



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:52 AM UTC

PDB ID : 4NWR / pdb_00004nwr
Title : Computationally Designed Two-Component Self-Assembling Tetrahedral Cage T33-28
Authors : McNamara, D.E.; King, N.P.; Bale, J.B.; Sheffler, W.; Baker, D.; Yeates, T.O.
Deposited on : 2013-12-06
Resolution : 3.50 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

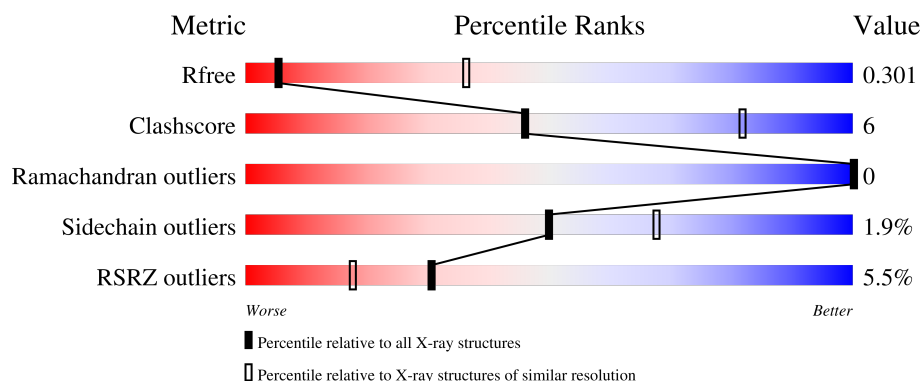
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	0	158	5% 77% 16% • •
1	2	158	5% 80% 15% • •
1	4	158	4% 80% 13% • •
1	6	158	5% 77% 17% • •
1	8	158	3% 73% 20% • 5%

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Mol	Chain	Length	Quality of chain
1	A	158	
1	AA	158	
1	AC	158	
1	AE	158	
1	AG	158	
1	AI	158	
1	AK	158	
1	AM	158	
1	AO	158	
1	AQ	158	
1	AS	158	
1	AU	158	
1	AW	158	
1	AY	158	
1	BA	158	
1	BC	158	
1	BE	158	
1	BG	158	
1	C	158	
1	E	158	
1	G	158	
1	I	158	
1	K	158	
1	M	158	
1	O	158	

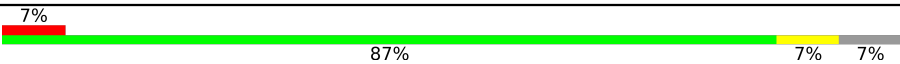
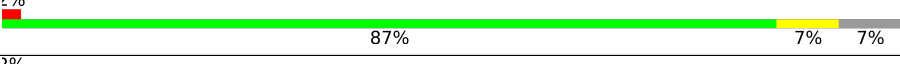
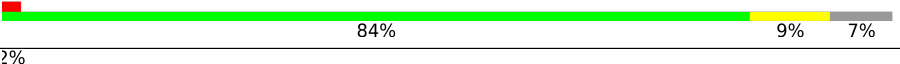
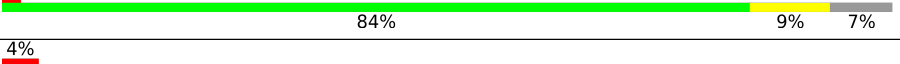
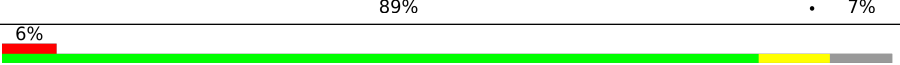
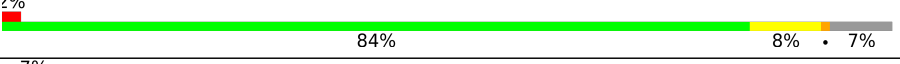
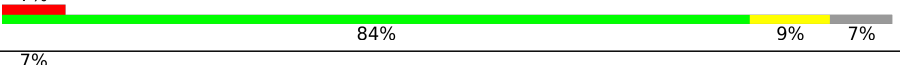
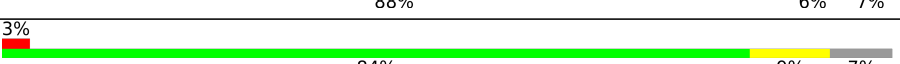
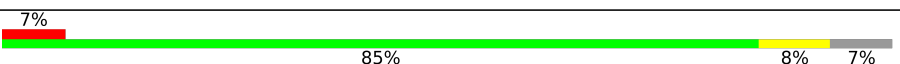
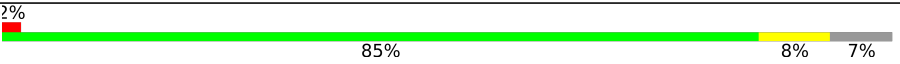
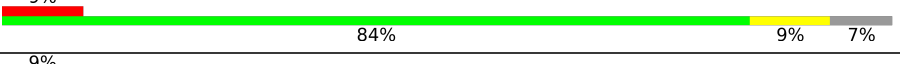
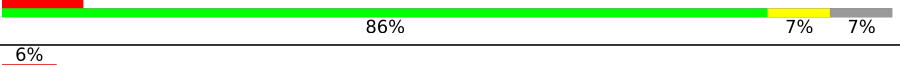
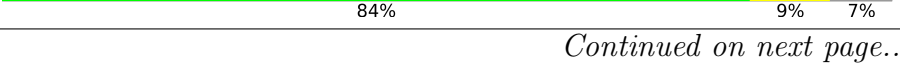
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Mol	Chain	Length	Quality of chain
1	Q	158	9% 80% 14% • •
1	S	158	4% 79% 15% • •
1	U	158	4% 77% 16% • •
1	W	158	5% 77% 17% • •
1	Y	158	% 80% 15% • •
1	a	158	5% 78% 16% • •
1	c	158	4% 78% 15% • •
1	e	158	3% 79% 15% • •
1	g	158	4% 78% 16% • •
1	i	158	2% 79% 15% • •
1	k	158	6% 77% 18% • •
1	m	158	8% 80% 14% • •
1	o	158	12% 80% 14% • •
1	q	158	6% 80% 13% • •
1	s	158	5% 78% 16% • •
1	u	158	3% 81% 14% • •
1	w	158	11% 78% 16% • •
1	y	158	6% 78% 15% • 5%
2	1	121	5% 84% 9% 7%
2	3	121	2% 86% 7% 7%
2	5	121	2% 87% 7% 7%
2	7	121	7% 84% 9% 7%
2	9	121	3% 85% 8% 7%
2	AB	121	3% 85% 8% 7%
2	AD	121	3% 84% 9% 7%

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Mol	Chain	Length	Quality of chain
2	AF	121	
2	AH	121	
2	AJ	121	
2	AL	121	
2	AN	121	
2	AP	121	
2	AR	121	
2	AT	121	
2	AV	121	
2	AX	121	
2	AZ	121	
2	B	121	
2	BB	121	
2	BD	121	
2	BF	121	
2	BH	121	
2	D	121	
2	F	121	
2	H	121	
2	J	121	
2	L	121	
2	N	121	
2	P	121	
2	R	121	
2	T	121	

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Mol	Chain	Length	Quality of chain
2	V	121	5% 86% 7% 7%
2	X	121	% 84% 9% 7%
2	Z	121	2% 85% 8% 7%
2	b	121	4% 88% 5% 7%
2	d	121	5% 85% 8% 7%
2	f	121	2% 85% 8% 7%
2	h	121	4% 83% 10% 7%
2	j	121	5% 87% 7% 6%
2	l	121	3% 83% 10% 7%
2	n	121	4% 86% 7% 7%
2	p	121	5% 85% 8% 7%
2	r	121	2% 85% 8% 7%
2	t	121	3% 85% 8% 7%
2	v	121	3% 84% 9% 7%
2	x	121	7% 87% 7% 7%
2	z	121	12% 86% 7% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 88858 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 integron gene cassette protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	C	152	Total	C	N	O	S	0	0	0
			1053	665	182	200	6			
1	E	153	Total	C	N	O	S	0	0	0
			1054	665	182	201	6			
1	G	152	Total	C	N	O	S	0	0	0
			1059	671	182	200	6			
1	I	151	Total	C	N	O	S	0	0	0
			1050	662	183	199	6			
1	K	151	Total	C	N	O	S	0	0	0
			1053	666	180	201	6			
1	M	152	Total	C	N	O	S	0	0	0
			1049	662	181	200	6			
1	O	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	Q	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	S	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	U	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	W	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	Y	152	Total	C	N	O	S	0	0	0
			1049	662	181	200	6			
1	a	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	c	151	Total	C	N	O	S	0	0	0
			1039	657	180	196	6			
1	e	151	Total	C	N	O	S	0	0	0
			1057	668	181	202	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	g	151	Total	C	N	O	S	0	0	0
			1050	662	183	199	6			
1	i	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	k	152	Total	C	N	O	S	0	0	0
			1055	667	182	200	6			
1	m	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	o	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	q	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	s	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	u	152	Total	C	N	O	S	0	0	0
			1049	662	181	200	6			
1	w	151	Total	C	N	O	S	0	0	0
			1043	659	180	198	6			
1	y	150	Total	C	N	O	S	0	0	0
			1039	656	179	198	6			
1	0	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	2	152	Total	C	N	O	S	0	0	0
			1048	662	181	199	6			
1	4	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	6	152	Total	C	N	O	S	0	0	0
			1048	661	180	201	6			
1	8	150	Total	C	N	O	S	0	0	0
			1049	664	179	200	6			
1	AA	152	Total	C	N	O	S	0	0	0
			1055	665	184	200	6			
1	AC	152	Total	C	N	O	S	0	0	0
			1059	667	185	201	6			
1	AE	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	AG	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	AI	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	AK	152	Total	C	N	O	S	0	0	0
			1056	666	182	202	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AM	152	Total	C	N	O	S	0	0	0
			1057	668	181	202	6			
1	AO	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	AQ	151	Total	C	N	O	S	0	0	0
			1048	663	181	199	5			
1	AS	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	AU	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	AW	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	AY	151	Total	C	N	O	S	0	0	0
			1043	659	180	198	6			
1	BA	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	BC	152	Total	C	N	O	S	0	0	0
			1048	662	181	199	6			
1	BE	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			
1	BG	151	Total	C	N	O	S	0	0	0
			1044	659	180	199	6			

There are 480 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	ILE	LYS	engineered mutation	UNP B0BGB0
A	53	ALA	ASP	engineered mutation	UNP B0BGB0
A	56	ILE	GLN	engineered mutation	UNP B0BGB0
A	57	PHE	SER	engineered mutation	UNP B0BGB0
A	58	LEU	ILE	engineered mutation	UNP B0BGB0
A	64	ASP	PHE	engineered mutation	UNP B0BGB0
A	109	GLU	LEU	engineered mutation	UNP B0BGB0
A	112	LEU	GLU	engineered mutation	UNP B0BGB0
A	113	ALA	LYS	engineered mutation	UNP B0BGB0
A	116	VAL	ALA	engineered mutation	UNP B0BGB0
C	49	ILE	LYS	engineered mutation	UNP B0BGB0
C	53	ALA	ASP	engineered mutation	UNP B0BGB0
C	56	ILE	GLN	engineered mutation	UNP B0BGB0
C	57	PHE	SER	engineered mutation	UNP B0BGB0
C	58	LEU	ILE	engineered mutation	UNP B0BGB0
C	64	ASP	PHE	engineered mutation	UNP B0BGB0
C	109	GLU	LEU	engineered mutation	UNP B0BGB0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	112	LEU	GLU	engineered mutation	UNP B0BGB0
C	113	ALA	LYS	engineered mutation	UNP B0BGB0
C	116	VAL	ALA	engineered mutation	UNP B0BGB0
E	49	ILE	LYS	engineered mutation	UNP B0BGB0
E	53	ALA	ASP	engineered mutation	UNP B0BGB0
E	56	ILE	GLN	engineered mutation	UNP B0BGB0
E	57	PHE	SER	engineered mutation	UNP B0BGB0
E	58	LEU	ILE	engineered mutation	UNP B0BGB0
E	64	ASP	PHE	engineered mutation	UNP B0BGB0
E	109	GLU	LEU	engineered mutation	UNP B0BGB0
E	112	LEU	GLU	engineered mutation	UNP B0BGB0
E	113	ALA	LYS	engineered mutation	UNP B0BGB0
E	116	VAL	ALA	engineered mutation	UNP B0BGB0
G	49	ILE	LYS	engineered mutation	UNP B0BGB0
G	53	ALA	ASP	engineered mutation	UNP B0BGB0
G	56	ILE	GLN	engineered mutation	UNP B0BGB0
G	57	PHE	SER	engineered mutation	UNP B0BGB0
G	58	LEU	ILE	engineered mutation	UNP B0BGB0
G	64	ASP	PHE	engineered mutation	UNP B0BGB0
G	109	GLU	LEU	engineered mutation	UNP B0BGB0
G	112	LEU	GLU	engineered mutation	UNP B0BGB0
G	113	ALA	LYS	engineered mutation	UNP B0BGB0
G	116	VAL	ALA	engineered mutation	UNP B0BGB0
I	49	ILE	LYS	engineered mutation	UNP B0BGB0
I	53	ALA	ASP	engineered mutation	UNP B0BGB0
I	56	ILE	GLN	engineered mutation	UNP B0BGB0
I	57	PHE	SER	engineered mutation	UNP B0BGB0
I	58	LEU	ILE	engineered mutation	UNP B0BGB0
I	64	ASP	PHE	engineered mutation	UNP B0BGB0
I	109	GLU	LEU	engineered mutation	UNP B0BGB0
I	112	LEU	GLU	engineered mutation	UNP B0BGB0
I	113	ALA	LYS	engineered mutation	UNP B0BGB0
I	116	VAL	ALA	engineered mutation	UNP B0BGB0
K	49	ILE	LYS	engineered mutation	UNP B0BGB0
K	53	ALA	ASP	engineered mutation	UNP B0BGB0
K	56	ILE	GLN	engineered mutation	UNP B0BGB0
K	57	PHE	SER	engineered mutation	UNP B0BGB0
K	58	LEU	ILE	engineered mutation	UNP B0BGB0
K	64	ASP	PHE	engineered mutation	UNP B0BGB0
K	109	GLU	LEU	engineered mutation	UNP B0BGB0
K	112	LEU	GLU	engineered mutation	UNP B0BGB0
K	113	ALA	LYS	engineered mutation	UNP B0BGB0

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Chain	Residue	Modelled	Actual	Comment	Reference
K	116	VAL	ALA	engineered mutation	UNP B0BGB0
M	49	ILE	LYS	engineered mutation	UNP B0BGB0
M	53	ALA	ASP	engineered mutation	UNP B0BGB0
M	56	ILE	GLN	engineered mutation	UNP B0BGB0
M	57	PHE	SER	engineered mutation	UNP B0BGB0
M	58	LEU	ILE	engineered mutation	UNP B0BGB0
M	64	ASP	PHE	engineered mutation	UNP B0BGB0
M	109	GLU	LEU	engineered mutation	UNP B0BGB0
M	112	LEU	GLU	engineered mutation	UNP B0BGB0
M	113	ALA	LYS	engineered mutation	UNP B0BGB0
M	116	VAL	ALA	engineered mutation	UNP B0BGB0
O	49	ILE	LYS	engineered mutation	UNP B0BGB0
O	53	ALA	ASP	engineered mutation	UNP B0BGB0
O	56	ILE	GLN	engineered mutation	UNP B0BGB0
O	57	PHE	SER	engineered mutation	UNP B0BGB0
O	58	LEU	ILE	engineered mutation	UNP B0BGB0
O	64	ASP	PHE	engineered mutation	UNP B0BGB0
O	109	GLU	LEU	engineered mutation	UNP B0BGB0
O	112	LEU	GLU	engineered mutation	UNP B0BGB0
O	113	ALA	LYS	engineered mutation	UNP B0BGB0
O	116	VAL	ALA	engineered mutation	UNP B0BGB0
Q	49	ILE	LYS	engineered mutation	UNP B0BGB0
Q	53	ALA	ASP	engineered mutation	UNP B0BGB0
Q	56	ILE	GLN	engineered mutation	UNP B0BGB0
Q	57	PHE	SER	engineered mutation	UNP B0BGB0
Q	58	LEU	ILE	engineered mutation	UNP B0BGB0
Q	64	ASP	PHE	engineered mutation	UNP B0BGB0
Q	109	GLU	LEU	engineered mutation	UNP B0BGB0
Q	112	LEU	GLU	engineered mutation	UNP B0BGB0
Q	113	ALA	LYS	engineered mutation	UNP B0BGB0
Q	116	VAL	ALA	engineered mutation	UNP B0BGB0
S	49	ILE	LYS	engineered mutation	UNP B0BGB0
S	53	ALA	ASP	engineered mutation	UNP B0BGB0
S	56	ILE	GLN	engineered mutation	UNP B0BGB0
S	57	PHE	SER	engineered mutation	UNP B0BGB0
S	58	LEU	ILE	engineered mutation	UNP B0BGB0
S	64	ASP	PHE	engineered mutation	UNP B0BGB0
S	109	GLU	LEU	engineered mutation	UNP B0BGB0
S	112	LEU	GLU	engineered mutation	UNP B0BGB0
S	113	ALA	LYS	engineered mutation	UNP B0BGB0
S	116	VAL	ALA	engineered mutation	UNP B0BGB0
U	49	ILE	LYS	engineered mutation	UNP B0BGB0

