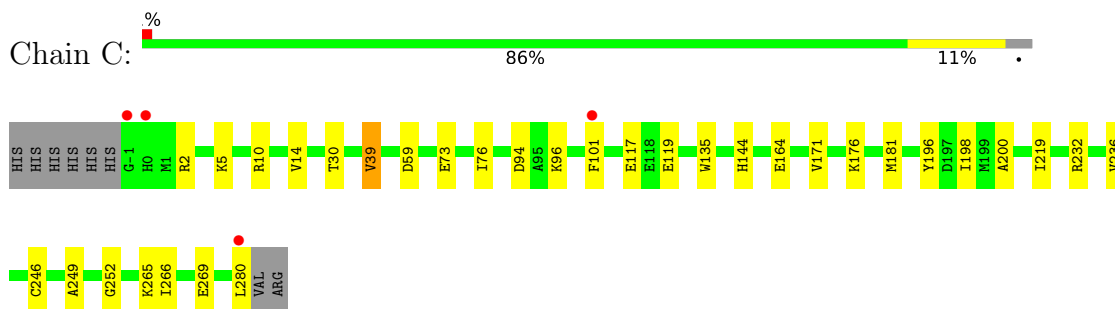
- Molecule 1: uncharacterized protein TM1086



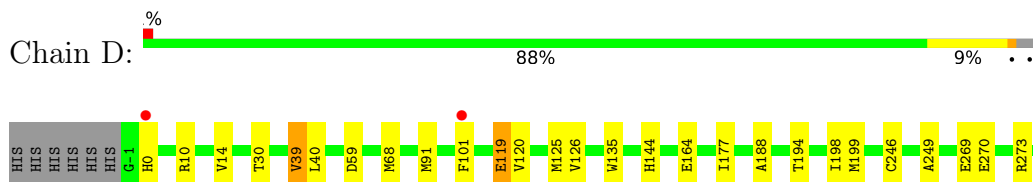
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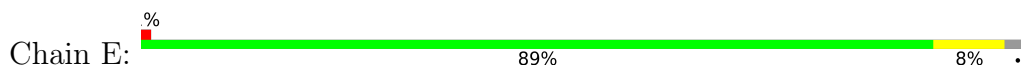
- Molecule 1: uncharacterized protein TM1086



- Molecule 1: uncharacterized protein TM1086

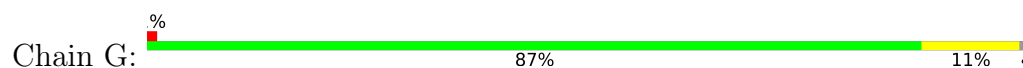


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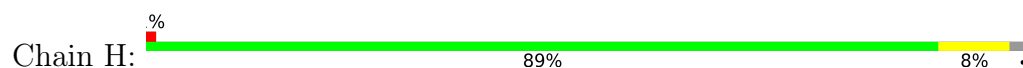




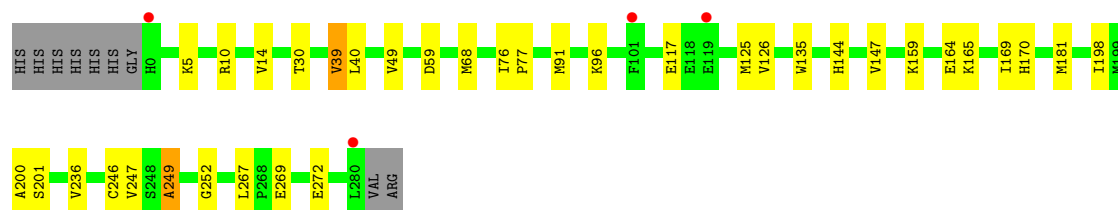
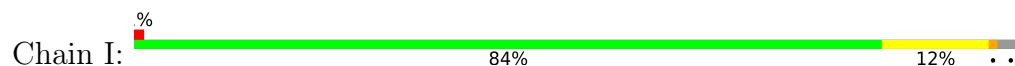
- Molecule 1: uncharacterized protein TM1086



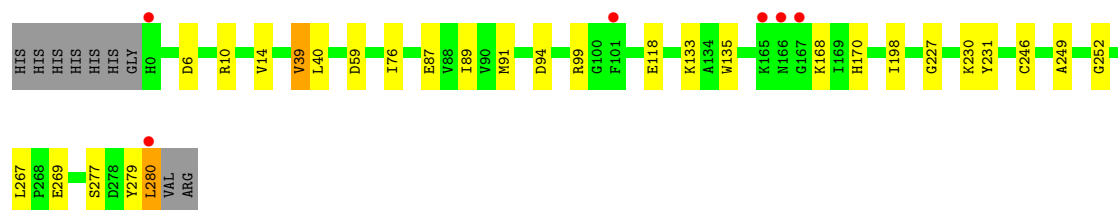
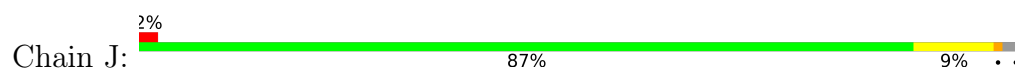
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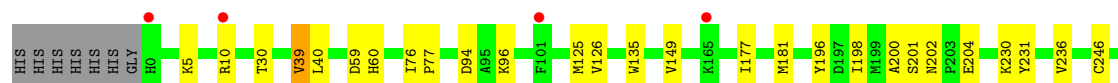
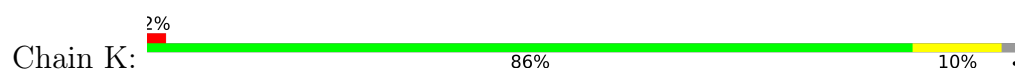
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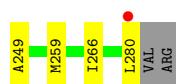