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Chain	Residue	Modelled	Actual	Comment	Reference
U	53	ALA	ASP	engineered mutation	UNP B0BGB0
U	56	ILE	GLN	engineered mutation	UNP B0BGB0
U	57	PHE	SER	engineered mutation	UNP B0BGB0
U	58	LEU	ILE	engineered mutation	UNP B0BGB0
U	64	ASP	PHE	engineered mutation	UNP B0BGB0
U	109	GLU	LEU	engineered mutation	UNP B0BGB0
U	112	LEU	GLU	engineered mutation	UNP B0BGB0
U	113	ALA	LYS	engineered mutation	UNP B0BGB0
U	116	VAL	ALA	engineered mutation	UNP B0BGB0
W	49	ILE	LYS	engineered mutation	UNP B0BGB0
W	53	ALA	ASP	engineered mutation	UNP B0BGB0
W	56	ILE	GLN	engineered mutation	UNP B0BGB0
W	57	PHE	SER	engineered mutation	UNP B0BGB0
W	58	LEU	ILE	engineered mutation	UNP B0BGB0
W	64	ASP	PHE	engineered mutation	UNP B0BGB0
W	109	GLU	LEU	engineered mutation	UNP B0BGB0
W	112	LEU	GLU	engineered mutation	UNP B0BGB0
W	113	ALA	LYS	engineered mutation	UNP B0BGB0
W	116	VAL	ALA	engineered mutation	UNP B0BGB0
Y	49	ILE	LYS	engineered mutation	UNP B0BGB0
Y	53	ALA	ASP	engineered mutation	UNP B0BGB0
Y	56	ILE	GLN	engineered mutation	UNP B0BGB0
Y	57	PHE	SER	engineered mutation	UNP B0BGB0
Y	58	LEU	ILE	engineered mutation	UNP B0BGB0
Y	64	ASP	PHE	engineered mutation	UNP B0BGB0
Y	109	GLU	LEU	engineered mutation	UNP B0BGB0
Y	112	LEU	GLU	engineered mutation	UNP B0BGB0
Y	113	ALA	LYS	engineered mutation	UNP B0BGB0
Y	116	VAL	ALA	engineered mutation	UNP B0BGB0
a	49	ILE	LYS	engineered mutation	UNP B0BGB0
a	53	ALA	ASP	engineered mutation	UNP B0BGB0
a	56	ILE	GLN	engineered mutation	UNP B0BGB0
a	57	PHE	SER	engineered mutation	UNP B0BGB0
a	58	LEU	ILE	engineered mutation	UNP B0BGB0
a	64	ASP	PHE	engineered mutation	UNP B0BGB0
a	109	GLU	LEU	engineered mutation	UNP B0BGB0
a	112	LEU	GLU	engineered mutation	UNP B0BGB0
a	113	ALA	LYS	engineered mutation	UNP B0BGB0
a	116	VAL	ALA	engineered mutation	UNP B0BGB0
c	49	ILE	LYS	engineered mutation	UNP B0BGB0
c	53	ALA	ASP	engineered mutation	UNP B0BGB0
c	56	ILE	GLN	engineered mutation	UNP B0BGB0

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Chain	Residue	Modelled	Actual	Comment	Reference
c	57	PHE	SER	engineered mutation	UNP B0BGB0
c	58	LEU	ILE	engineered mutation	UNP B0BGB0
c	64	ASP	PHE	engineered mutation	UNP B0BGB0
c	109	GLU	LEU	engineered mutation	UNP B0BGB0
c	112	LEU	GLU	engineered mutation	UNP B0BGB0
c	113	ALA	LYS	engineered mutation	UNP B0BGB0
c	116	VAL	ALA	engineered mutation	UNP B0BGB0
e	49	ILE	LYS	engineered mutation	UNP B0BGB0
e	53	ALA	ASP	engineered mutation	UNP B0BGB0
e	56	ILE	GLN	engineered mutation	UNP B0BGB0
e	57	PHE	SER	engineered mutation	UNP B0BGB0
e	58	LEU	ILE	engineered mutation	UNP B0BGB0
e	64	ASP	PHE	engineered mutation	UNP B0BGB0
e	109	GLU	LEU	engineered mutation	UNP B0BGB0
e	112	LEU	GLU	engineered mutation	UNP B0BGB0
e	113	ALA	LYS	engineered mutation	UNP B0BGB0
e	116	VAL	ALA	engineered mutation	UNP B0BGB0
g	49	ILE	LYS	engineered mutation	UNP B0BGB0
g	53	ALA	ASP	engineered mutation	UNP B0BGB0
g	56	ILE	GLN	engineered mutation	UNP B0BGB0
g	57	PHE	SER	engineered mutation	UNP B0BGB0
g	58	LEU	ILE	engineered mutation	UNP B0BGB0
g	64	ASP	PHE	engineered mutation	UNP B0BGB0
g	109	GLU	LEU	engineered mutation	UNP B0BGB0
g	112	LEU	GLU	engineered mutation	UNP B0BGB0
g	113	ALA	LYS	engineered mutation	UNP B0BGB0
g	116	VAL	ALA	engineered mutation	UNP B0BGB0
i	49	ILE	LYS	engineered mutation	UNP B0BGB0
i	53	ALA	ASP	engineered mutation	UNP B0BGB0
i	56	ILE	GLN	engineered mutation	UNP B0BGB0
i	57	PHE	SER	engineered mutation	UNP B0BGB0
i	58	LEU	ILE	engineered mutation	UNP B0BGB0
i	64	ASP	PHE	engineered mutation	UNP B0BGB0
i	109	GLU	LEU	engineered mutation	UNP B0BGB0
i	112	LEU	GLU	engineered mutation	UNP B0BGB0
i	113	ALA	LYS	engineered mutation	UNP B0BGB0
i	116	VAL	ALA	engineered mutation	UNP B0BGB0
k	49	ILE	LYS	engineered mutation	UNP B0BGB0
k	53	ALA	ASP	engineered mutation	UNP B0BGB0
k	56	ILE	GLN	engineered mutation	UNP B0BGB0
k	57	PHE	SER	engineered mutation	UNP B0BGB0
k	58	LEU	ILE	engineered mutation	UNP B0BGB0

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Chain	Residue	Modelled	Actual	Comment	Reference
k	64	ASP	PHE	engineered mutation	UNP B0BGB0
k	109	GLU	LEU	engineered mutation	UNP B0BGB0
k	112	LEU	GLU	engineered mutation	UNP B0BGB0
k	113	ALA	LYS	engineered mutation	UNP B0BGB0
k	116	VAL	ALA	engineered mutation	UNP B0BGB0
m	49	ILE	LYS	engineered mutation	UNP B0BGB0
m	53	ALA	ASP	engineered mutation	UNP B0BGB0
m	56	ILE	GLN	engineered mutation	UNP B0BGB0
m	57	PHE	SER	engineered mutation	UNP B0BGB0
m	58	LEU	ILE	engineered mutation	UNP B0BGB0
m	64	ASP	PHE	engineered mutation	UNP B0BGB0
m	109	GLU	LEU	engineered mutation	UNP B0BGB0
m	112	LEU	GLU	engineered mutation	UNP B0BGB0
m	113	ALA	LYS	engineered mutation	UNP B0BGB0
m	116	VAL	ALA	engineered mutation	UNP B0BGB0
o	49	ILE	LYS	engineered mutation	UNP B0BGB0
o	53	ALA	ASP	engineered mutation	UNP B0BGB0
o	56	ILE	GLN	engineered mutation	UNP B0BGB0
o	57	PHE	SER	engineered mutation	UNP B0BGB0
o	58	LEU	ILE	engineered mutation	UNP B0BGB0
o	64	ASP	PHE	engineered mutation	UNP B0BGB0
o	109	GLU	LEU	engineered mutation	UNP B0BGB0
o	112	LEU	GLU	engineered mutation	UNP B0BGB0
o	113	ALA	LYS	engineered mutation	UNP B0BGB0
o	116	VAL	ALA	engineered mutation	UNP B0BGB0
q	49	ILE	LYS	engineered mutation	UNP B0BGB0
q	53	ALA	ASP	engineered mutation	UNP B0BGB0
q	56	ILE	GLN	engineered mutation	UNP B0BGB0
q	57	PHE	SER	engineered mutation	UNP B0BGB0
q	58	LEU	ILE	engineered mutation	UNP B0BGB0
q	64	ASP	PHE	engineered mutation	UNP B0BGB0
q	109	GLU	LEU	engineered mutation	UNP B0BGB0
q	112	LEU	GLU	engineered mutation	UNP B0BGB0
q	113	ALA	LYS	engineered mutation	UNP B0BGB0
q	116	VAL	ALA	engineered mutation	UNP B0BGB0
s	49	ILE	LYS	engineered mutation	UNP B0BGB0
s	53	ALA	ASP	engineered mutation	UNP B0BGB0
s	56	ILE	GLN	engineered mutation	UNP B0BGB0
s	57	PHE	SER	engineered mutation	UNP B0BGB0
s	58	LEU	ILE	engineered mutation	UNP B0BGB0
s	64	ASP	PHE	engineered mutation	UNP B0BGB0
s	109	GLU	LEU	engineered mutation	UNP B0BGB0

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Chain	Residue	Modelled	Actual	Comment	Reference
s	112	LEU	GLU	engineered mutation	UNP B0BGB0
s	113	ALA	LYS	engineered mutation	UNP B0BGB0
s	116	VAL	ALA	engineered mutation	UNP B0BGB0
u	49	ILE	LYS	engineered mutation	UNP B0BGB0
u	53	ALA	ASP	engineered mutation	UNP B0BGB0
u	56	ILE	GLN	engineered mutation	UNP B0BGB0
u	57	PHE	SER	engineered mutation	UNP B0BGB0
u	58	LEU	ILE	engineered mutation	UNP B0BGB0
u	64	ASP	PHE	engineered mutation	UNP B0BGB0
u	109	GLU	LEU	engineered mutation	UNP B0BGB0
u	112	LEU	GLU	engineered mutation	UNP B0BGB0
u	113	ALA	LYS	engineered mutation	UNP B0BGB0
u	116	VAL	ALA	engineered mutation	UNP B0BGB0
w	49	ILE	LYS	engineered mutation	UNP B0BGB0
w	53	ALA	ASP	engineered mutation	UNP B0BGB0
w	56	ILE	GLN	engineered mutation	UNP B0BGB0
w	57	PHE	SER	engineered mutation	UNP B0BGB0
w	58	LEU	ILE	engineered mutation	UNP B0BGB0
w	64	ASP	PHE	engineered mutation	UNP B0BGB0
w	109	GLU	LEU	engineered mutation	UNP B0BGB0
w	112	LEU	GLU	engineered mutation	UNP B0BGB0
w	113	ALA	LYS	engineered mutation	UNP B0BGB0
w	116	VAL	ALA	engineered mutation	UNP B0BGB0
y	49	ILE	LYS	engineered mutation	UNP B0BGB0
y	53	ALA	ASP	engineered mutation	UNP B0BGB0
y	56	ILE	GLN	engineered mutation	UNP B0BGB0
y	57	PHE	SER	engineered mutation	UNP B0BGB0
y	58	LEU	ILE	engineered mutation	UNP B0BGB0
y	64	ASP	PHE	engineered mutation	UNP B0BGB0
y	109	GLU	LEU	engineered mutation	UNP B0BGB0
y	112	LEU	GLU	engineered mutation	UNP B0BGB0
y	113	ALA	LYS	engineered mutation	UNP B0BGB0
y	116	VAL	ALA	engineered mutation	UNP B0BGB0
0	49	ILE	LYS	engineered mutation	UNP B0BGB0
0	53	ALA	ASP	engineered mutation	UNP B0BGB0
0	56	ILE	GLN	engineered mutation	UNP B0BGB0
0	57	PHE	SER	engineered mutation	UNP B0BGB0
0	58	LEU	ILE	engineered mutation	UNP B0BGB0
0	64	ASP	PHE	engineered mutation	UNP B0BGB0
0	109	GLU	LEU	engineered mutation	UNP B0BGB0
0	112	LEU	GLU	engineered mutation	UNP B0BGB0
0	113	ALA	LYS	engineered mutation	UNP B0BGB0

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Chain	Residue	Modelled	Actual	Comment	Reference
0	116	VAL	ALA	engineered mutation	UNP B0BGB0
2	49	ILE	LYS	engineered mutation	UNP B0BGB0
2	53	ALA	ASP	engineered mutation	UNP B0BGB0
2	56	ILE	GLN	engineered mutation	UNP B0BGB0
2	57	PHE	SER	engineered mutation	UNP B0BGB0
2	58	LEU	ILE	engineered mutation	UNP B0BGB0
2	64	ASP	PHE	engineered mutation	UNP B0BGB0
2	109	GLU	LEU	engineered mutation	UNP B0BGB0
2	112	LEU	GLU	engineered mutation	UNP B0BGB0
2	113	ALA	LYS	engineered mutation	UNP B0BGB0
2	116	VAL	ALA	engineered mutation	UNP B0BGB0
4	49	ILE	LYS	engineered mutation	UNP B0BGB0
4	53	ALA	ASP	engineered mutation	UNP B0BGB0
4	56	ILE	GLN	engineered mutation	UNP B0BGB0
4	57	PHE	SER	engineered mutation	UNP B0BGB0
4	58	LEU	ILE	engineered mutation	UNP B0BGB0
4	64	ASP	PHE	engineered mutation	UNP B0BGB0
4	109	GLU	LEU	engineered mutation	UNP B0BGB0
4	112	LEU	GLU	engineered mutation	UNP B0BGB0
4	113	ALA	LYS	engineered mutation	UNP B0BGB0
4	116	VAL	ALA	engineered mutation	UNP B0BGB0
6	49	ILE	LYS	engineered mutation	UNP B0BGB0
6	53	ALA	ASP	engineered mutation	UNP B0BGB0
6	56	ILE	GLN	engineered mutation	UNP B0BGB0
6	57	PHE	SER	engineered mutation	UNP B0BGB0
6	58	LEU	ILE	engineered mutation	UNP B0BGB0
6	64	ASP	PHE	engineered mutation	UNP B0BGB0
6	109	GLU	LEU	engineered mutation	UNP B0BGB0
6	112	LEU	GLU	engineered mutation	UNP B0BGB0
6	113	ALA	LYS	engineered mutation	UNP B0BGB0
6	116	VAL	ALA	engineered mutation	UNP B0BGB0
8	49	ILE	LYS	engineered mutation	UNP B0BGB0
8	53	ALA	ASP	engineered mutation	UNP B0BGB0
8	56	ILE	GLN	engineered mutation	UNP B0BGB0
8	57	PHE	SER	engineered mutation	UNP B0BGB0
8	58	LEU	ILE	engineered mutation	UNP B0BGB0
8	64	ASP	PHE	engineered mutation	UNP B0BGB0
8	109	GLU	LEU	engineered mutation	UNP B0BGB0
8	112	LEU	GLU	engineered mutation	UNP B0BGB0
8	113	ALA	LYS	engineered mutation	UNP B0BGB0
8	116	VAL	ALA	engineered mutation	UNP B0BGB0
AA	49	ILE	LYS	engineered mutation	UNP B0BGB0

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Chain	Residue	Modelled	Actual	Comment	Reference
AA	53	ALA	ASP	engineered mutation	UNP B0BGB0
AA	56	ILE	GLN	engineered mutation	UNP B0BGB0
AA	57	PHE	SER	engineered mutation	UNP B0BGB0
AA	58	LEU	ILE	engineered mutation	UNP B0BGB0
AA	64	ASP	PHE	engineered mutation	UNP B0BGB0
AA	109	GLU	LEU	engineered mutation	UNP B0BGB0
AA	112	LEU	GLU	engineered mutation	UNP B0BGB0
AA	113	ALA	LYS	engineered mutation	UNP B0BGB0
AA	116	VAL	ALA	engineered mutation	UNP B0BGB0
AC	49	ILE	LYS	engineered mutation	UNP B0BGB0
AC	53	ALA	ASP	engineered mutation	UNP B0BGB0
AC	56	ILE	GLN	engineered mutation	UNP B0BGB0
AC	57	PHE	SER	engineered mutation	UNP B0BGB0
AC	58	LEU	ILE	engineered mutation	UNP B0BGB0
AC	64	ASP	PHE	engineered mutation	UNP B0BGB0
AC	109	GLU	LEU	engineered mutation	UNP B0BGB0
AC	112	LEU	GLU	engineered mutation	UNP B0BGB0
AC	113	ALA	LYS	engineered mutation	UNP B0BGB0
AC	116	VAL	ALA	engineered mutation	UNP B0BGB0
AE	49	ILE	LYS	engineered mutation	UNP B0BGB0
AE	53	ALA	ASP	engineered mutation	UNP B0BGB0
AE	56	ILE	GLN	engineered mutation	UNP B0BGB0
AE	57	PHE	SER	engineered mutation	UNP B0BGB0
AE	58	LEU	ILE	engineered mutation	UNP B0BGB0
AE	64	ASP	PHE	engineered mutation	UNP B0BGB0
AE	109	GLU	LEU	engineered mutation	UNP B0BGB0
AE	112	LEU	GLU	engineered mutation	UNP B0BGB0
AE	113	ALA	LYS	engineered mutation	UNP B0BGB0
AE	116	VAL	ALA	engineered mutation	UNP B0BGB0
AG	49	ILE	LYS	engineered mutation	UNP B0BGB0
AG	53	ALA	ASP	engineered mutation	UNP B0BGB0
AG	56	ILE	GLN	engineered mutation	UNP B0BGB0
AG	57	PHE	SER	engineered mutation	UNP B0BGB0
AG	58	LEU	ILE	engineered mutation	UNP B0BGB0
AG	64	ASP	PHE	engineered mutation	UNP B0BGB0
AG	109	GLU	LEU	engineered mutation	UNP B0BGB0
AG	112	LEU	GLU	engineered mutation	UNP B0BGB0
AG	113	ALA	LYS	engineered mutation	UNP B0BGB0
AG	116	VAL	ALA	engineered mutation	UNP B0BGB0
AI	49	ILE	LYS	engineered mutation	UNP B0BGB0
AI	53	ALA	ASP	engineered mutation	UNP B0BGB0
AI	56	ILE	GLN	engineered mutation	UNP B0BGB0

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Chain	Residue	Modelled	Actual	Comment	Reference
AI	57	PHE	SER	engineered mutation	UNP B0BGB0
AI	58	LEU	ILE	engineered mutation	UNP B0BGB0
AI	64	ASP	PHE	engineered mutation	UNP B0BGB0
AI	109	GLU	LEU	engineered mutation	UNP B0BGB0
AI	112	LEU	GLU	engineered mutation	UNP B0BGB0
AI	113	ALA	LYS	engineered mutation	UNP B0BGB0
AI	116	VAL	ALA	engineered mutation	UNP B0BGB0
AK	49	ILE	LYS	engineered mutation	UNP B0BGB0
AK	53	ALA	ASP	engineered mutation	UNP B0BGB0
AK	56	ILE	GLN	engineered mutation	UNP B0BGB0
AK	57	PHE	SER	engineered mutation	UNP B0BGB0
AK	58	LEU	ILE	engineered mutation	UNP B0BGB0
AK	64	ASP	PHE	engineered mutation	UNP B0BGB0
AK	109	GLU	LEU	engineered mutation	UNP B0BGB0
AK	112	LEU	GLU	engineered mutation	UNP B0BGB0
AK	113	ALA	LYS	engineered mutation	UNP B0BGB0
AK	116	VAL	ALA	engineered mutation	UNP B0BGB0
AM	49	ILE	LYS	engineered mutation	UNP B0BGB0
AM	53	ALA	ASP	engineered mutation	UNP B0BGB0
AM	56	ILE	GLN	engineered mutation	UNP B0BGB0
AM	57	PHE	SER	engineered mutation	UNP B0BGB0
AM	58	LEU	ILE	engineered mutation	UNP B0BGB0
AM	64	ASP	PHE	engineered mutation	UNP B0BGB0
AM	109	GLU	LEU	engineered mutation	UNP B0BGB0
AM	112	LEU	GLU	engineered mutation	UNP B0BGB0
AM	113	ALA	LYS	engineered mutation	UNP B0BGB0
AM	116	VAL	ALA	engineered mutation	UNP B0BGB0
AO	49	ILE	LYS	engineered mutation	UNP B0BGB0
AO	53	ALA	ASP	engineered mutation	UNP B0BGB0
AO	56	ILE	GLN	engineered mutation	UNP B0BGB0
AO	57	PHE	SER	engineered mutation	UNP B0BGB0
AO	58	LEU	ILE	engineered mutation	UNP B0BGB0
AO	64	ASP	PHE	engineered mutation	UNP B0BGB0
AO	109	GLU	LEU	engineered mutation	UNP B0BGB0
AO	112	LEU	GLU	engineered mutation	UNP B0BGB0
AO	113	ALA	LYS	engineered mutation	UNP B0BGB0
AO	116	VAL	ALA	engineered mutation	UNP B0BGB0
AQ	49	ILE	LYS	engineered mutation	UNP B0BGB0
AQ	53	ALA	ASP	engineered mutation	UNP B0BGB0
AQ	56	ILE	GLN	engineered mutation	UNP B0BGB0
AQ	57	PHE	SER	engineered mutation	UNP B0BGB0
AQ	58	LEU	ILE	engineered mutation	UNP B0BGB0