- Molecule 1: uncharacterized protein TM1086

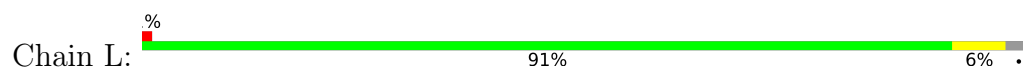


- Molecule 1: uncharacterized protein TM1086

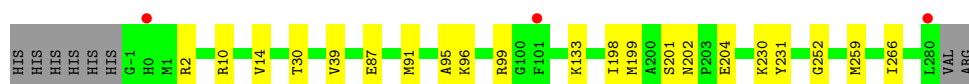




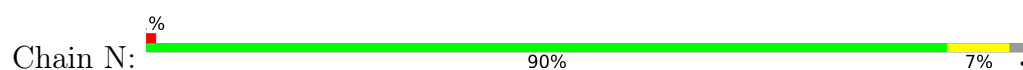
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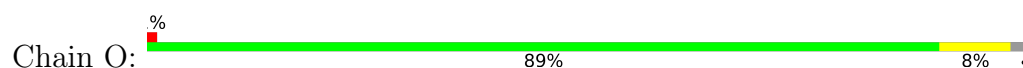
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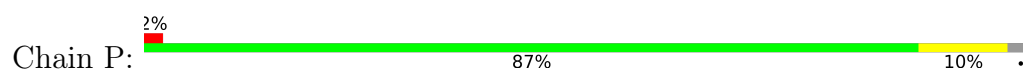
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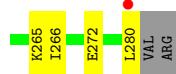
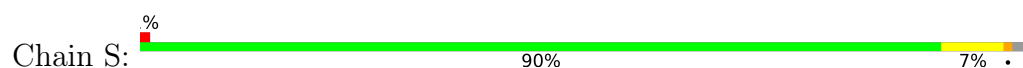
- Molecule 1: uncharacterized protein TM1086



- Molecule 1: uncharacterized protein TM1086

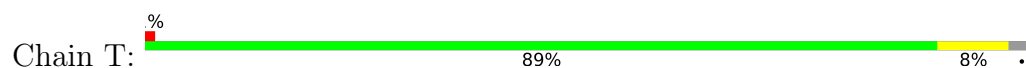


- Molecule 1: uncharacterized protein TM1086

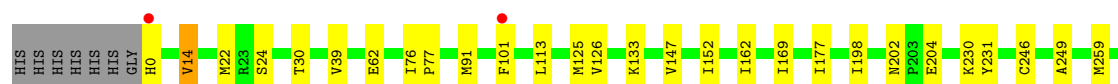
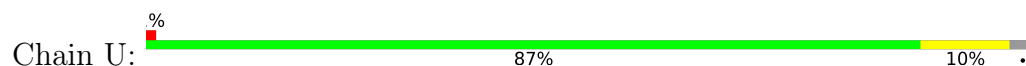




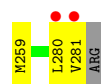
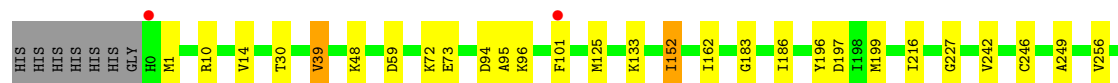
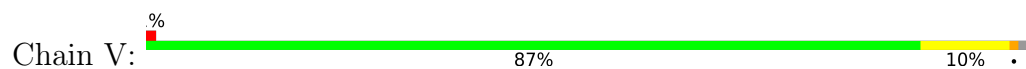
- Molecule 1: uncharacterized protein TM1086