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Chain	Residue	Modelled	Actual	Comment	Reference
AQ	64	ASP	PHE	engineered mutation	UNP B0BGB0
AQ	109	GLU	LEU	engineered mutation	UNP B0BGB0
AQ	112	LEU	GLU	engineered mutation	UNP B0BGB0
AQ	113	ALA	LYS	engineered mutation	UNP B0BGB0
AQ	116	VAL	ALA	engineered mutation	UNP B0BGB0
AS	49	ILE	LYS	engineered mutation	UNP B0BGB0
AS	53	ALA	ASP	engineered mutation	UNP B0BGB0
AS	56	ILE	GLN	engineered mutation	UNP B0BGB0
AS	57	PHE	SER	engineered mutation	UNP B0BGB0
AS	58	LEU	ILE	engineered mutation	UNP B0BGB0
AS	64	ASP	PHE	engineered mutation	UNP B0BGB0
AS	109	GLU	LEU	engineered mutation	UNP B0BGB0
AS	112	LEU	GLU	engineered mutation	UNP B0BGB0
AS	113	ALA	LYS	engineered mutation	UNP B0BGB0
AS	116	VAL	ALA	engineered mutation	UNP B0BGB0
AU	49	ILE	LYS	engineered mutation	UNP B0BGB0
AU	53	ALA	ASP	engineered mutation	UNP B0BGB0
AU	56	ILE	GLN	engineered mutation	UNP B0BGB0
AU	57	PHE	SER	engineered mutation	UNP B0BGB0
AU	58	LEU	ILE	engineered mutation	UNP B0BGB0
AU	64	ASP	PHE	engineered mutation	UNP B0BGB0
AU	109	GLU	LEU	engineered mutation	UNP B0BGB0
AU	112	LEU	GLU	engineered mutation	UNP B0BGB0
AU	113	ALA	LYS	engineered mutation	UNP B0BGB0
AU	116	VAL	ALA	engineered mutation	UNP B0BGB0
AW	49	ILE	LYS	engineered mutation	UNP B0BGB0
AW	53	ALA	ASP	engineered mutation	UNP B0BGB0
AW	56	ILE	GLN	engineered mutation	UNP B0BGB0
AW	57	PHE	SER	engineered mutation	UNP B0BGB0
AW	58	LEU	ILE	engineered mutation	UNP B0BGB0
AW	64	ASP	PHE	engineered mutation	UNP B0BGB0
AW	109	GLU	LEU	engineered mutation	UNP B0BGB0
AW	112	LEU	GLU	engineered mutation	UNP B0BGB0
AW	113	ALA	LYS	engineered mutation	UNP B0BGB0
AW	116	VAL	ALA	engineered mutation	UNP B0BGB0
AY	49	ILE	LYS	engineered mutation	UNP B0BGB0
AY	53	ALA	ASP	engineered mutation	UNP B0BGB0
AY	56	ILE	GLN	engineered mutation	UNP B0BGB0
AY	57	PHE	SER	engineered mutation	UNP B0BGB0
AY	58	LEU	ILE	engineered mutation	UNP B0BGB0
AY	64	ASP	PHE	engineered mutation	UNP B0BGB0
AY	109	GLU	LEU	engineered mutation	UNP B0BGB0

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Chain	Residue	Modelled	Actual	Comment	Reference
AY	112	LEU	GLU	engineered mutation	UNP B0BGB0
AY	113	ALA	LYS	engineered mutation	UNP B0BGB0
AY	116	VAL	ALA	engineered mutation	UNP B0BGB0
BA	49	ILE	LYS	engineered mutation	UNP B0BGB0
BA	53	ALA	ASP	engineered mutation	UNP B0BGB0
BA	56	ILE	GLN	engineered mutation	UNP B0BGB0
BA	57	PHE	SER	engineered mutation	UNP B0BGB0
BA	58	LEU	ILE	engineered mutation	UNP B0BGB0
BA	64	ASP	PHE	engineered mutation	UNP B0BGB0
BA	109	GLU	LEU	engineered mutation	UNP B0BGB0
BA	112	LEU	GLU	engineered mutation	UNP B0BGB0
BA	113	ALA	LYS	engineered mutation	UNP B0BGB0
BA	116	VAL	ALA	engineered mutation	UNP B0BGB0
BC	49	ILE	LYS	engineered mutation	UNP B0BGB0
BC	53	ALA	ASP	engineered mutation	UNP B0BGB0
BC	56	ILE	GLN	engineered mutation	UNP B0BGB0
BC	57	PHE	SER	engineered mutation	UNP B0BGB0
BC	58	LEU	ILE	engineered mutation	UNP B0BGB0
BC	64	ASP	PHE	engineered mutation	UNP B0BGB0
BC	109	GLU	LEU	engineered mutation	UNP B0BGB0
BC	112	LEU	GLU	engineered mutation	UNP B0BGB0
BC	113	ALA	LYS	engineered mutation	UNP B0BGB0
BC	116	VAL	ALA	engineered mutation	UNP B0BGB0
BE	49	ILE	LYS	engineered mutation	UNP B0BGB0
BE	53	ALA	ASP	engineered mutation	UNP B0BGB0
BE	56	ILE	GLN	engineered mutation	UNP B0BGB0
BE	57	PHE	SER	engineered mutation	UNP B0BGB0
BE	58	LEU	ILE	engineered mutation	UNP B0BGB0
BE	64	ASP	PHE	engineered mutation	UNP B0BGB0
BE	109	GLU	LEU	engineered mutation	UNP B0BGB0
BE	112	LEU	GLU	engineered mutation	UNP B0BGB0
BE	113	ALA	LYS	engineered mutation	UNP B0BGB0
BE	116	VAL	ALA	engineered mutation	UNP B0BGB0
BG	49	ILE	LYS	engineered mutation	UNP B0BGB0
BG	53	ALA	ASP	engineered mutation	UNP B0BGB0
BG	56	ILE	GLN	engineered mutation	UNP B0BGB0
BG	57	PHE	SER	engineered mutation	UNP B0BGB0
BG	58	LEU	ILE	engineered mutation	UNP B0BGB0
BG	64	ASP	PHE	engineered mutation	UNP B0BGB0
BG	109	GLU	LEU	engineered mutation	UNP B0BGB0
BG	112	LEU	GLU	engineered mutation	UNP B0BGB0
BG	113	ALA	LYS	engineered mutation	UNP B0BGB0

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Chain	Residue	Modelled	Actual	Comment	Reference
BG	116	VAL	ALA	engineered mutation	UNP B0BGB0

- Molecule 2 is a protein called Macrophage migration inhibitory factor-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	113	Total	C	N	O	S	0	0	0
			806	524	135	141	6			
2	D	113	Total	C	N	O	S	0	0	0
			805	521	137	141	6			
2	F	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	H	113	Total	C	N	O	S	0	0	0
			804	522	135	141	6			
2	J	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	L	113	Total	C	N	O	S	0	0	0
			814	530	137	141	6			
2	N	113	Total	C	N	O	S	0	0	0
			808	524	137	141	6			
2	P	113	Total	C	N	O	S	0	0	0
			811	527	137	141	6			
2	R	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	T	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	V	113	Total	C	N	O	S	0	0	0
			807	525	135	141	6			
2	X	113	Total	C	N	O	S	0	0	0
			804	520	135	143	6			
2	Z	113	Total	C	N	O	S	0	0	0
			807	525	135	141	6			
2	b	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	d	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	f	113	Total	C	N	O	S	0	0	0
			811	527	137	141	6			
2	h	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	j	114	Total	C	N	O	S	0	0	0
			816	530	138	142	6			
2	l	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	n	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	p	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	r	113	Total	C	N	O	S	0	0	0
			805	521	137	141	6			
2	t	113	Total	C	N	O	S	0	0	0
			807	525	135	141	6			
2	v	113	Total	C	N	O	S	0	0	0
			808	524	137	141	6			
2	x	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	z	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	1	113	Total	C	N	O	S	0	0	0
			805	521	137	141	6			
2	3	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	5	113	Total	C	N	O	S	0	0	0
			807	525	135	141	6			
2	7	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	9	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	AB	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	AD	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	AF	113	Total	C	N	O	S	0	0	0
			805	521	137	141	6			
2	AH	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	AJ	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	AL	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	AN	113	Total	C	N	O	S	0	0	0
			803	521	135	141	6			
2	AP	113	Total	C	N	O	S	0	0	0
			810	526	135	143	6			
2	AR	113	Total	C	N	O	S	0	0	0
			804	520	135	143	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AT	113	Total	C	N	O	S	0	0	0
			807	525	135	141	6			
2	AV	113	Total	C	N	O	S	0	0	0
			805	521	137	141	6			
2	AX	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	AZ	113	Total	C	N	O	S	0	0	0
			808	524	137	141	6			
2	BB	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	BD	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	BF	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			
2	BH	113	Total	C	N	O	S	0	0	0
			801	519	135	141	6			

There are 768 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	18	LEU	GLU	engineered mutation	UNP Q4Q413
B	19	LEU	ASN	engineered mutation	UNP Q4Q413
B	22	ILE	GLN	engineered mutation	UNP Q4Q413
B	23	ILE	VAL	engineered mutation	UNP Q4Q413
B	26	ILE	ALA	engineered mutation	UNP Q4Q413
B	30	VAL	ASP	engineered mutation	UNP Q4Q413
B	87	ALA	LYS	engineered mutation	UNP Q4Q413
B	88	VAL	GLU	engineered mutation	UNP Q4Q413
B	114	LEU	-	expression tag	UNP Q4Q413
B	115	GLU	-	expression tag	UNP Q4Q413
B	116	HIS	-	expression tag	UNP Q4Q413
B	117	HIS	-	expression tag	UNP Q4Q413
B	118	HIS	-	expression tag	UNP Q4Q413
B	119	HIS	-	expression tag	UNP Q4Q413
B	120	HIS	-	expression tag	UNP Q4Q413
B	121	HIS	-	expression tag	UNP Q4Q413
D	18	LEU	GLU	engineered mutation	UNP Q4Q413
D	19	LEU	ASN	engineered mutation	UNP Q4Q413
D	22	ILE	GLN	engineered mutation	UNP Q4Q413
D	23	ILE	VAL	engineered mutation	UNP Q4Q413
D	26	ILE	ALA	engineered mutation	UNP Q4Q413
D	30	VAL	ASP	engineered mutation	UNP Q4Q413
D	87	ALA	LYS	engineered mutation	UNP Q4Q413

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Chain	Residue	Modelled	Actual	Comment	Reference
D	88	VAL	GLU	engineered mutation	UNP Q4Q413
D	114	LEU	-	expression tag	UNP Q4Q413
D	115	GLU	-	expression tag	UNP Q4Q413
D	116	HIS	-	expression tag	UNP Q4Q413
D	117	HIS	-	expression tag	UNP Q4Q413
D	118	HIS	-	expression tag	UNP Q4Q413
D	119	HIS	-	expression tag	UNP Q4Q413
D	120	HIS	-	expression tag	UNP Q4Q413
D	121	HIS	-	expression tag	UNP Q4Q413
F	18	LEU	GLU	engineered mutation	UNP Q4Q413
F	19	LEU	ASN	engineered mutation	UNP Q4Q413
F	22	ILE	GLN	engineered mutation	UNP Q4Q413
F	23	ILE	VAL	engineered mutation	UNP Q4Q413
F	26	ILE	ALA	engineered mutation	UNP Q4Q413
F	30	VAL	ASP	engineered mutation	UNP Q4Q413
F	87	ALA	LYS	engineered mutation	UNP Q4Q413
F	88	VAL	GLU	engineered mutation	UNP Q4Q413
F	114	LEU	-	expression tag	UNP Q4Q413
F	115	GLU	-	expression tag	UNP Q4Q413
F	116	HIS	-	expression tag	UNP Q4Q413
F	117	HIS	-	expression tag	UNP Q4Q413
F	118	HIS	-	expression tag	UNP Q4Q413
F	119	HIS	-	expression tag	UNP Q4Q413
F	120	HIS	-	expression tag	UNP Q4Q413
F	121	HIS	-	expression tag	UNP Q4Q413
H	18	LEU	GLU	engineered mutation	UNP Q4Q413
H	19	LEU	ASN	engineered mutation	UNP Q4Q413
H	22	ILE	GLN	engineered mutation	UNP Q4Q413
H	23	ILE	VAL	engineered mutation	UNP Q4Q413
H	26	ILE	ALA	engineered mutation	UNP Q4Q413
H	30	VAL	ASP	engineered mutation	UNP Q4Q413
H	87	ALA	LYS	engineered mutation	UNP Q4Q413
H	88	VAL	GLU	engineered mutation	UNP Q4Q413
H	114	LEU	-	expression tag	UNP Q4Q413
H	115	GLU	-	expression tag	UNP Q4Q413
H	116	HIS	-	expression tag	UNP Q4Q413
H	117	HIS	-	expression tag	UNP Q4Q413
H	118	HIS	-	expression tag	UNP Q4Q413
H	119	HIS	-	expression tag	UNP Q4Q413
H	120	HIS	-	expression tag	UNP Q4Q413
H	121	HIS	-	expression tag	UNP Q4Q413
J	18	LEU	GLU	engineered mutation	UNP Q4Q413

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Chain	Residue	Modelled	Actual	Comment	Reference
J	19	LEU	ASN	engineered mutation	UNP Q4Q413
J	22	ILE	GLN	engineered mutation	UNP Q4Q413
J	23	ILE	VAL	engineered mutation	UNP Q4Q413
J	26	ILE	ALA	engineered mutation	UNP Q4Q413
J	30	VAL	ASP	engineered mutation	UNP Q4Q413
J	87	ALA	LYS	engineered mutation	UNP Q4Q413
J	88	VAL	GLU	engineered mutation	UNP Q4Q413
J	114	LEU	-	expression tag	UNP Q4Q413
J	115	GLU	-	expression tag	UNP Q4Q413
J	116	HIS	-	expression tag	UNP Q4Q413
J	117	HIS	-	expression tag	UNP Q4Q413
J	118	HIS	-	expression tag	UNP Q4Q413
J	119	HIS	-	expression tag	UNP Q4Q413
J	120	HIS	-	expression tag	UNP Q4Q413
J	121	HIS	-	expression tag	UNP Q4Q413
L	18	LEU	GLU	engineered mutation	UNP Q4Q413
L	19	LEU	ASN	engineered mutation	UNP Q4Q413
L	22	ILE	GLN	engineered mutation	UNP Q4Q413
L	23	ILE	VAL	engineered mutation	UNP Q4Q413
L	26	ILE	ALA	engineered mutation	UNP Q4Q413
L	30	VAL	ASP	engineered mutation	UNP Q4Q413
L	87	ALA	LYS	engineered mutation	UNP Q4Q413
L	88	VAL	GLU	engineered mutation	UNP Q4Q413
L	114	LEU	-	expression tag	UNP Q4Q413
L	115	GLU	-	expression tag	UNP Q4Q413
L	116	HIS	-	expression tag	UNP Q4Q413
L	117	HIS	-	expression tag	UNP Q4Q413
L	118	HIS	-	expression tag	UNP Q4Q413
L	119	HIS	-	expression tag	UNP Q4Q413
L	120	HIS	-	expression tag	UNP Q4Q413
L	121	HIS	-	expression tag	UNP Q4Q413
N	18	LEU	GLU	engineered mutation	UNP Q4Q413
N	19	LEU	ASN	engineered mutation	UNP Q4Q413
N	22	ILE	GLN	engineered mutation	UNP Q4Q413
N	23	ILE	VAL	engineered mutation	UNP Q4Q413
N	26	ILE	ALA	engineered mutation	UNP Q4Q413
N	30	VAL	ASP	engineered mutation	UNP Q4Q413
N	87	ALA	LYS	engineered mutation	UNP Q4Q413
N	88	VAL	GLU	engineered mutation	UNP Q4Q413
N	114	LEU	-	expression tag	UNP Q4Q413
N	115	GLU	-	expression tag	UNP Q4Q413
N	116	HIS	-	expression tag	UNP Q4Q413

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Chain	Residue	Modelled	Actual	Comment	Reference
N	117	HIS	-	expression tag	UNP Q4Q413
N	118	HIS	-	expression tag	UNP Q4Q413
N	119	HIS	-	expression tag	UNP Q4Q413
N	120	HIS	-	expression tag	UNP Q4Q413
N	121	HIS	-	expression tag	UNP Q4Q413
P	18	LEU	GLU	engineered mutation	UNP Q4Q413
P	19	LEU	ASN	engineered mutation	UNP Q4Q413
P	22	ILE	GLN	engineered mutation	UNP Q4Q413
P	23	ILE	VAL	engineered mutation	UNP Q4Q413
P	26	ILE	ALA	engineered mutation	UNP Q4Q413
P	30	VAL	ASP	engineered mutation	UNP Q4Q413
P	87	ALA	LYS	engineered mutation	UNP Q4Q413
P	88	VAL	GLU	engineered mutation	UNP Q4Q413
P	114	LEU	-	expression tag	UNP Q4Q413
P	115	GLU	-	expression tag	UNP Q4Q413
P	116	HIS	-	expression tag	UNP Q4Q413
P	117	HIS	-	expression tag	UNP Q4Q413
P	118	HIS	-	expression tag	UNP Q4Q413
P	119	HIS	-	expression tag	UNP Q4Q413
P	120	HIS	-	expression tag	UNP Q4Q413
P	121	HIS	-	expression tag	UNP Q4Q413
R	18	LEU	GLU	engineered mutation	UNP Q4Q413
R	19	LEU	ASN	engineered mutation	UNP Q4Q413
R	22	ILE	GLN	engineered mutation	UNP Q4Q413
R	23	ILE	VAL	engineered mutation	UNP Q4Q413
R	26	ILE	ALA	engineered mutation	UNP Q4Q413
R	30	VAL	ASP	engineered mutation	UNP Q4Q413
R	87	ALA	LYS	engineered mutation	UNP Q4Q413
R	88	VAL	GLU	engineered mutation	UNP Q4Q413
R	114	LEU	-	expression tag	UNP Q4Q413
R	115	GLU	-	expression tag	UNP Q4Q413
R	116	HIS	-	expression tag	UNP Q4Q413
R	117	HIS	-	expression tag	UNP Q4Q413
R	118	HIS	-	expression tag	UNP Q4Q413
R	119	HIS	-	expression tag	UNP Q4Q413
R	120	HIS	-	expression tag	UNP Q4Q413
R	121	HIS	-	expression tag	UNP Q4Q413
T	18	LEU	GLU	engineered mutation	UNP Q4Q413
T	19	LEU	ASN	engineered mutation	UNP Q4Q413
T	22	ILE	GLN	engineered mutation	UNP Q4Q413
T	23	ILE	VAL	engineered mutation	UNP Q4Q413
T	26	ILE	ALA	engineered mutation	UNP Q4Q413

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Chain	Residue	Modelled	Actual	Comment	Reference
T	30	VAL	ASP	engineered mutation	UNP Q4Q413
T	87	ALA	LYS	engineered mutation	UNP Q4Q413
T	88	VAL	GLU	engineered mutation	UNP Q4Q413
T	114	LEU	-	expression tag	UNP Q4Q413
T	115	GLU	-	expression tag	UNP Q4Q413
T	116	HIS	-	expression tag	UNP Q4Q413
T	117	HIS	-	expression tag	UNP Q4Q413
T	118	HIS	-	expression tag	UNP Q4Q413
T	119	HIS	-	expression tag	UNP Q4Q413
T	120	HIS	-	expression tag	UNP Q4Q413
T	121	HIS	-	expression tag	UNP Q4Q413
V	18	LEU	GLU	engineered mutation	UNP Q4Q413
V	19	LEU	ASN	engineered mutation	UNP Q4Q413
V	22	ILE	GLN	engineered mutation	UNP Q4Q413
V	23	ILE	VAL	engineered mutation	UNP Q4Q413
V	26	ILE	ALA	engineered mutation	UNP Q4Q413
V	30	VAL	ASP	engineered mutation	UNP Q4Q413
V	87	ALA	LYS	engineered mutation	UNP Q4Q413
V	88	VAL	GLU	engineered mutation	UNP Q4Q413
V	114	LEU	-	expression tag	UNP Q4Q413
V	115	GLU	-	expression tag	UNP Q4Q413
V	116	HIS	-	expression tag	UNP Q4Q413
V	117	HIS	-	expression tag	UNP Q4Q413
V	118	HIS	-	expression tag	UNP Q4Q413
V	119	HIS	-	expression tag	UNP Q4Q413
V	120	HIS	-	expression tag	UNP Q4Q413
V	121	HIS	-	expression tag	UNP Q4Q413
X	18	LEU	GLU	engineered mutation	UNP Q4Q413
X	19	LEU	ASN	engineered mutation	UNP Q4Q413
X	22	ILE	GLN	engineered mutation	UNP Q4Q413
X	23	ILE	VAL	engineered mutation	UNP Q4Q413
X	26	ILE	ALA	engineered mutation	UNP Q4Q413
X	30	VAL	ASP	engineered mutation	UNP Q4Q413
X	87	ALA	LYS	engineered mutation	UNP Q4Q413
X	88	VAL	GLU	engineered mutation	UNP Q4Q413
X	114	LEU	-	expression tag	UNP Q4Q413
X	115	GLU	-	expression tag	UNP Q4Q413
X	116	HIS	-	expression tag	UNP Q4Q413
X	117	HIS	-	expression tag	UNP Q4Q413
X	118	HIS	-	expression tag	UNP Q4Q413
X	119	HIS	-	expression tag	UNP Q4Q413
X	120	HIS	-	expression tag	UNP Q4Q413

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Chain	Residue	Modelled	Actual	Comment	Reference
X	121	HIS	-	expression tag	UNP Q4Q413
Z	18	LEU	GLU	engineered mutation	UNP Q4Q413
Z	19	LEU	ASN	engineered mutation	UNP Q4Q413
Z	22	ILE	GLN	engineered mutation	UNP Q4Q413
Z	23	ILE	VAL	engineered mutation	UNP Q4Q413
Z	26	ILE	ALA	engineered mutation	UNP Q4Q413
Z	30	VAL	ASP	engineered mutation	UNP Q4Q413
Z	87	ALA	LYS	engineered mutation	UNP Q4Q413
Z	88	VAL	GLU	engineered mutation	UNP Q4Q413
Z	114	LEU	-	expression tag	UNP Q4Q413
Z	115	GLU	-	expression tag	UNP Q4Q413
Z	116	HIS	-	expression tag	UNP Q4Q413
Z	117	HIS	-	expression tag	UNP Q4Q413
Z	118	HIS	-	expression tag	UNP Q4Q413
Z	119	HIS	-	expression tag	UNP Q4Q413
Z	120	HIS	-	expression tag	UNP Q4Q413
Z	121	HIS	-	expression tag	UNP Q4Q413
b	18	LEU	GLU	engineered mutation	UNP Q4Q413
b	19	LEU	ASN	engineered mutation	UNP Q4Q413
b	22	ILE	GLN	engineered mutation	UNP Q4Q413
b	23	ILE	VAL	engineered mutation	UNP Q4Q413
b	26	ILE	ALA	engineered mutation	UNP Q4Q413
b	30	VAL	ASP	engineered mutation	UNP Q4Q413
b	87	ALA	LYS	engineered mutation	UNP Q4Q413
b	88	VAL	GLU	engineered mutation	UNP Q4Q413
b	114	LEU	-	expression tag	UNP Q4Q413
b	115	GLU	-	expression tag	UNP Q4Q413
b	116	HIS	-	expression tag	UNP Q4Q413
b	117	HIS	-	expression tag	UNP Q4Q413
b	118	HIS	-	expression tag	UNP Q4Q413
b	119	HIS	-	expression tag	UNP Q4Q413
b	120	HIS	-	expression tag	UNP Q4Q413
b	121	HIS	-	expression tag	UNP Q4Q413
d	18	LEU	GLU	engineered mutation	UNP Q4Q413
d	19	LEU	ASN	engineered mutation	UNP Q4Q413
d	22	ILE	GLN	engineered mutation	UNP Q4Q413
d	23	ILE	VAL	engineered mutation	UNP Q4Q413
d	26	ILE	ALA	engineered mutation	UNP Q4Q413
d	30	VAL	ASP	engineered mutation	UNP Q4Q413
d	87	ALA	LYS	engineered mutation	UNP Q4Q413
d	88	VAL	GLU	engineered mutation	UNP Q4Q413
d	114	LEU	-	expression tag	UNP Q4Q413

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Chain	Residue	Modelled	Actual	Comment	Reference
d	115	GLU	-	expression tag	UNP Q4Q413
d	116	HIS	-	expression tag	UNP Q4Q413
d	117	HIS	-	expression tag	UNP Q4Q413
d	118	HIS	-	expression tag	UNP Q4Q413
d	119	HIS	-	expression tag	UNP Q4Q413
d	120	HIS	-	expression tag	UNP Q4Q413
d	121	HIS	-	expression tag	UNP Q4Q413
f	18	LEU	GLU	engineered mutation	UNP Q4Q413
f	19	LEU	ASN	engineered mutation	UNP Q4Q413
f	22	ILE	GLN	engineered mutation	UNP Q4Q413
f	23	ILE	VAL	engineered mutation	UNP Q4Q413
f	26	ILE	ALA	engineered mutation	UNP Q4Q413
f	30	VAL	ASP	engineered mutation	UNP Q4Q413
f	87	ALA	LYS	engineered mutation	UNP Q4Q413
f	88	VAL	GLU	engineered mutation	UNP Q4Q413
f	114	LEU	-	expression tag	UNP Q4Q413
f	115	GLU	-	expression tag	UNP Q4Q413
f	116	HIS	-	expression tag	UNP Q4Q413
f	117	HIS	-	expression tag	UNP Q4Q413
f	118	HIS	-	expression tag	UNP Q4Q413
f	119	HIS	-	expression tag	UNP Q4Q413
f	120	HIS	-	expression tag	UNP Q4Q413
f	121	HIS	-	expression tag	UNP Q4Q413
h	18	LEU	GLU	engineered mutation	UNP Q4Q413
h	19	LEU	ASN	engineered mutation	UNP Q4Q413
h	22	ILE	GLN	engineered mutation	UNP Q4Q413
h	23	ILE	VAL	engineered mutation	UNP Q4Q413
h	26	ILE	ALA	engineered mutation	UNP Q4Q413
h	30	VAL	ASP	engineered mutation	UNP Q4Q413
h	87	ALA	LYS	engineered mutation	UNP Q4Q413
h	88	VAL	GLU	engineered mutation	UNP Q4Q413
h	114	LEU	-	expression tag	UNP Q4Q413
h	115	GLU	-	expression tag	UNP Q4Q413
h	116	HIS	-	expression tag	UNP Q4Q413
h	117	HIS	-	expression tag	UNP Q4Q413
h	118	HIS	-	expression tag	UNP Q4Q413
h	119	HIS	-	expression tag	UNP Q4Q413
h	120	HIS	-	expression tag	UNP Q4Q413
h	121	HIS	-	expression tag	UNP Q4Q413
j	18	LEU	GLU	engineered mutation	UNP Q4Q413
j	19	LEU	ASN	engineered mutation	UNP Q4Q413
j	22	ILE	GLN	engineered mutation	UNP Q4Q413

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Chain	Residue	Modelled	Actual	Comment	Reference
j	23	ILE	VAL	engineered mutation	UNP Q4Q413
j	26	ILE	ALA	engineered mutation	UNP Q4Q413
j	30	VAL	ASP	engineered mutation	UNP Q4Q413
j	87	ALA	LYS	engineered mutation	UNP Q4Q413
j	88	VAL	GLU	engineered mutation	UNP Q4Q413
j	114	LEU	-	expression tag	UNP Q4Q413
j	115	GLU	-	expression tag	UNP Q4Q413
j	116	HIS	-	expression tag	UNP Q4Q413
j	117	HIS	-	expression tag	UNP Q4Q413
j	118	HIS	-	expression tag	UNP Q4Q413
j	119	HIS	-	expression tag	UNP Q4Q413
j	120	HIS	-	expression tag	UNP Q4Q413
j	121	HIS	-	expression tag	UNP Q4Q413
l	18	LEU	GLU	engineered mutation	UNP Q4Q413
l	19	LEU	ASN	engineered mutation	UNP Q4Q413
l	22	ILE	GLN	engineered mutation	UNP Q4Q413
l	23	ILE	VAL	engineered mutation	UNP Q4Q413
l	26	ILE	ALA	engineered mutation	UNP Q4Q413
l	30	VAL	ASP	engineered mutation	UNP Q4Q413
l	87	ALA	LYS	engineered mutation	UNP Q4Q413
l	88	VAL	GLU	engineered mutation	UNP Q4Q413
l	114	LEU	-	expression tag	UNP Q4Q413
l	115	GLU	-	expression tag	UNP Q4Q413
l	116	HIS	-	expression tag	UNP Q4Q413
l	117	HIS	-	expression tag	UNP Q4Q413
l	118	HIS	-	expression tag	UNP Q4Q413
l	119	HIS	-	expression tag	UNP Q4Q413
l	120	HIS	-	expression tag	UNP Q4Q413
l	121	HIS	-	expression tag	UNP Q4Q413
n	18	LEU	GLU	engineered mutation	UNP Q4Q413
n	19	LEU	ASN	engineered mutation	UNP Q4Q413
n	22	ILE	GLN	engineered mutation	UNP Q4Q413
n	23	ILE	VAL	engineered mutation	UNP Q4Q413
n	26	ILE	ALA	engineered mutation	UNP Q4Q413
n	30	VAL	ASP	engineered mutation	UNP Q4Q413
n	87	ALA	LYS	engineered mutation	UNP Q4Q413
n	88	VAL	GLU	engineered mutation	UNP Q4Q413
n	114	LEU	-	expression tag	UNP Q4Q413
n	115	GLU	-	expression tag	UNP Q4Q413
n	116	HIS	-	expression tag	UNP Q4Q413
n	117	HIS	-	expression tag	UNP Q4Q413
n	118	HIS	-	expression tag	UNP Q4Q413

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Chain	Residue	Modelled	Actual	Comment	Reference
n	119	HIS	-	expression tag	UNP Q4Q413
n	120	HIS	-	expression tag	UNP Q4Q413
n	121	HIS	-	expression tag	UNP Q4Q413
p	18	LEU	GLU	engineered mutation	UNP Q4Q413
p	19	LEU	ASN	engineered mutation	UNP Q4Q413
p	22	ILE	GLN	engineered mutation	UNP Q4Q413
p	23	ILE	VAL	engineered mutation	UNP Q4Q413
p	26	ILE	ALA	engineered mutation	UNP Q4Q413
p	30	VAL	ASP	engineered mutation	UNP Q4Q413
p	87	ALA	LYS	engineered mutation	UNP Q4Q413
p	88	VAL	GLU	engineered mutation	UNP Q4Q413
p	114	LEU	-	expression tag	UNP Q4Q413
p	115	GLU	-	expression tag	UNP Q4Q413
p	116	HIS	-	expression tag	UNP Q4Q413
p	117	HIS	-	expression tag	UNP Q4Q413
p	118	HIS	-	expression tag	UNP Q4Q413
p	119	HIS	-	expression tag	UNP Q4Q413
p	120	HIS	-	expression tag	UNP Q4Q413
p	121	HIS	-	expression tag	UNP Q4Q413
r	18	LEU	GLU	engineered mutation	UNP Q4Q413
r	19	LEU	ASN	engineered mutation	UNP Q4Q413
r	22	ILE	GLN	engineered mutation	UNP Q4Q413
r	23	ILE	VAL	engineered mutation	UNP Q4Q413
r	26	ILE	ALA	engineered mutation	UNP Q4Q413
r	30	VAL	ASP	engineered mutation	UNP Q4Q413
r	87	ALA	LYS	engineered mutation	UNP Q4Q413
r	88	VAL	GLU	engineered mutation	UNP Q4Q413
r	114	LEU	-	expression tag	UNP Q4Q413
r	115	GLU	-	expression tag	UNP Q4Q413
r	116	HIS	-	expression tag	UNP Q4Q413
r	117	HIS	-	expression tag	UNP Q4Q413
r	118	HIS	-	expression tag	UNP Q4Q413
r	119	HIS	-	expression tag	UNP Q4Q413
r	120	HIS	-	expression tag	UNP Q4Q413
r	121	HIS	-	expression tag	UNP Q4Q413
t	18	LEU	GLU	engineered mutation	UNP Q4Q413
t	19	LEU	ASN	engineered mutation	UNP Q4Q413
t	22	ILE	GLN	engineered mutation	UNP Q4Q413
t	23	ILE	VAL	engineered mutation	UNP Q4Q413
t	26	ILE	ALA	engineered mutation	UNP Q4Q413
t	30	VAL	ASP	engineered mutation	UNP Q4Q413
t	87	ALA	LYS	engineered mutation	UNP Q4Q413

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Chain	Residue	Modelled	Actual	Comment	Reference
t	88	VAL	GLU	engineered mutation	UNP Q4Q413
t	114	LEU	-	expression tag	UNP Q4Q413
t	115	GLU	-	expression tag	UNP Q4Q413
t	116	HIS	-	expression tag	UNP Q4Q413
t	117	HIS	-	expression tag	UNP Q4Q413
t	118	HIS	-	expression tag	UNP Q4Q413
t	119	HIS	-	expression tag	UNP Q4Q413
t	120	HIS	-	expression tag	UNP Q4Q413
t	121	HIS	-	expression tag	UNP Q4Q413
v	18	LEU	GLU	engineered mutation	UNP Q4Q413
v	19	LEU	ASN	engineered mutation	UNP Q4Q413
v	22	ILE	GLN	engineered mutation	UNP Q4Q413
v	23	ILE	VAL	engineered mutation	UNP Q4Q413
v	26	ILE	ALA	engineered mutation	UNP Q4Q413
v	30	VAL	ASP	engineered mutation	UNP Q4Q413
v	87	ALA	LYS	engineered mutation	UNP Q4Q413
v	88	VAL	GLU	engineered mutation	UNP Q4Q413
v	114	LEU	-	expression tag	UNP Q4Q413
v	115	GLU	-	expression tag	UNP Q4Q413
v	116	HIS	-	expression tag	UNP Q4Q413
v	117	HIS	-	expression tag	UNP Q4Q413
v	118	HIS	-	expression tag	UNP Q4Q413
v	119	HIS	-	expression tag	UNP Q4Q413
v	120	HIS	-	expression tag	UNP Q4Q413
v	121	HIS	-	expression tag	UNP Q4Q413
x	18	LEU	GLU	engineered mutation	UNP Q4Q413
x	19	LEU	ASN	engineered mutation	UNP Q4Q413
x	22	ILE	GLN	engineered mutation	UNP Q4Q413
x	23	ILE	VAL	engineered mutation	UNP Q4Q413
x	26	ILE	ALA	engineered mutation	UNP Q4Q413
x	30	VAL	ASP	engineered mutation	UNP Q4Q413
x	87	ALA	LYS	engineered mutation	UNP Q4Q413
x	88	VAL	GLU	engineered mutation	UNP Q4Q413
x	114	LEU	-	expression tag	UNP Q4Q413
x	115	GLU	-	expression tag	UNP Q4Q413
x	116	HIS	-	expression tag	UNP Q4Q413
x	117	HIS	-	expression tag	UNP Q4Q413
x	118	HIS	-	expression tag	UNP Q4Q413
x	119	HIS	-	expression tag	UNP Q4Q413
x	120	HIS	-	expression tag	UNP Q4Q413
x	121	HIS	-	expression tag	UNP Q4Q413
z	18	LEU	GLU	engineered mutation	UNP Q4Q413