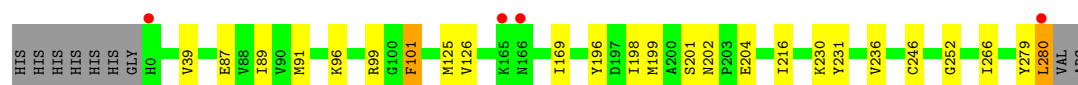
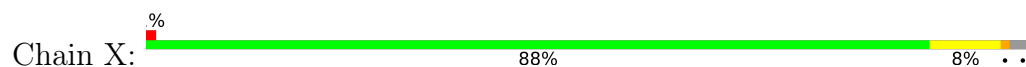
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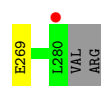
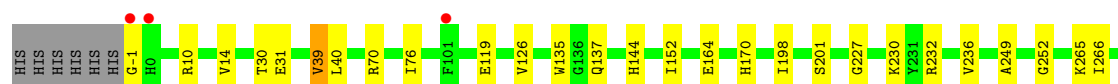
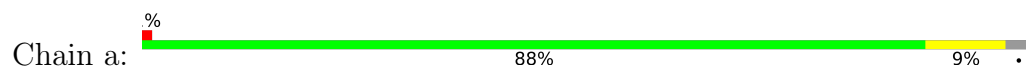
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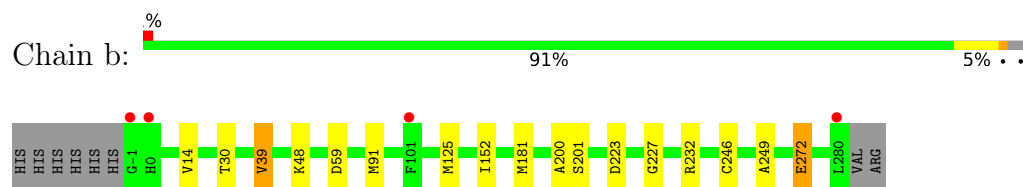
- Molecule 1: uncharacterized protein TM1086



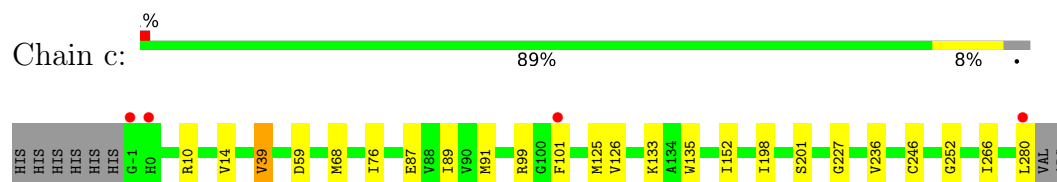
- Molecule 1: uncharacterized protein TM1086



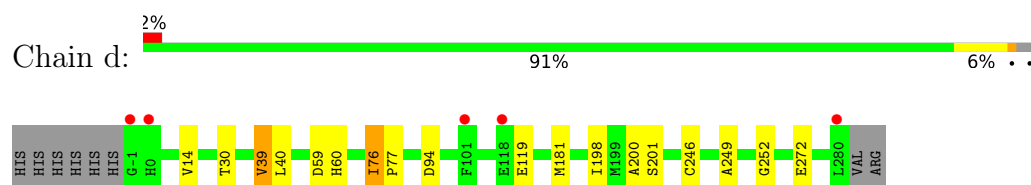
- Molecule 1: uncharacterized protein TM1086