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Chain	Residue	Modelled	Actual	Comment	Reference
z	19	LEU	ASN	engineered mutation	UNP Q4Q413
z	22	ILE	GLN	engineered mutation	UNP Q4Q413
z	23	ILE	VAL	engineered mutation	UNP Q4Q413
z	26	ILE	ALA	engineered mutation	UNP Q4Q413
z	30	VAL	ASP	engineered mutation	UNP Q4Q413
z	87	ALA	LYS	engineered mutation	UNP Q4Q413
z	88	VAL	GLU	engineered mutation	UNP Q4Q413
z	114	LEU	-	expression tag	UNP Q4Q413
z	115	GLU	-	expression tag	UNP Q4Q413
z	116	HIS	-	expression tag	UNP Q4Q413
z	117	HIS	-	expression tag	UNP Q4Q413
z	118	HIS	-	expression tag	UNP Q4Q413
z	119	HIS	-	expression tag	UNP Q4Q413
z	120	HIS	-	expression tag	UNP Q4Q413
z	121	HIS	-	expression tag	UNP Q4Q413
1	18	LEU	GLU	engineered mutation	UNP Q4Q413
1	19	LEU	ASN	engineered mutation	UNP Q4Q413
1	22	ILE	GLN	engineered mutation	UNP Q4Q413
1	23	ILE	VAL	engineered mutation	UNP Q4Q413
1	26	ILE	ALA	engineered mutation	UNP Q4Q413
1	30	VAL	ASP	engineered mutation	UNP Q4Q413
1	87	ALA	LYS	engineered mutation	UNP Q4Q413
1	88	VAL	GLU	engineered mutation	UNP Q4Q413
1	114	LEU	-	expression tag	UNP Q4Q413
1	115	GLU	-	expression tag	UNP Q4Q413
1	116	HIS	-	expression tag	UNP Q4Q413
1	117	HIS	-	expression tag	UNP Q4Q413
1	118	HIS	-	expression tag	UNP Q4Q413
1	119	HIS	-	expression tag	UNP Q4Q413
1	120	HIS	-	expression tag	UNP Q4Q413
1	121	HIS	-	expression tag	UNP Q4Q413
3	18	LEU	GLU	engineered mutation	UNP Q4Q413
3	19	LEU	ASN	engineered mutation	UNP Q4Q413
3	22	ILE	GLN	engineered mutation	UNP Q4Q413
3	23	ILE	VAL	engineered mutation	UNP Q4Q413
3	26	ILE	ALA	engineered mutation	UNP Q4Q413
3	30	VAL	ASP	engineered mutation	UNP Q4Q413
3	87	ALA	LYS	engineered mutation	UNP Q4Q413
3	88	VAL	GLU	engineered mutation	UNP Q4Q413
3	114	LEU	-	expression tag	UNP Q4Q413
3	115	GLU	-	expression tag	UNP Q4Q413
3	116	HIS	-	expression tag	UNP Q4Q413

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Chain	Residue	Modelled	Actual	Comment	Reference
3	117	HIS	-	expression tag	UNP Q4Q413
3	118	HIS	-	expression tag	UNP Q4Q413
3	119	HIS	-	expression tag	UNP Q4Q413
3	120	HIS	-	expression tag	UNP Q4Q413
3	121	HIS	-	expression tag	UNP Q4Q413
5	18	LEU	GLU	engineered mutation	UNP Q4Q413
5	19	LEU	ASN	engineered mutation	UNP Q4Q413
5	22	ILE	GLN	engineered mutation	UNP Q4Q413
5	23	ILE	VAL	engineered mutation	UNP Q4Q413
5	26	ILE	ALA	engineered mutation	UNP Q4Q413
5	30	VAL	ASP	engineered mutation	UNP Q4Q413
5	87	ALA	LYS	engineered mutation	UNP Q4Q413
5	88	VAL	GLU	engineered mutation	UNP Q4Q413
5	114	LEU	-	expression tag	UNP Q4Q413
5	115	GLU	-	expression tag	UNP Q4Q413
5	116	HIS	-	expression tag	UNP Q4Q413
5	117	HIS	-	expression tag	UNP Q4Q413
5	118	HIS	-	expression tag	UNP Q4Q413
5	119	HIS	-	expression tag	UNP Q4Q413
5	120	HIS	-	expression tag	UNP Q4Q413
5	121	HIS	-	expression tag	UNP Q4Q413
7	18	LEU	GLU	engineered mutation	UNP Q4Q413
7	19	LEU	ASN	engineered mutation	UNP Q4Q413
7	22	ILE	GLN	engineered mutation	UNP Q4Q413
7	23	ILE	VAL	engineered mutation	UNP Q4Q413
7	26	ILE	ALA	engineered mutation	UNP Q4Q413
7	30	VAL	ASP	engineered mutation	UNP Q4Q413
7	87	ALA	LYS	engineered mutation	UNP Q4Q413
7	88	VAL	GLU	engineered mutation	UNP Q4Q413
7	114	LEU	-	expression tag	UNP Q4Q413
7	115	GLU	-	expression tag	UNP Q4Q413
7	116	HIS	-	expression tag	UNP Q4Q413
7	117	HIS	-	expression tag	UNP Q4Q413
7	118	HIS	-	expression tag	UNP Q4Q413
7	119	HIS	-	expression tag	UNP Q4Q413
7	120	HIS	-	expression tag	UNP Q4Q413
7	121	HIS	-	expression tag	UNP Q4Q413
9	18	LEU	GLU	engineered mutation	UNP Q4Q413
9	19	LEU	ASN	engineered mutation	UNP Q4Q413
9	22	ILE	GLN	engineered mutation	UNP Q4Q413
9	23	ILE	VAL	engineered mutation	UNP Q4Q413
9	26	ILE	ALA	engineered mutation	UNP Q4Q413

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Chain	Residue	Modelled	Actual	Comment	Reference
9	30	VAL	ASP	engineered mutation	UNP Q4Q413
9	87	ALA	LYS	engineered mutation	UNP Q4Q413
9	88	VAL	GLU	engineered mutation	UNP Q4Q413
9	114	LEU	-	expression tag	UNP Q4Q413
9	115	GLU	-	expression tag	UNP Q4Q413
9	116	HIS	-	expression tag	UNP Q4Q413
9	117	HIS	-	expression tag	UNP Q4Q413
9	118	HIS	-	expression tag	UNP Q4Q413
9	119	HIS	-	expression tag	UNP Q4Q413
9	120	HIS	-	expression tag	UNP Q4Q413
9	121	HIS	-	expression tag	UNP Q4Q413
AB	18	LEU	GLU	engineered mutation	UNP Q4Q413
AB	19	LEU	ASN	engineered mutation	UNP Q4Q413
AB	22	ILE	GLN	engineered mutation	UNP Q4Q413
AB	23	ILE	VAL	engineered mutation	UNP Q4Q413
AB	26	ILE	ALA	engineered mutation	UNP Q4Q413
AB	30	VAL	ASP	engineered mutation	UNP Q4Q413
AB	87	ALA	LYS	engineered mutation	UNP Q4Q413
AB	88	VAL	GLU	engineered mutation	UNP Q4Q413
AB	114	LEU	-	expression tag	UNP Q4Q413
AB	115	GLU	-	expression tag	UNP Q4Q413
AB	116	HIS	-	expression tag	UNP Q4Q413
AB	117	HIS	-	expression tag	UNP Q4Q413
AB	118	HIS	-	expression tag	UNP Q4Q413
AB	119	HIS	-	expression tag	UNP Q4Q413
AB	120	HIS	-	expression tag	UNP Q4Q413
AB	121	HIS	-	expression tag	UNP Q4Q413
AD	18	LEU	GLU	engineered mutation	UNP Q4Q413
AD	19	LEU	ASN	engineered mutation	UNP Q4Q413
AD	22	ILE	GLN	engineered mutation	UNP Q4Q413
AD	23	ILE	VAL	engineered mutation	UNP Q4Q413
AD	26	ILE	ALA	engineered mutation	UNP Q4Q413
AD	30	VAL	ASP	engineered mutation	UNP Q4Q413
AD	87	ALA	LYS	engineered mutation	UNP Q4Q413
AD	88	VAL	GLU	engineered mutation	UNP Q4Q413
AD	114	LEU	-	expression tag	UNP Q4Q413
AD	115	GLU	-	expression tag	UNP Q4Q413
AD	116	HIS	-	expression tag	UNP Q4Q413
AD	117	HIS	-	expression tag	UNP Q4Q413
AD	118	HIS	-	expression tag	UNP Q4Q413
AD	119	HIS	-	expression tag	UNP Q4Q413
AD	120	HIS	-	expression tag	UNP Q4Q413

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Chain	Residue	Modelled	Actual	Comment	Reference
AD	121	HIS	-	expression tag	UNP Q4Q413
AF	18	LEU	GLU	engineered mutation	UNP Q4Q413
AF	19	LEU	ASN	engineered mutation	UNP Q4Q413
AF	22	ILE	GLN	engineered mutation	UNP Q4Q413
AF	23	ILE	VAL	engineered mutation	UNP Q4Q413
AF	26	ILE	ALA	engineered mutation	UNP Q4Q413
AF	30	VAL	ASP	engineered mutation	UNP Q4Q413
AF	87	ALA	LYS	engineered mutation	UNP Q4Q413
AF	88	VAL	GLU	engineered mutation	UNP Q4Q413
AF	114	LEU	-	expression tag	UNP Q4Q413
AF	115	GLU	-	expression tag	UNP Q4Q413
AF	116	HIS	-	expression tag	UNP Q4Q413
AF	117	HIS	-	expression tag	UNP Q4Q413
AF	118	HIS	-	expression tag	UNP Q4Q413
AF	119	HIS	-	expression tag	UNP Q4Q413
AF	120	HIS	-	expression tag	UNP Q4Q413
AF	121	HIS	-	expression tag	UNP Q4Q413
AH	18	LEU	GLU	engineered mutation	UNP Q4Q413
AH	19	LEU	ASN	engineered mutation	UNP Q4Q413
AH	22	ILE	GLN	engineered mutation	UNP Q4Q413
AH	23	ILE	VAL	engineered mutation	UNP Q4Q413
AH	26	ILE	ALA	engineered mutation	UNP Q4Q413
AH	30	VAL	ASP	engineered mutation	UNP Q4Q413
AH	87	ALA	LYS	engineered mutation	UNP Q4Q413
AH	88	VAL	GLU	engineered mutation	UNP Q4Q413
AH	114	LEU	-	expression tag	UNP Q4Q413
AH	115	GLU	-	expression tag	UNP Q4Q413
AH	116	HIS	-	expression tag	UNP Q4Q413
AH	117	HIS	-	expression tag	UNP Q4Q413
AH	118	HIS	-	expression tag	UNP Q4Q413
AH	119	HIS	-	expression tag	UNP Q4Q413
AH	120	HIS	-	expression tag	UNP Q4Q413
AH	121	HIS	-	expression tag	UNP Q4Q413
AJ	18	LEU	GLU	engineered mutation	UNP Q4Q413
AJ	19	LEU	ASN	engineered mutation	UNP Q4Q413
AJ	22	ILE	GLN	engineered mutation	UNP Q4Q413
AJ	23	ILE	VAL	engineered mutation	UNP Q4Q413
AJ	26	ILE	ALA	engineered mutation	UNP Q4Q413
AJ	30	VAL	ASP	engineered mutation	UNP Q4Q413
AJ	87	ALA	LYS	engineered mutation	UNP Q4Q413
AJ	88	VAL	GLU	engineered mutation	UNP Q4Q413
AJ	114	LEU	-	expression tag	UNP Q4Q413

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Chain	Residue	Modelled	Actual	Comment	Reference
AJ	115	GLU	-	expression tag	UNP Q4Q413
AJ	116	HIS	-	expression tag	UNP Q4Q413
AJ	117	HIS	-	expression tag	UNP Q4Q413
AJ	118	HIS	-	expression tag	UNP Q4Q413
AJ	119	HIS	-	expression tag	UNP Q4Q413
AJ	120	HIS	-	expression tag	UNP Q4Q413
AJ	121	HIS	-	expression tag	UNP Q4Q413
AL	18	LEU	GLU	engineered mutation	UNP Q4Q413
AL	19	LEU	ASN	engineered mutation	UNP Q4Q413
AL	22	ILE	GLN	engineered mutation	UNP Q4Q413
AL	23	ILE	VAL	engineered mutation	UNP Q4Q413
AL	26	ILE	ALA	engineered mutation	UNP Q4Q413
AL	30	VAL	ASP	engineered mutation	UNP Q4Q413
AL	87	ALA	LYS	engineered mutation	UNP Q4Q413
AL	88	VAL	GLU	engineered mutation	UNP Q4Q413
AL	114	LEU	-	expression tag	UNP Q4Q413
AL	115	GLU	-	expression tag	UNP Q4Q413
AL	116	HIS	-	expression tag	UNP Q4Q413
AL	117	HIS	-	expression tag	UNP Q4Q413
AL	118	HIS	-	expression tag	UNP Q4Q413
AL	119	HIS	-	expression tag	UNP Q4Q413
AL	120	HIS	-	expression tag	UNP Q4Q413
AL	121	HIS	-	expression tag	UNP Q4Q413
AN	18	LEU	GLU	engineered mutation	UNP Q4Q413
AN	19	LEU	ASN	engineered mutation	UNP Q4Q413
AN	22	ILE	GLN	engineered mutation	UNP Q4Q413
AN	23	ILE	VAL	engineered mutation	UNP Q4Q413
AN	26	ILE	ALA	engineered mutation	UNP Q4Q413
AN	30	VAL	ASP	engineered mutation	UNP Q4Q413
AN	87	ALA	LYS	engineered mutation	UNP Q4Q413
AN	88	VAL	GLU	engineered mutation	UNP Q4Q413
AN	114	LEU	-	expression tag	UNP Q4Q413
AN	115	GLU	-	expression tag	UNP Q4Q413
AN	116	HIS	-	expression tag	UNP Q4Q413
AN	117	HIS	-	expression tag	UNP Q4Q413
AN	118	HIS	-	expression tag	UNP Q4Q413
AN	119	HIS	-	expression tag	UNP Q4Q413
AN	120	HIS	-	expression tag	UNP Q4Q413
AN	121	HIS	-	expression tag	UNP Q4Q413
AP	18	LEU	GLU	engineered mutation	UNP Q4Q413
AP	19	LEU	ASN	engineered mutation	UNP Q4Q413
AP	22	ILE	GLN	engineered mutation	UNP Q4Q413

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Chain	Residue	Modelled	Actual	Comment	Reference
AP	23	ILE	VAL	engineered mutation	UNP Q4Q413
AP	26	ILE	ALA	engineered mutation	UNP Q4Q413
AP	30	VAL	ASP	engineered mutation	UNP Q4Q413
AP	87	ALA	LYS	engineered mutation	UNP Q4Q413
AP	88	VAL	GLU	engineered mutation	UNP Q4Q413
AP	114	LEU	-	expression tag	UNP Q4Q413
AP	115	GLU	-	expression tag	UNP Q4Q413
AP	116	HIS	-	expression tag	UNP Q4Q413
AP	117	HIS	-	expression tag	UNP Q4Q413
AP	118	HIS	-	expression tag	UNP Q4Q413
AP	119	HIS	-	expression tag	UNP Q4Q413
AP	120	HIS	-	expression tag	UNP Q4Q413
AP	121	HIS	-	expression tag	UNP Q4Q413
AR	18	LEU	GLU	engineered mutation	UNP Q4Q413
AR	19	LEU	ASN	engineered mutation	UNP Q4Q413
AR	22	ILE	GLN	engineered mutation	UNP Q4Q413
AR	23	ILE	VAL	engineered mutation	UNP Q4Q413
AR	26	ILE	ALA	engineered mutation	UNP Q4Q413
AR	30	VAL	ASP	engineered mutation	UNP Q4Q413
AR	87	ALA	LYS	engineered mutation	UNP Q4Q413
AR	88	VAL	GLU	engineered mutation	UNP Q4Q413
AR	114	LEU	-	expression tag	UNP Q4Q413
AR	115	GLU	-	expression tag	UNP Q4Q413
AR	116	HIS	-	expression tag	UNP Q4Q413
AR	117	HIS	-	expression tag	UNP Q4Q413
AR	118	HIS	-	expression tag	UNP Q4Q413
AR	119	HIS	-	expression tag	UNP Q4Q413
AR	120	HIS	-	expression tag	UNP Q4Q413
AR	121	HIS	-	expression tag	UNP Q4Q413
AT	18	LEU	GLU	engineered mutation	UNP Q4Q413
AT	19	LEU	ASN	engineered mutation	UNP Q4Q413
AT	22	ILE	GLN	engineered mutation	UNP Q4Q413
AT	23	ILE	VAL	engineered mutation	UNP Q4Q413
AT	26	ILE	ALA	engineered mutation	UNP Q4Q413
AT	30	VAL	ASP	engineered mutation	UNP Q4Q413
AT	87	ALA	LYS	engineered mutation	UNP Q4Q413
AT	88	VAL	GLU	engineered mutation	UNP Q4Q413
AT	114	LEU	-	expression tag	UNP Q4Q413
AT	115	GLU	-	expression tag	UNP Q4Q413
AT	116	HIS	-	expression tag	UNP Q4Q413
AT	117	HIS	-	expression tag	UNP Q4Q413
AT	118	HIS	-	expression tag	UNP Q4Q413

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Chain	Residue	Modelled	Actual	Comment	Reference
AT	119	HIS	-	expression tag	UNP Q4Q413
AT	120	HIS	-	expression tag	UNP Q4Q413
AT	121	HIS	-	expression tag	UNP Q4Q413
AV	18	LEU	GLU	engineered mutation	UNP Q4Q413
AV	19	LEU	ASN	engineered mutation	UNP Q4Q413
AV	22	ILE	GLN	engineered mutation	UNP Q4Q413
AV	23	ILE	VAL	engineered mutation	UNP Q4Q413
AV	26	ILE	ALA	engineered mutation	UNP Q4Q413
AV	30	VAL	ASP	engineered mutation	UNP Q4Q413
AV	87	ALA	LYS	engineered mutation	UNP Q4Q413
AV	88	VAL	GLU	engineered mutation	UNP Q4Q413
AV	114	LEU	-	expression tag	UNP Q4Q413
AV	115	GLU	-	expression tag	UNP Q4Q413
AV	116	HIS	-	expression tag	UNP Q4Q413
AV	117	HIS	-	expression tag	UNP Q4Q413
AV	118	HIS	-	expression tag	UNP Q4Q413
AV	119	HIS	-	expression tag	UNP Q4Q413
AV	120	HIS	-	expression tag	UNP Q4Q413
AV	121	HIS	-	expression tag	UNP Q4Q413
AX	18	LEU	GLU	engineered mutation	UNP Q4Q413
AX	19	LEU	ASN	engineered mutation	UNP Q4Q413
AX	22	ILE	GLN	engineered mutation	UNP Q4Q413
AX	23	ILE	VAL	engineered mutation	UNP Q4Q413
AX	26	ILE	ALA	engineered mutation	UNP Q4Q413
AX	30	VAL	ASP	engineered mutation	UNP Q4Q413
AX	87	ALA	LYS	engineered mutation	UNP Q4Q413
AX	88	VAL	GLU	engineered mutation	UNP Q4Q413
AX	114	LEU	-	expression tag	UNP Q4Q413
AX	115	GLU	-	expression tag	UNP Q4Q413
AX	116	HIS	-	expression tag	UNP Q4Q413
AX	117	HIS	-	expression tag	UNP Q4Q413
AX	118	HIS	-	expression tag	UNP Q4Q413
AX	119	HIS	-	expression tag	UNP Q4Q413
AX	120	HIS	-	expression tag	UNP Q4Q413
AX	121	HIS	-	expression tag	UNP Q4Q413
AZ	18	LEU	GLU	engineered mutation	UNP Q4Q413
AZ	19	LEU	ASN	engineered mutation	UNP Q4Q413
AZ	22	ILE	GLN	engineered mutation	UNP Q4Q413
AZ	23	ILE	VAL	engineered mutation	UNP Q4Q413
AZ	26	ILE	ALA	engineered mutation	UNP Q4Q413
AZ	30	VAL	ASP	engineered mutation	UNP Q4Q413
AZ	87	ALA	LYS	engineered mutation	UNP Q4Q413

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Chain	Residue	Modelled	Actual	Comment	Reference
AZ	88	VAL	GLU	engineered mutation	UNP Q4Q413
AZ	114	LEU	-	expression tag	UNP Q4Q413
AZ	115	GLU	-	expression tag	UNP Q4Q413
AZ	116	HIS	-	expression tag	UNP Q4Q413
AZ	117	HIS	-	expression tag	UNP Q4Q413
AZ	118	HIS	-	expression tag	UNP Q4Q413
AZ	119	HIS	-	expression tag	UNP Q4Q413
AZ	120	HIS	-	expression tag	UNP Q4Q413
AZ	121	HIS	-	expression tag	UNP Q4Q413
BB	18	LEU	GLU	engineered mutation	UNP Q4Q413
BB	19	LEU	ASN	engineered mutation	UNP Q4Q413
BB	22	ILE	GLN	engineered mutation	UNP Q4Q413
BB	23	ILE	VAL	engineered mutation	UNP Q4Q413
BB	26	ILE	ALA	engineered mutation	UNP Q4Q413
BB	30	VAL	ASP	engineered mutation	UNP Q4Q413
BB	87	ALA	LYS	engineered mutation	UNP Q4Q413
BB	88	VAL	GLU	engineered mutation	UNP Q4Q413
BB	114	LEU	-	expression tag	UNP Q4Q413
BB	115	GLU	-	expression tag	UNP Q4Q413
BB	116	HIS	-	expression tag	UNP Q4Q413
BB	117	HIS	-	expression tag	UNP Q4Q413
BB	118	HIS	-	expression tag	UNP Q4Q413
BB	119	HIS	-	expression tag	UNP Q4Q413
BB	120	HIS	-	expression tag	UNP Q4Q413
BB	121	HIS	-	expression tag	UNP Q4Q413
BD	18	LEU	GLU	engineered mutation	UNP Q4Q413
BD	19	LEU	ASN	engineered mutation	UNP Q4Q413
BD	22	ILE	GLN	engineered mutation	UNP Q4Q413
BD	23	ILE	VAL	engineered mutation	UNP Q4Q413
BD	26	ILE	ALA	engineered mutation	UNP Q4Q413
BD	30	VAL	ASP	engineered mutation	UNP Q4Q413
BD	87	ALA	LYS	engineered mutation	UNP Q4Q413
BD	88	VAL	GLU	engineered mutation	UNP Q4Q413
BD	114	LEU	-	expression tag	UNP Q4Q413
BD	115	GLU	-	expression tag	UNP Q4Q413
BD	116	HIS	-	expression tag	UNP Q4Q413
BD	117	HIS	-	expression tag	UNP Q4Q413
BD	118	HIS	-	expression tag	UNP Q4Q413
BD	119	HIS	-	expression tag	UNP Q4Q413
BD	120	HIS	-	expression tag	UNP Q4Q413
BD	121	HIS	-	expression tag	UNP Q4Q413
BF	18	LEU	GLU	engineered mutation	UNP Q4Q413

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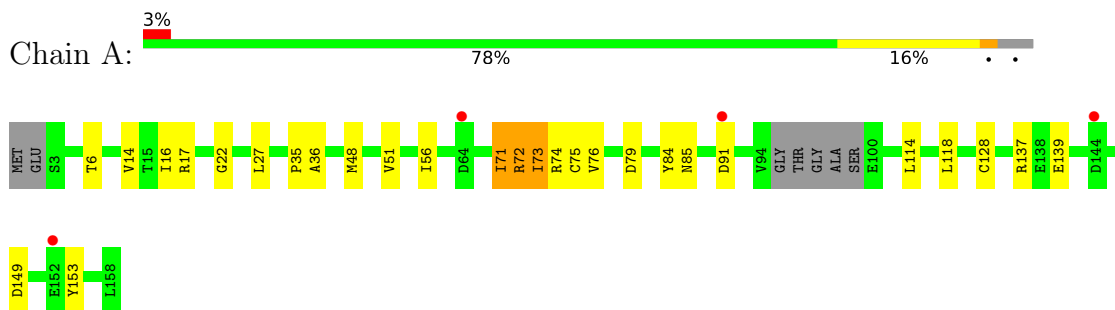
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Chain	Residue	Modelled	Actual	Comment	Reference
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BF	22	ILE	GLN	engineered mutation	UNP Q4Q413
BF	23	ILE	VAL	engineered mutation	UNP Q4Q413
BF	26	ILE	ALA	engineered mutation	UNP Q4Q413
BF	30	VAL	ASP	engineered mutation	UNP Q4Q413
BF	87	ALA	LYS	engineered mutation	UNP Q4Q413
BF	88	VAL	GLU	engineered mutation	UNP Q4Q413
BF	114	LEU	-	expression tag	UNP Q4Q413
BF	115	GLU	-	expression tag	UNP Q4Q413
BF	116	HIS	-	expression tag	UNP Q4Q413
BF	117	HIS	-	expression tag	UNP Q4Q413
BF	118	HIS	-	expression tag	UNP Q4Q413
BF	119	HIS	-	expression tag	UNP Q4Q413
BF	120	HIS	-	expression tag	UNP Q4Q413
BF	121	HIS	-	expression tag	UNP Q4Q413
BH	18	LEU	GLU	engineered mutation	UNP Q4Q413
BH	19	LEU	ASN	engineered mutation	UNP Q4Q413
BH	22	ILE	GLN	engineered mutation	UNP Q4Q413
BH	23	ILE	VAL	engineered mutation	UNP Q4Q413
BH	26	ILE	ALA	engineered mutation	UNP Q4Q413
BH	30	VAL	ASP	engineered mutation	UNP Q4Q413
BH	87	ALA	LYS	engineered mutation	UNP Q4Q413
BH	88	VAL	GLU	engineered mutation	UNP Q4Q413
BH	114	LEU	-	expression tag	UNP Q4Q413
BH	115	GLU	-	expression tag	UNP Q4Q413
BH	116	HIS	-	expression tag	UNP Q4Q413
BH	117	HIS	-	expression tag	UNP Q4Q413
BH	118	HIS	-	expression tag	UNP Q4Q413
BH	119	HIS	-	expression tag	UNP Q4Q413
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BH	121	HIS	-	expression tag	UNP Q4Q413

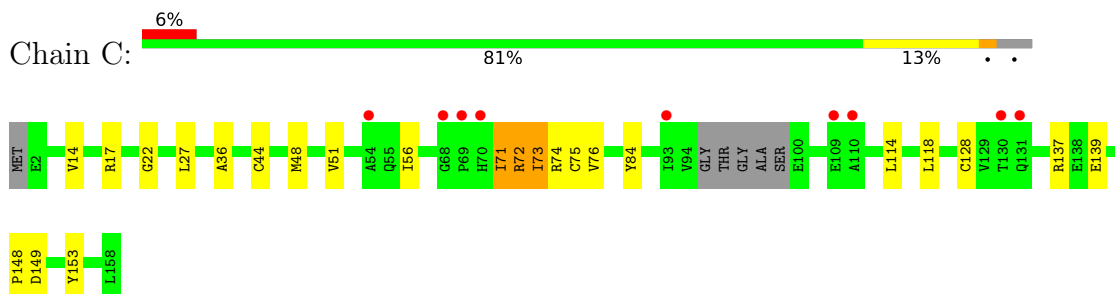
3 Residue-property plots [i](#)

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.

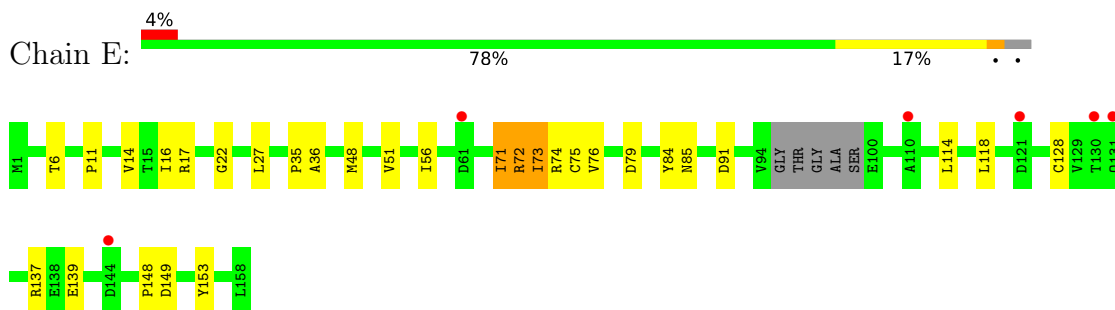
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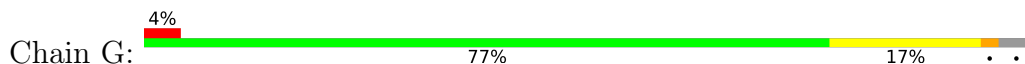
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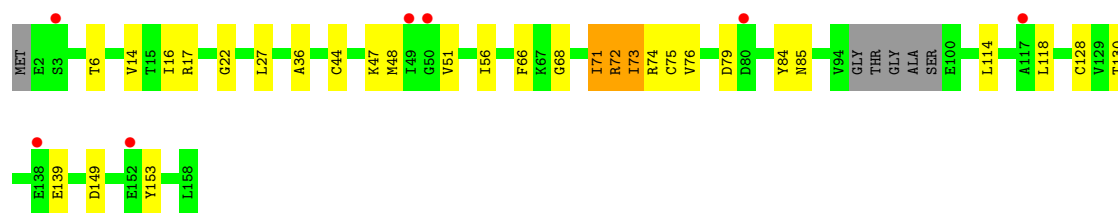


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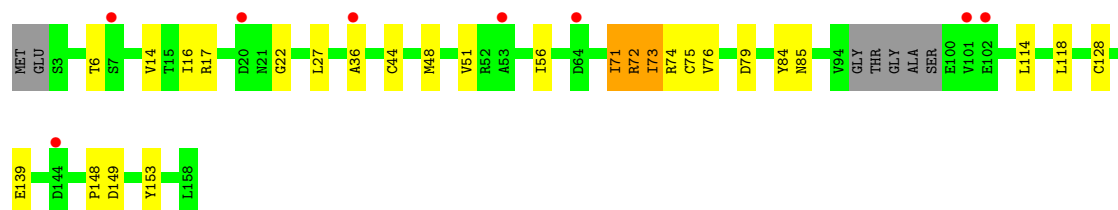
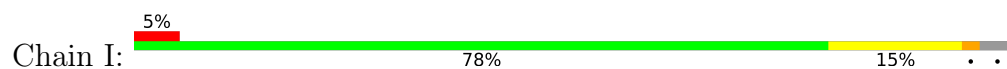


- Molecule 1: integron gene cassette protein

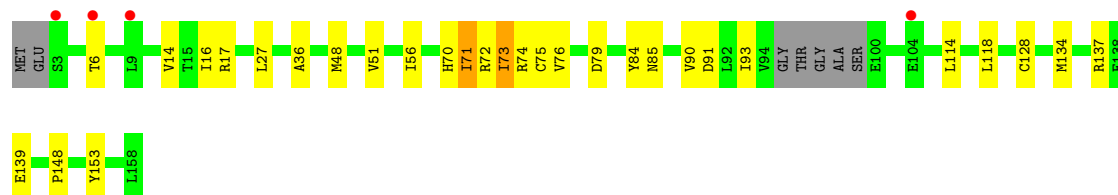
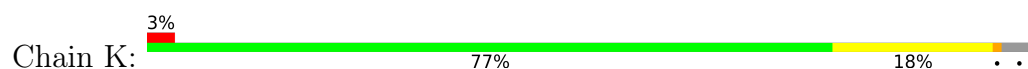




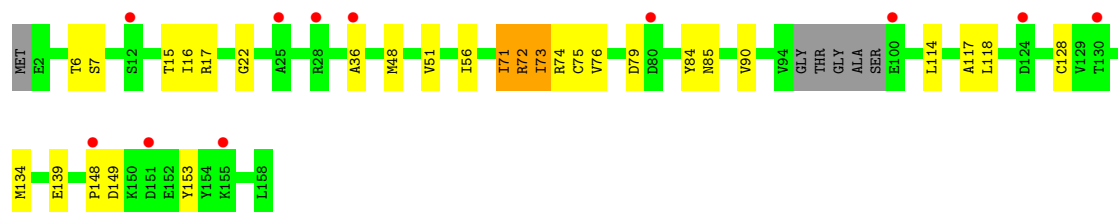
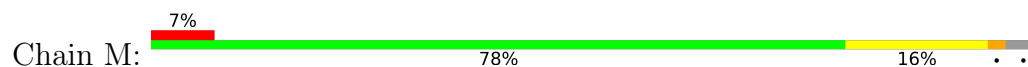
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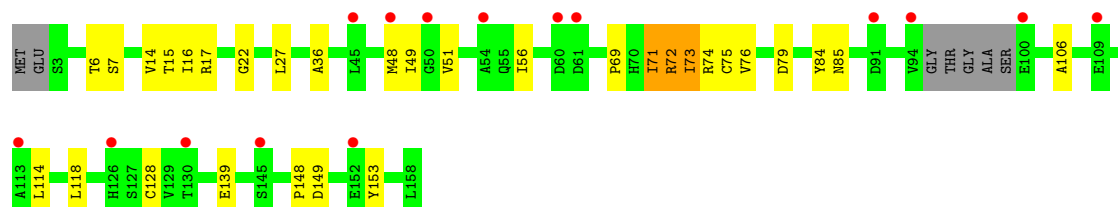
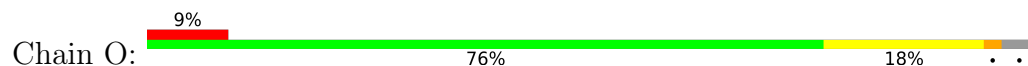
- Molecule 1: integron gene cassette protein



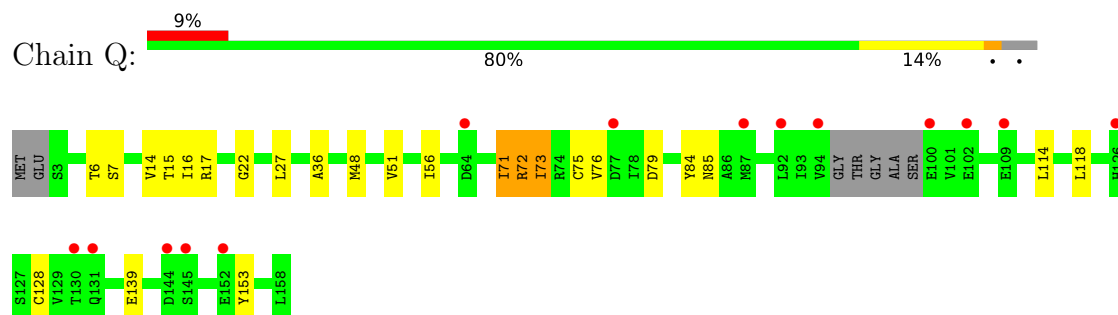
- Molecule 1: integron gene cassette protein



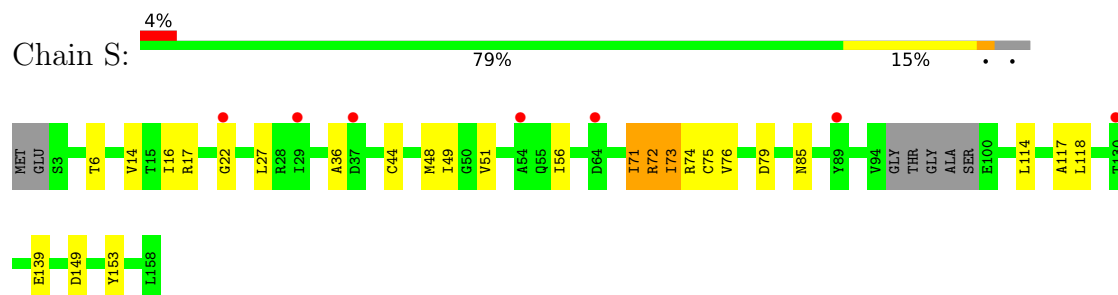
- Molecule 1: integron gene cassette protein