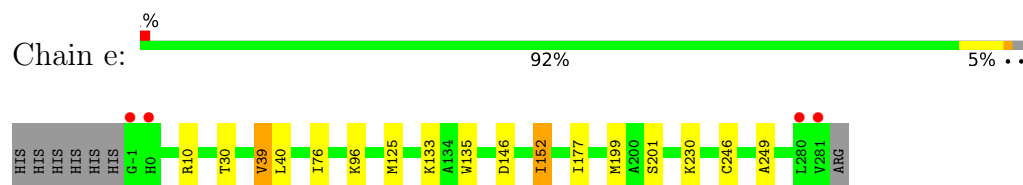
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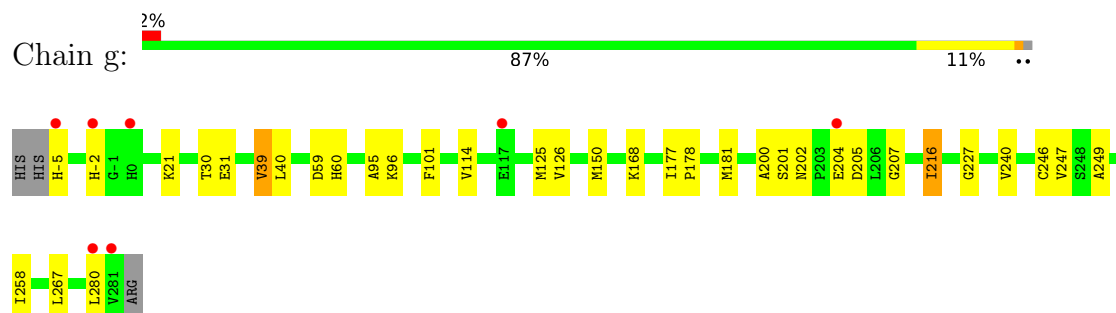
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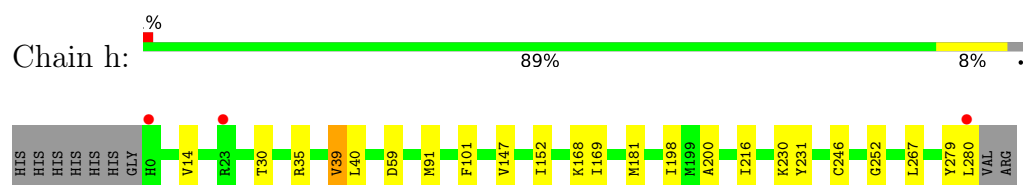
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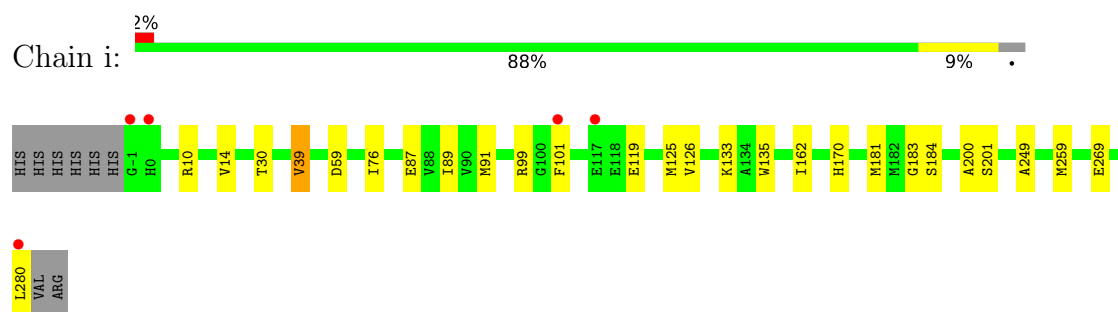
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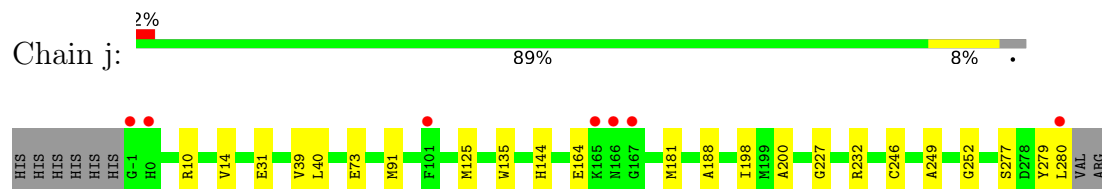
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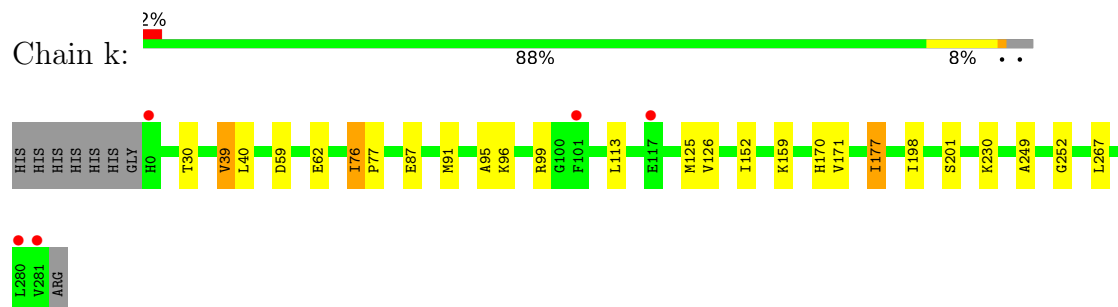
- Molecule 1: uncharacterized protein TM1086



- 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, α , β , γ	289.84Å 299.52Å 316.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.38 50.00 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.38) 99.1 (50.00-2.38)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.151 , 0.191 0.154 , 0.193	Depositor DCC
R_{free} test set	26930 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.15	1/2155 (0.0%)	0.96	1/2912 (0.0%)
1	B	1.10	0/2169	0.95	1/2931 (0.0%)
1	C	1.17	5/2165 (0.2%)	0.99	0/2926
1	D	1.18	3/2143 (0.1%)	1.02	1/2897 (0.0%)
1	E	1.15	2/2147 (0.1%)	0.98	0/2902
1	G	1.09	0/2197	0.99	0/2970
1	H	1.07	0/2149	0.99	0/2905
1	I	1.09	3/2163 (0.1%)	0.99	1/2923 (0.0%)
1	J	1.11	1/2154 (0.0%)	0.99	0/2911
1	K	1.03	0/2160	0.98	0/2919
1	L	1.14	0/2153	0.98	1/2910 (0.0%)
1	M	1.14	0/2171	1.00	0/2934
1	N	1.10	1/2158 (0.0%)	0.98	1/2916 (0.0%)
1	O	1.12	0/2147	1.00	0/2902
1	P	1.14	0/2165	1.00	0/2926
1	S	1.07	1/2148 (0.0%)	0.98	1/2903 (0.0%)
1	T	1.07	0/2158	0.98	0/2917
1	U	1.06	0/2143	0.99	2/2897 (0.1%)
1	V	1.09	1/2150 (0.0%)	1.00	3/2907 (0.1%)
1	X	1.09	0/2140	1.01	1/2893 (0.0%)
1	a	1.12	2/2171 (0.1%)	0.98	0/2934
1	b	1.11	0/2158	0.98	0/2916
1	c	1.11	1/2147 (0.0%)	0.97	1/2902 (0.0%)
1	d	1.11	1/2158 (0.0%)	0.99	0/2916
1	e	1.08	2/2165 (0.1%)	0.97	1/2926 (0.0%)
1	g	1.08	0/2215	0.97	1/2994 (0.0%)
1	h	1.05	0/2132	0.99	0/2883
1	i	1.10	1/2147 (0.0%)	1.00	0/2902
1	j	1.10	1/2158 (0.0%)	1.00	0/2916
1	k	1.16	3/2161 (0.1%)	1.00	0/2921
All	All	1.11	29/64747 (0.0%)	0.99	16/87511 (0.0%)