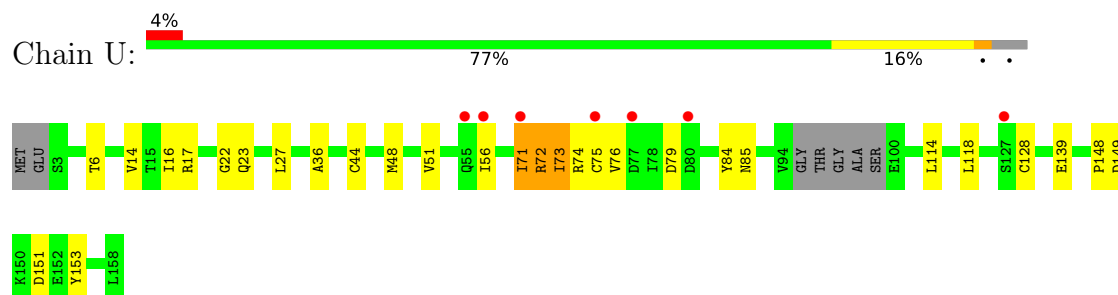
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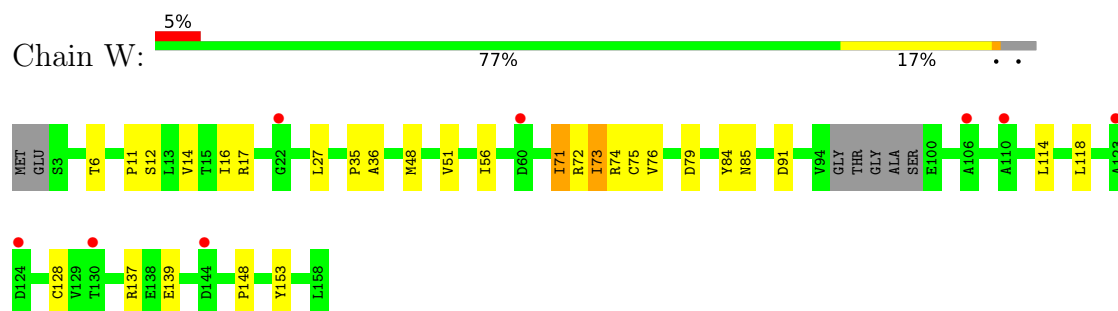
- Molecule 1: integron gene cassette protein



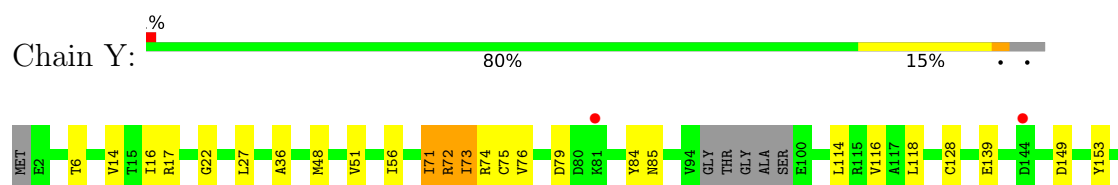
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- Molecule 1: integron gene cassette protein



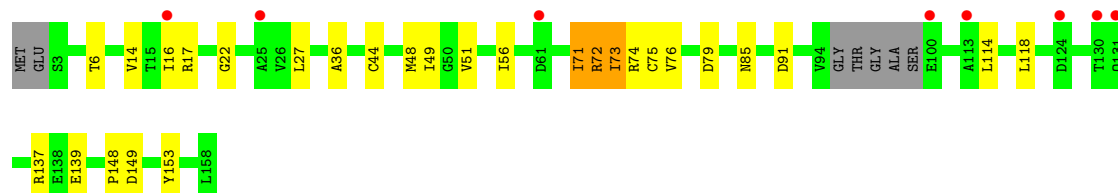
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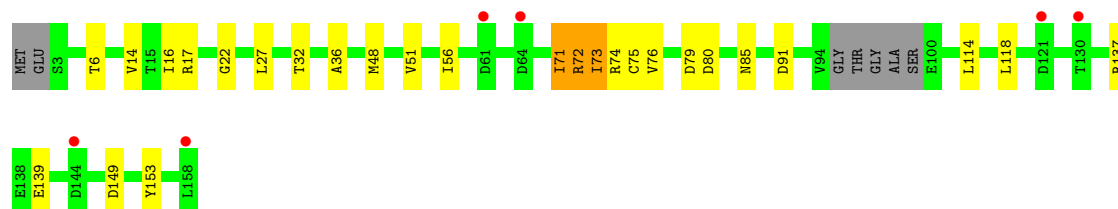
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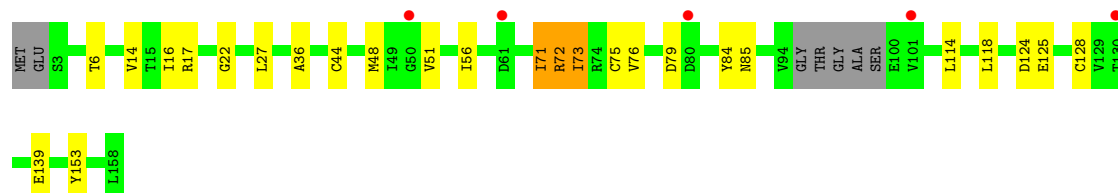
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Chain c: 



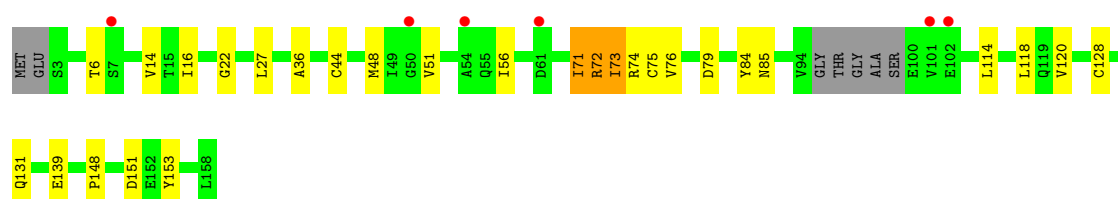
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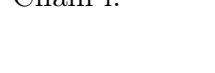
- Molecule 1: integron gene cassette protein

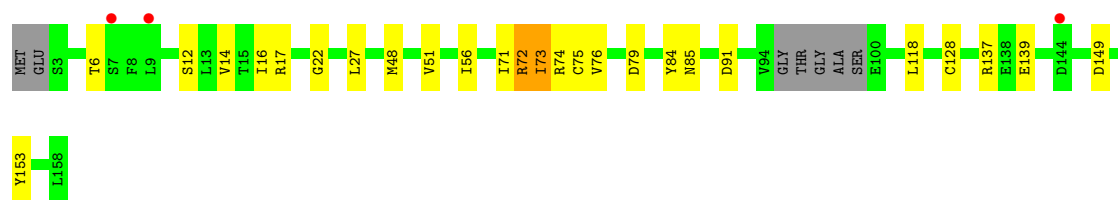
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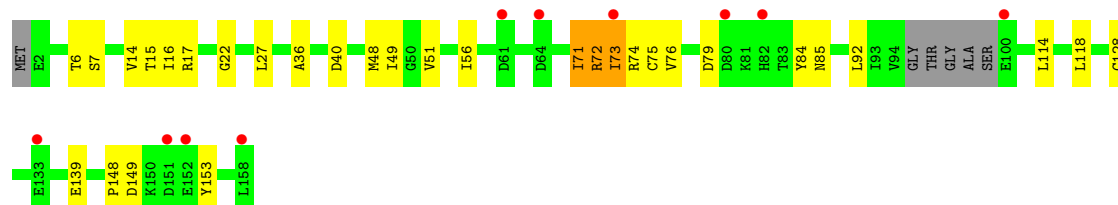
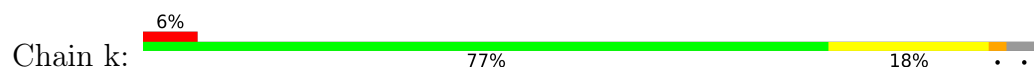
- Molecule 1: integron gene cassette protein

Chain i: 

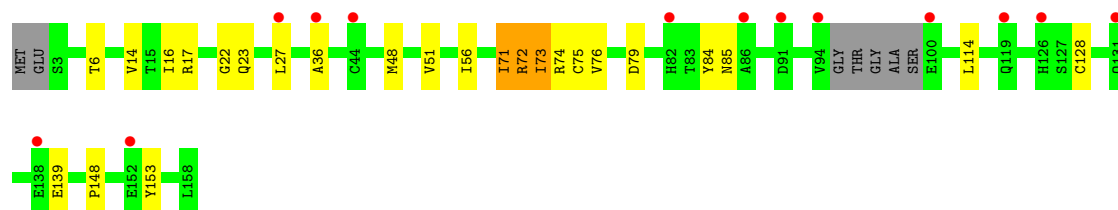
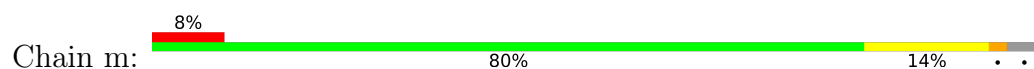




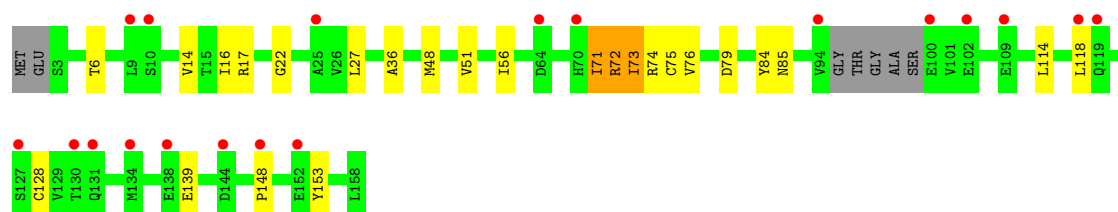
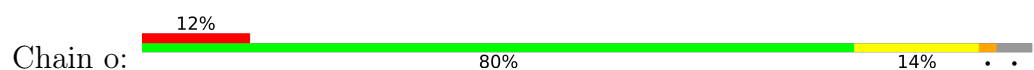
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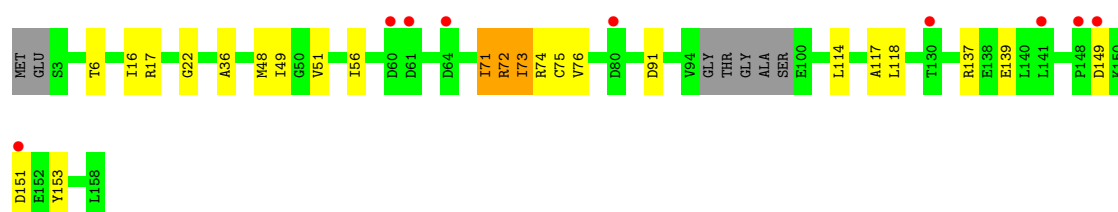
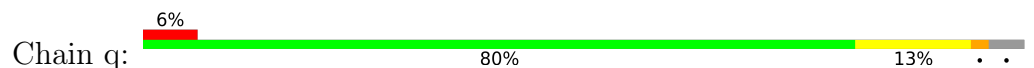
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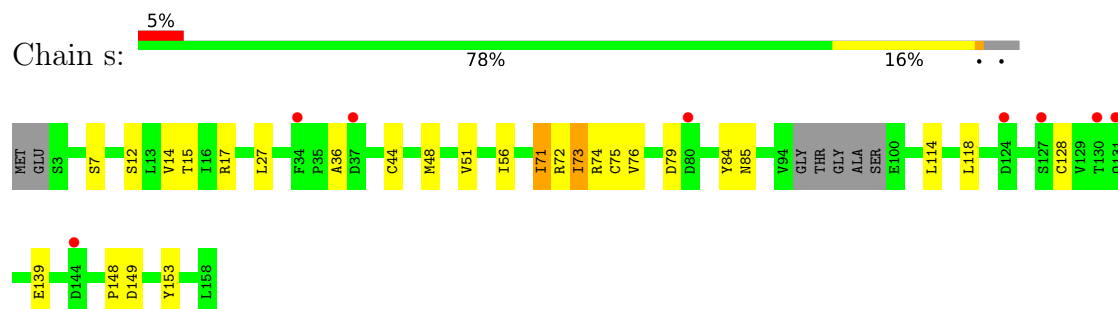
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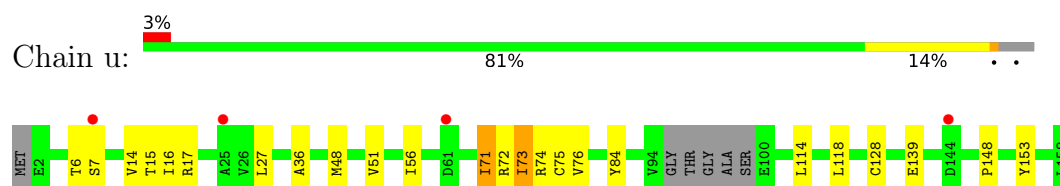
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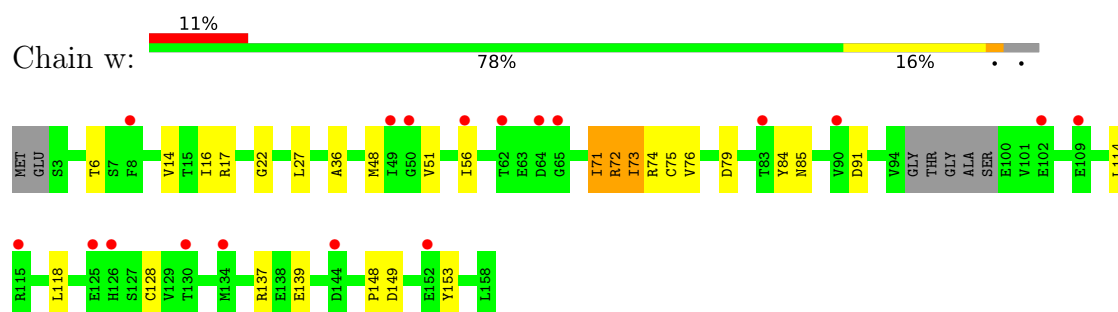
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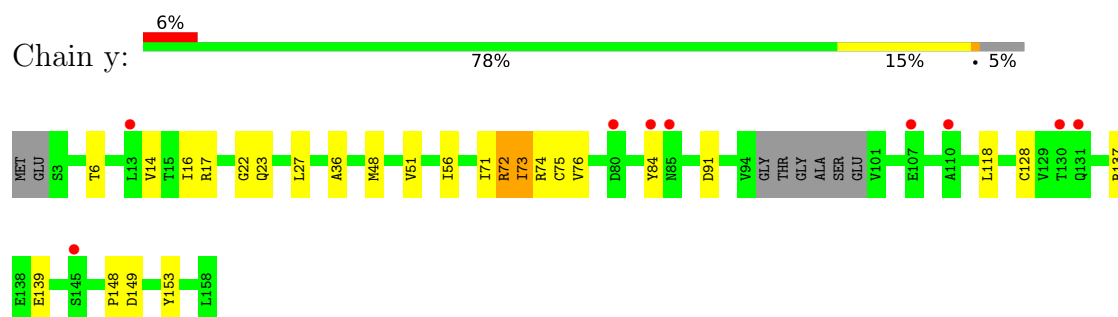
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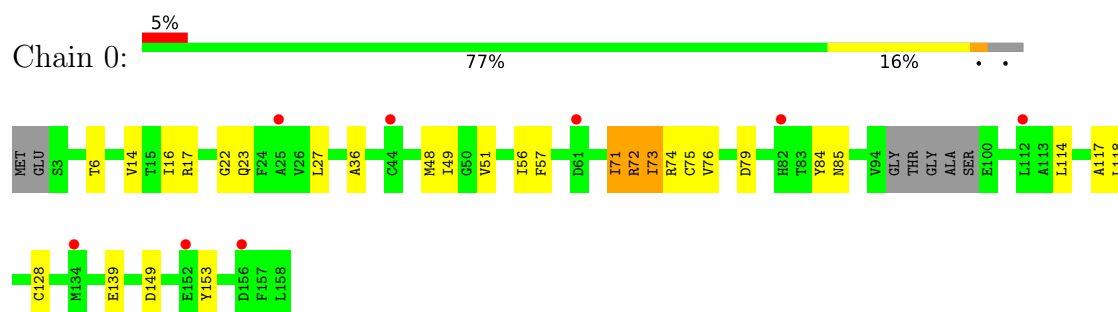
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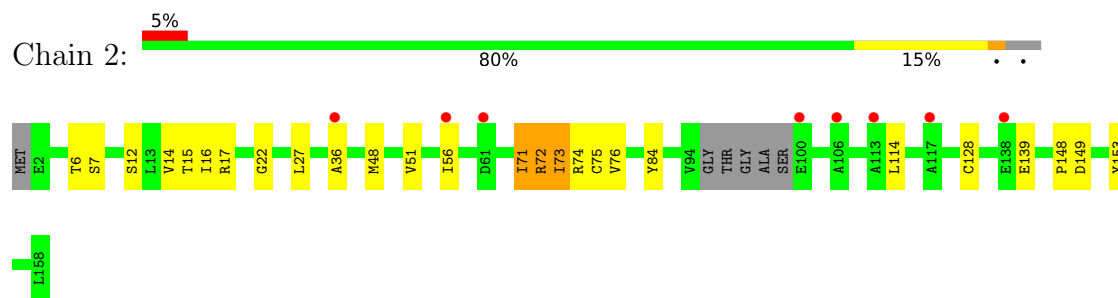
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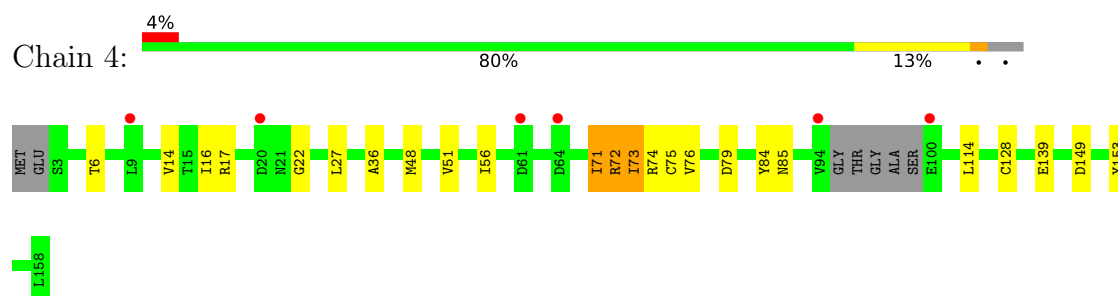
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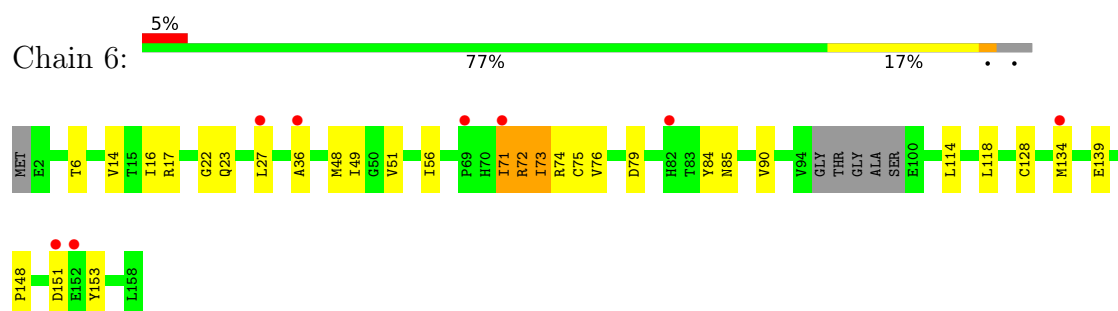
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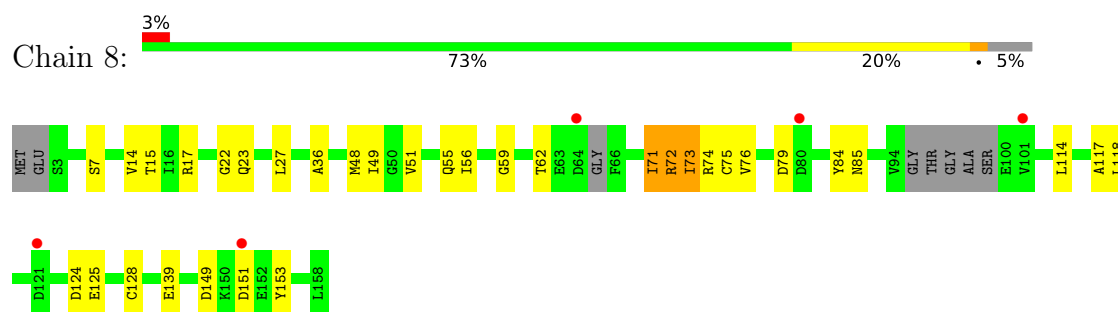
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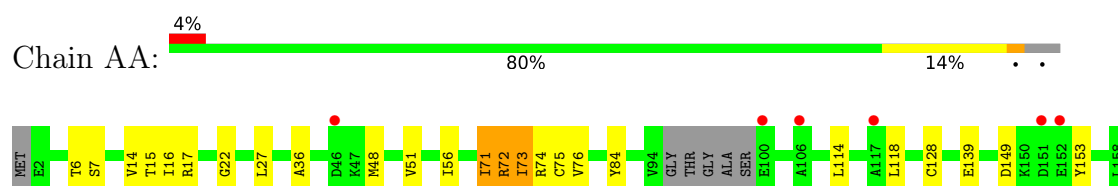
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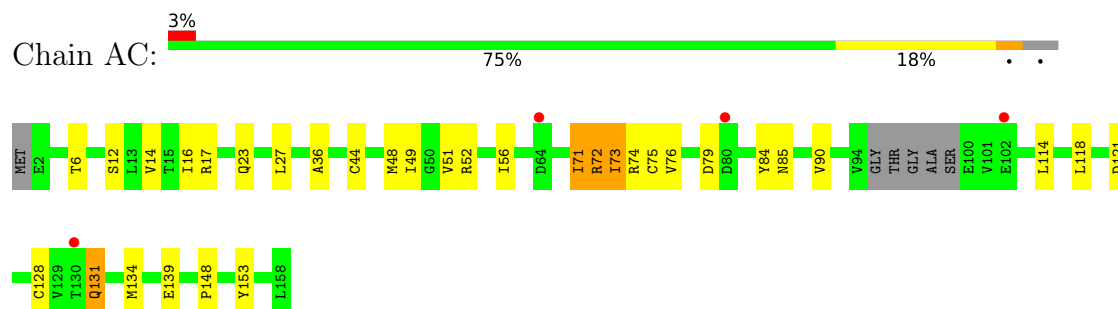
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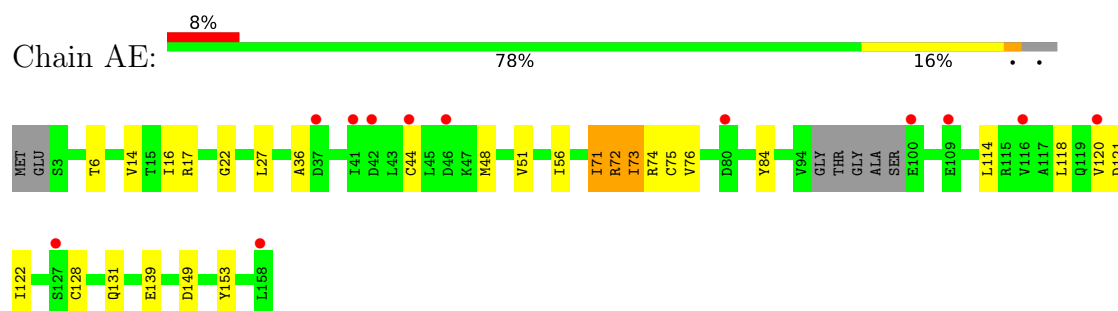
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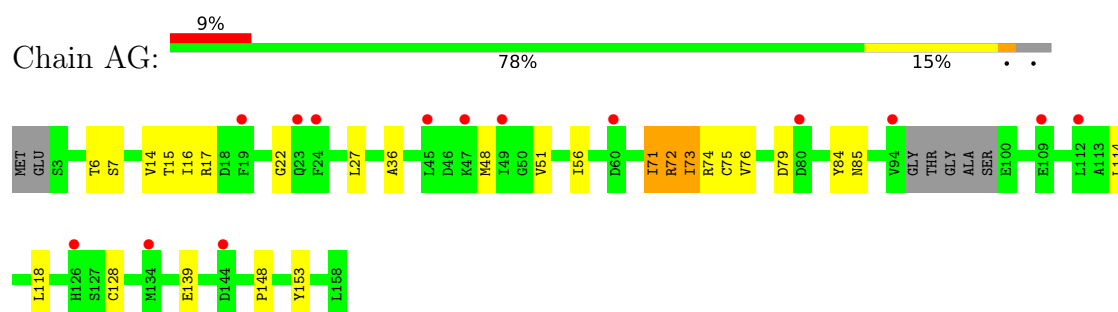
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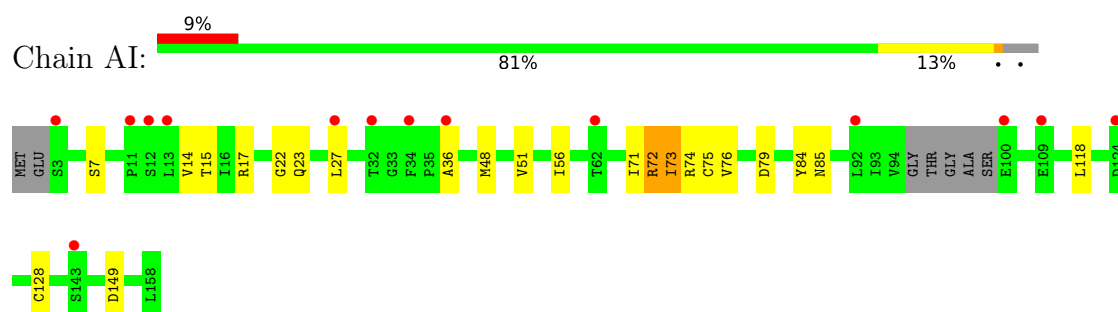
- Molecule 1: integron gene cassette protein