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	76	ILE	CA-CB	-8.62	1.49	1.54
1	k	76	ILE	CA-CB	-8.47	1.49	1.54
1	S	171	VAL	CA-C	-6.95	1.47	1.52
1	C	171	VAL	CA-CB	6.53	1.59	1.54
1	D	273	ARG	C-O	-6.45	1.16	1.23

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	72	LYS	N-CA-C	6.80	118.69	111.28
1	A	198	ILE	CB-CA-C	-6.48	104.23	111.23
1	N	242	VAL	CB-CA-C	-6.13	104.64	110.65
1	c	152	ILE	N-CA-C	5.77	116.42	108.12
1	U	152	ILE	N-CA-C	5.43	116.09	108.17

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	2113	0	2153	31	0
1	B	2121	0	2171	22	0
1	C	2123	0	2165	17	0
1	D	2104	0	2140	26	0
1	E	2108	0	2144	24	0
1	G	2151	0	2177	34	0
1	H	2107	0	2146	27	0
1	I	2121	0	2159	27	0
1	J	2112	0	2154	24	0
1	K	2115	0	2159	25	0
1	L	2111	0	2149	16	0
1	M	2123	0	2169	27	0
1	N	2119	0	2156	20	0
1	O	2108	0	2144	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	2120	0	2166	32	0
1	S	2106	0	2141	24	0
1	T	2116	0	2159	23	0
1	U	2107	0	2140	28	0
1	V	2111	0	2150	26	0
1	X	2101	0	2137	29	0
1	a	2123	0	2171	23	0
1	b	2116	0	2157	21	0
1	c	2111	0	2143	21	0
1	d	2116	0	2157	13	0
1	e	2123	0	2166	22	0
1	g	2166	0	2199	28	0
1	h	2096	0	2128	23	0
1	i	2108	0	2144	20	0
1	j	2116	0	2157	18	0
1	k	2119	0	2163	17	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
2	G	3	0	0	1	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	3	0	0	0	0
2	M	3	0	0	0	0
2	N	3	0	0	0	0
2	O	3	0	0	1	0
2	P	2	0	0	1	0
2	S	3	0	0	0	0
2	T	3	0	0	0	0
2	U	3	0	0	0	0
2	V	3	0	0	0	0
2	X	3	0	0	0	0
2	a	3	0	0	0	0
2	b	3	0	0	0	0
2	c	3	0	0	0	0
2	d	3	0	0	0	0
2	e	3	0	0	1	0
2	g	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	h	3	0	0	0	0
2	i	3	0	0	0	0
2	j	3	0	0	0	0
2	k	4	0	0	0	0
3	A	175	0	0	6	0
3	B	182	0	0	3	0
3	C	185	0	0	3	0
3	D	190	0	0	6	0
3	E	192	0	0	4	0
3	G	145	0	0	2	0
3	H	153	0	0	2	0
3	I	164	0	0	4	0
3	J	135	0	0	2	0
3	K	156	0	0	0	0
3	L	179	0	0	2	0
3	M	176	0	0	2	0
3	N	174	0	0	2	0
3	O	183	0	0	5	0
3	P	170	0	0	5	0
3	S	166	0	0	5	0
3	T	158	0	0	1	0
3	U	147	0	0	3	0
3	V	148	0	0	5	0
3	X	155	0	0	3	0
3	a	194	0	0	4	0
3	b	195	0	0	5	0
3	c	196	0	0	3	0
3	d	179	0	0	2	0
3	e	183	0	0	4	0
3	g	152	0	0	1	0
3	h	158	0	0	3	0
3	i	139	0	0	0	0
3	j	151	0	0	2	0
3	k	174	0	0	1	0
All	All	68631	0	64664	577	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 4.

The worst 5 of 577 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:g:126:VAL:HB	1:j:14:VAL:HG11	1.37	1.05
1:I:14:VAL:HG11	1:K:126:VAL:HB	1.41	0.99
1:B:199[A]:MET:HE1	1:K:231:TYR:H	1.31	0.94
1:U:14:VAL:HG11	1:X:126:VAL:HB	1.46	0.94
1:c:68:MET:HE1	3:c:3399:HOH:O	1.68	0.94

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	282/290 (97%)	272 (96%)	9 (3%)	1 (0%)	30	40
1	B	284/290 (98%)	274 (96%)	9 (3%)	1 (0%)	30	40
1	C	283/290 (98%)	273 (96%)	9 (3%)	1 (0%)	30	40
1	D	281/290 (97%)	270 (96%)	10 (4%)	1 (0%)	30	40
1	E	281/290 (97%)	271 (96%)	9 (3%)	1 (0%)	30	40
1	G	286/290 (99%)	277 (97%)	8 (3%)	1 (0%)	36	48
1	H	281/290 (97%)	271 (96%)	9 (3%)	1 (0%)	30	40
1	I	282/290 (97%)	272 (96%)	9 (3%)	1 (0%)	30	40
1	J	281/290 (97%)	269 (96%)	11 (4%)	1 (0%)	30	40
1	K	282/290 (97%)	270 (96%)	11 (4%)	1 (0%)	30	40
1	L	282/290 (97%)	271 (96%)	10 (4%)	1 (0%)	30	40
1	M	284/290 (98%)	275 (97%)	8 (3%)	1 (0%)	30	40
1	N	282/290 (97%)	273 (97%)	8 (3%)	1 (0%)	30	40
1	O	281/290 (97%)	273 (97%)	7 (2%)	1 (0%)	30	40
1	P	283/290 (98%)	275 (97%)	7 (2%)	1 (0%)	30	40
1	S	281/290 (97%)	269 (96%)	11 (4%)	1 (0%)	30	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	282/290 (97%)	271 (96%)	10 (4%)	1 (0%)	30	40
1	U	280/290 (97%)	268 (96%)	11 (4%)	1 (0%)	30	40
1	V	281/290 (97%)	272 (97%)	8 (3%)	1 (0%)	30	40
1	X	280/290 (97%)	271 (97%)	8 (3%)	1 (0%)	30	40
1	a	284/290 (98%)	275 (97%)	8 (3%)	1 (0%)	30	40
1	b	282/290 (97%)	272 (96%)	9 (3%)	1 (0%)	30	40
1	c	281/290 (97%)	271 (96%)	9 (3%)	1 (0%)	30	40
1	d	282/290 (97%)	271 (96%)	10 (4%)	1 (0%)	30	40
1	e	283/290 (98%)	272 (96%)	10 (4%)	1 (0%)	30	40
1	g	288/290 (99%)	277 (96%)	9 (3%)	2 (1%)	18	26
1	h	279/290 (96%)	266 (95%)	12 (4%)	1 (0%)	30	40
1	i	281/290 (97%)	269 (96%)	11 (4%)	1 (0%)	30	40
1	j	282/290 (97%)	271 (96%)	10 (4%)	1 (0%)	30	40
1	k	282/290 (97%)	272 (96%)	9 (3%)	1 (0%)	30	40
All	All	8463/8700 (97%)	8153 (96%)	279 (3%)	31 (0%)	30	40

5 of 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

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%)	228 (99%)	3 (1%)	61	78
1	B	232/237 (98%)	229 (99%)	3 (1%)	61	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	232/237 (98%)	226 (97%)	6 (3%)	40	60
1	D	229/237 (97%)	226 (99%)	3 (1%)	61	78
1	E	230/237 (97%)	227 (99%)	3 (1%)	61	78
1	G	235/237 (99%)	229 (97%)	6 (3%)	40	60
1	H	231/237 (98%)	228 (99%)	3 (1%)	61	78
1	I	232/237 (98%)	229 (99%)	3 (1%)	61	78
1	J	231/237 (98%)	229 (99%)	2 (1%)	70	84
1	K	232/237 (98%)	228 (98%)	4 (2%)	53	72
1	L	231/237 (98%)	229 (99%)	2 (1%)	70	84
1	M	233/237 (98%)	231 (99%)	2 (1%)	70	84
1	N	231/237 (98%)	230 (100%)	1 (0%)	84	91
1	O	230/237 (97%)	229 (100%)	1 (0%)	84	91
1	P	232/237 (98%)	227 (98%)	5 (2%)	45	65
1	S	230/237 (97%)	230 (100%)	0	100	100
1	T	232/237 (98%)	230 (99%)	2 (1%)	70	84
1	U	230/237 (97%)	230 (100%)	0	100	100
1	V	231/237 (98%)	227 (98%)	4 (2%)	53	72
1	X	230/237 (97%)	226 (98%)	4 (2%)	53	72
1	a	233/237 (98%)	231 (99%)	2 (1%)	70	84
1	b	231/237 (98%)	228 (99%)	3 (1%)	61	78
1	c	230/237 (97%)	229 (100%)	1 (0%)	84	91
1	d	231/237 (98%)	229 (99%)	2 (1%)	70	84
1	e	232/237 (98%)	230 (99%)	2 (1%)	70	84
1	g	237/237 (100%)	233 (98%)	4 (2%)	53	72
1	h	229/237 (97%)	228 (100%)	1 (0%)	84	91
1	i	230/237 (97%)	229 (100%)	1 (0%)	84	91
1	j	231/237 (98%)	230 (100%)	1 (0%)	84	91
1	k	232/237 (98%)	230 (99%)	2 (1%)	70	84
All	All	6941/7110 (98%)	6865 (99%)	76 (1%)	65	81

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	152	ILE
1	h	152	ILE
1	b	152	ILE
1	e	152	ILE
1	k	201	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	e	0	HIS
1	j	166	ASN
1	J	220	GLN
1	N	202	ASN
1	O	202	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	282/290 (97%)	-0.43	3 (1%) 78 77	16, 29, 47, 57	2 (0%)
1	B	282/290 (97%)	-0.48	3 (1%) 78 77	16, 28, 46, 57	4 (1%)
1	C	282/290 (97%)	-0.48	4 (1%) 73 72	12, 26, 42, 55	3 (1%)
1	D	282/290 (97%)	-0.44	3 (1%) 78 77	18, 27, 44, 55	1 (0%)
1	E	282/290 (97%)	-0.45	4 (1%) 73 72	17, 27, 45, 56	1 (0%)
1	G	286/290 (98%)	-0.26	4 (1%) 73 72	18, 33, 56, 64	2 (0%)
1	H	281/290 (96%)	-0.32	3 (1%) 78 77	19, 31, 55, 68	2 (0%)
1	I	281/290 (96%)	-0.40	4 (1%) 73 72	14, 29, 46, 58	3 (1%)
1	J	281/290 (96%)	-0.20	6 (2%) 63 62	23, 35, 58, 74	2 (0%)
1	K	281/290 (96%)	-0.30	5 (1%) 67 66	20, 32, 57, 69	3 (1%)
1	L	282/290 (97%)	-0.46	3 (1%) 78 77	16, 27, 45, 56	2 (0%)
1	M	282/290 (97%)	-0.44	3 (1%) 78 77	16, 28, 44, 57	4 (1%)
1	N	282/290 (97%)	-0.47	3 (1%) 78 77	15, 28, 46, 56	2 (0%)
1	O	282/290 (97%)	-0.45	4 (1%) 73 72	16, 27, 45, 57	1 (0%)
1	P	282/290 (97%)	-0.48	5 (1%) 67 66	14, 27, 44, 55	3 (1%)
1	S	281/290 (96%)	-0.30	4 (1%) 73 72	19, 33, 56, 70	2 (0%)
1	T	282/290 (97%)	-0.34	4 (1%) 73 72	18, 32, 54, 63	2 (0%)
1	U	281/290 (96%)	-0.30	3 (1%) 78 77	18, 33, 57, 70	1 (0%)
1	V	282/290 (97%)	-0.33	4 (1%) 73 72	19, 31, 53, 62	1 (0%)
1	X	281/290 (96%)	-0.29	4 (1%) 73 72	18, 27, 45, 62	1 (0%)
1	a	282/290 (97%)	-0.47	4 (1%) 73 72	13, 27, 45, 56	4 (1%)
1	b	282/290 (97%)	-0.52	4 (1%) 73 72	15, 25, 42, 56	2 (0%)
1	c	282/290 (97%)	-0.41	4 (1%) 73 72	15, 27, 45, 58	1 (0%)
1	d	282/290 (97%)	-0.44	5 (1%) 67 66	16, 28, 45, 57	2 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	e	283/290 (97%)	-0.40	4 (1%)	73 72	16, 28, 47, 58	2 (0%)
1	g	287/290 (98%)	-0.17	7 (2%)	59 59	20, 34, 57, 66	3 (1%)
1	h	281/290 (96%)	-0.29	3 (1%)	78 77	23, 33, 56, 69	0
1	i	282/290 (97%)	-0.26	5 (1%)	67 66	19, 33, 56, 68	1 (0%)
1	j	282/290 (97%)	-0.24	7 (2%)	58 58	22, 32, 58, 71	2 (0%)
1	k	282/290 (97%)	-0.41	5 (1%)	67 66	17, 29, 47, 57	2 (0%)
All	All	8462/8700 (97%)	-0.37	124 (1%)	72 71	12, 30, 50, 74	61 (0%)

The worst 5 of 124 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	280	LEU	6.5
1	g	281	VAL	6.4
1	L	280	LEU	6.1
1	V	281	VAL	6.1
1	X	280	LEU	5.7

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	k	284	1/1	0.91	0.17	63,63,63,63	0
2	CL	P	284	1/1	0.93	0.10	44,44,44,44	0
2	CL	S	283	1/1	0.94	0.10	42,42,42,42	0
2	CL	d	283	1/1	0.94	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	C	284	1/1	0.94	0.12	45,45,45,45	0
2	CL	S	285	1/1	0.95	0.08	52,52,52,52	0
2	CL	T	283	1/1	0.95	0.10	44,44,44,44	0
2	CL	b	285	1/1	0.95	0.12	40,40,40,40	0
2	CL	E	284	1/1	0.95	0.09	40,40,40,40	0
2	CL	e	284	1/1	0.95	0.08	43,43,43,43	0
2	CL	h	283	1/1	0.95	0.09	48,48,48,48	0
2	CL	G	285	1/1	0.95	0.08	59,59,59,59	0
2	CL	A	285	1/1	0.96	0.10	45,45,45,45	0
2	CL	A	283	1/1	0.96	0.07	40,40,40,40	0
2	CL	U	285	1/1	0.96	0.08	37,37,37,37	0
2	CL	b	283	1/1	0.96	0.08	36,36,36,36	0
2	CL	H	285	1/1	0.96	0.08	51,51,51,51	0
2	CL	J	283	1/1	0.96	0.07	47,47,47,47	0
2	CL	N	284	1/1	0.96	0.07	43,43,43,43	0
2	CL	C	285	1/1	0.96	0.07	37,37,37,37	0
2	CL	h	285	1/1	0.96	0.09	47,47,47,47	0
2	CL	i	285	1/1	0.96	0.07	42,42,42,42	0
2	CL	j	283	1/1	0.96	0.07	43,43,43,43	0
2	CL	D	283	1/1	0.96	0.10	42,42,42,42	0
2	CL	k	285	1/1	0.96	0.07	40,40,40,40	0
2	CL	U	284	1/1	0.97	0.07	58,58,58,58	0
2	CL	G	283	1/1	0.97	0.09	40,40,40,40	0
2	CL	V	285	1/1	0.97	0.09	45,45,45,45	0
2	CL	X	285	1/1	0.97	0.07	44,44,44,44	0
2	CL	a	285	1/1	0.97	0.08	43,43,43,43	0
2	CL	L	283	1/1	0.97	0.08	37,37,37,37	0
2	CL	L	285	1/1	0.97	0.06	43,43,43,43	0
2	CL	c	284	1/1	0.97	0.07	39,39,39,39	0
2	CL	c	285	1/1	0.97	0.10	36,36,36,36	0
2	CL	M	283	1/1	0.97	0.08	42,42,42,42	0
2	CL	d	285	1/1	0.97	0.10	41,41,41,41	0
2	CL	B	283	1/1	0.97	0.07	44,44,44,44	0
2	CL	g	283	1/1	0.97	0.07	43,43,43,43	0
2	CL	N	285	1/1	0.97	0.07	41,41,41,41	0
2	CL	O	285	1/1	0.97	0.08	41,41,41,41	0
2	CL	i	284	1/1	0.97	0.05	51,51,51,51	0
2	CL	H	283	1/1	0.97	0.06	46,46,46,46	0
2	CL	B	285	1/1	0.97	0.09	40,40,40,40	0
2	CL	j	285	1/1	0.97	0.07	57,57,57,57	0
2	CL	I	284	1/1	0.97	0.06	48,48,48,48	0
2	CL	I	285	1/1	0.97	0.09	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	k	286	1/1	0.97	0.07	47,47,47,47	0
2	CL	D	285	1/1	0.98	0.08	42,42,42,42	0
2	CL	h	284	1/1	0.98	0.08	40,40,40,40	0
2	CL	T	285	1/1	0.98	0.09	47,47,47,47	0
2	CL	A	284	1/1	0.98	0.09	32,32,32,32	0
2	CL	I	283	1/1	0.98	0.11	34,34,34,34	0
2	CL	V	283	1/1	0.98	0.07	42,42,42,42	0
2	CL	M	285	1/1	0.98	0.06	42,42,42,42	0
2	CL	X	284	1/1	0.98	0.06	56,56,56,56	0
2	CL	K	284	1/1	0.98	0.10	48,48,48,48	0
2	CL	a	283	1/1	0.98	0.09	43,43,43,43	0
2	CL	B	284	1/1	0.99	0.12	33,33,33,33	0
2	CL	b	284	1/1	0.99	0.06	32,32,32,32	0
2	CL	S	284	1/1	0.99	0.09	39,39,39,39	0
2	CL	c	283	1/1	0.99	0.09	32,32,32,32	0
2	CL	D	284	1/1	0.99	0.09	32,32,32,32	0
2	CL	G	284	1/1	0.99	0.09	33,33,33,33	0
2	CL	T	284	1/1	0.99	0.13	36,36,36,36	0
2	CL	d	284	1/1	0.99	0.07	29,29,29,29	0
2	CL	M	284	1/1	0.99	0.12	32,32,32,32	0
2	CL	e	283	1/1	0.99	0.07	33,33,33,33	0
2	CL	U	283	1/1	0.99	0.11	36,36,36,36	0
2	CL	e	285	1/1	0.99	0.07	39,39,39,39	0
2	CL	C	283	1/1	0.99	0.11	29,29,29,29	0
2	CL	g	284	1/1	0.99	0.10	37,37,37,37	0
2	CL	N	283	1/1	0.99	0.05	34,34,34,34	0
2	CL	E	283	1/1	0.99	0.09	31,31,31,31	0
2	CL	V	284	1/1	0.99	0.09	41,41,41,41	0
2	CL	i	283	1/1	0.99	0.10	35,35,35,35	0
2	CL	J	284	1/1	0.99	0.14	38,38,38,38	0
2	CL	X	283	1/1	0.99	0.08	39,39,39,39	0
2	CL	O	283	1/1	0.99	0.04	44,44,44,44	0
2	CL	j	284	1/1	0.99	0.12	37,37,37,37	0
2	CL	K	283	1/1	0.99	0.05	34,34,34,34	0
2	CL	k	283	1/1	0.99	0.07	38,38,38,38	0
2	CL	P	283	1/1	0.99	0.08	32,32,32,32	0
2	CL	a	284	1/1	0.99	0.08	31,31,31,31	0
2	CL	H	284	1/1	0.99	0.07	35,35,35,35	0
2	CL	L	284	1/1	1.00	0.08	31,31,31,31	0
2	CL	O	284	1/1	1.00	0.11	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.