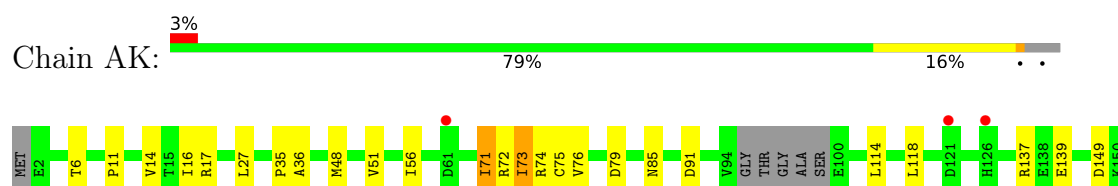
- Molecule 1: integron gene cassette protein

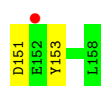


- Molecule 1: integron gene cassette protein

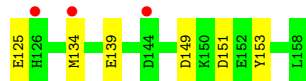
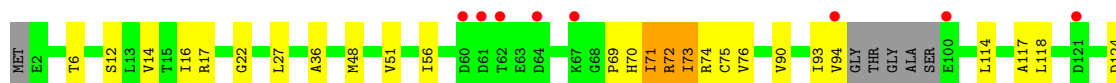
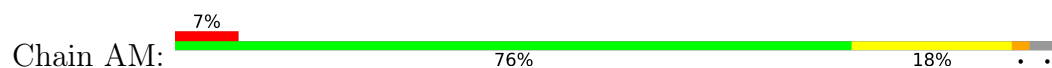


- Molecule 1: integron gene cassette protein

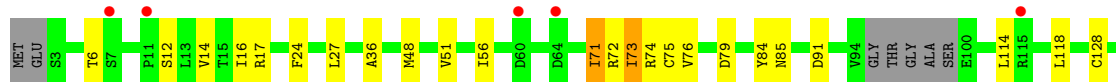
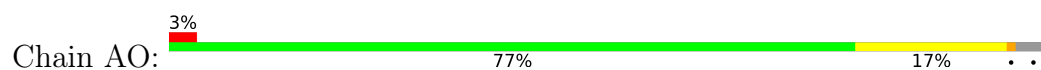




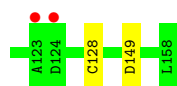
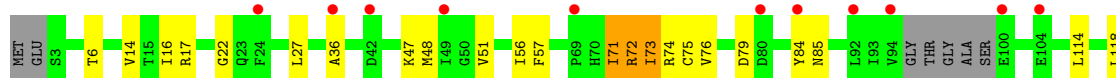
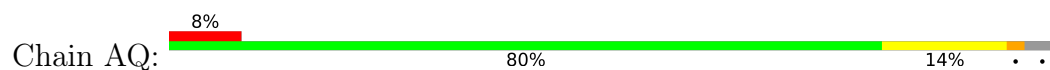
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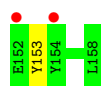
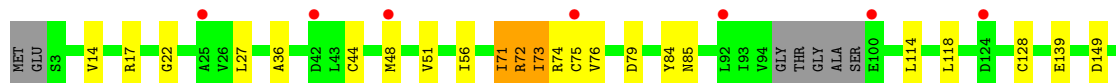
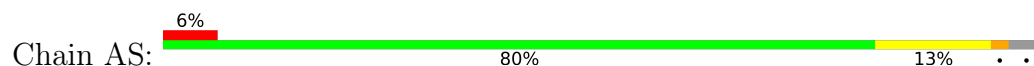
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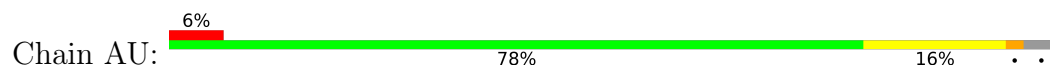
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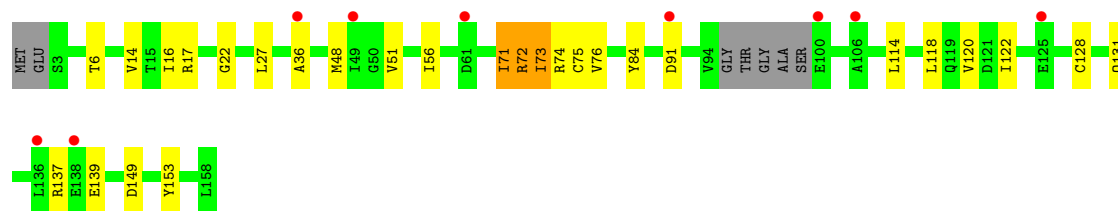


- Molecule 1: integron gene cassette protein

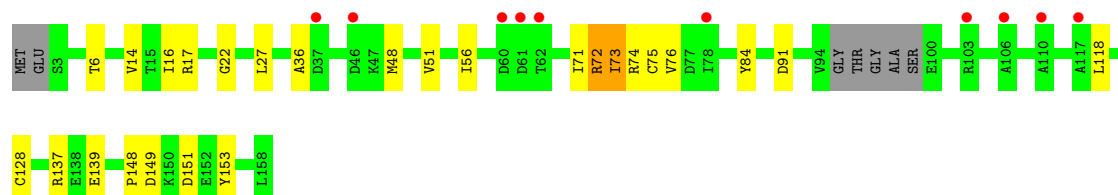
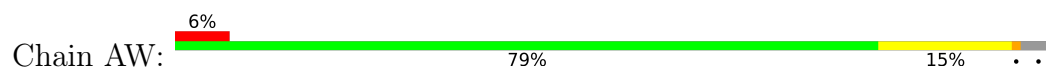


- Molecule 1: integron gene cassette protein

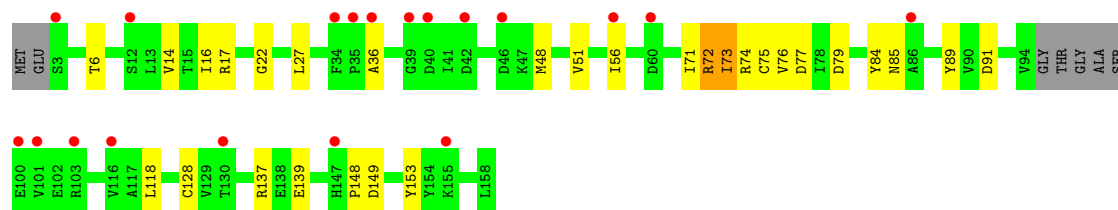
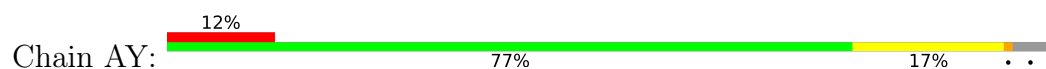




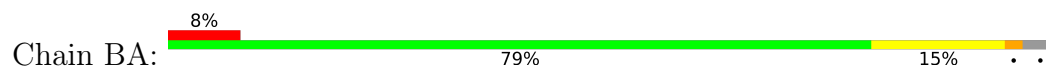
• Molecule 1: integron gene cassette protein



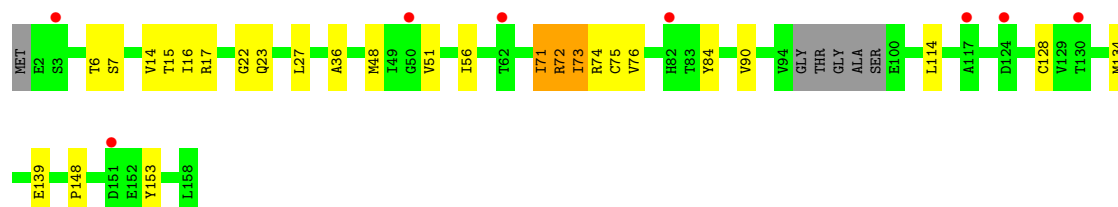
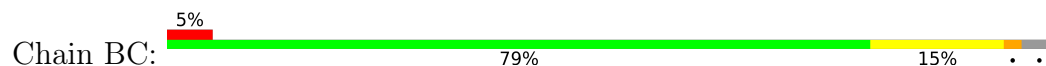
• Molecule 1: integron gene cassette protein



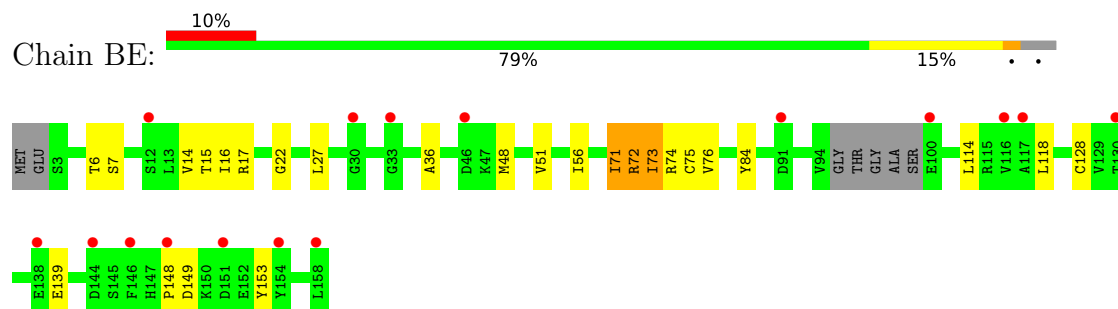
• Molecule 1: integron gene cassette protein



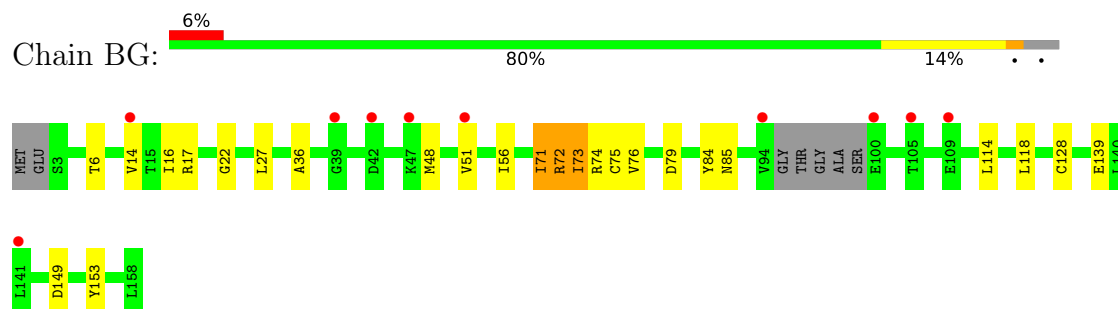
• Molecule 1: integron gene cassette protein



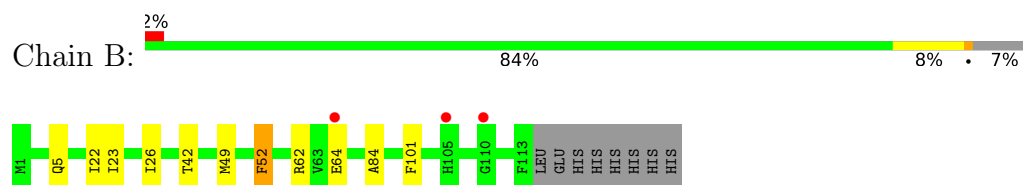
- Molecule 1: integron gene cassette protein



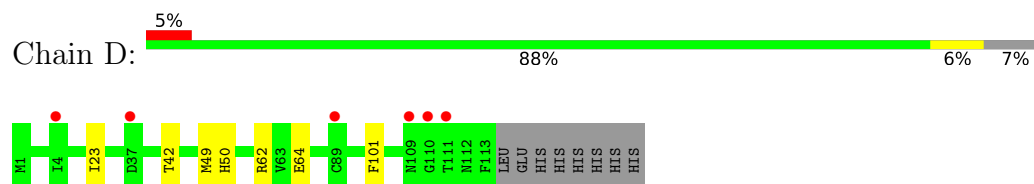
- Molecule 1: integron gene cassette protein



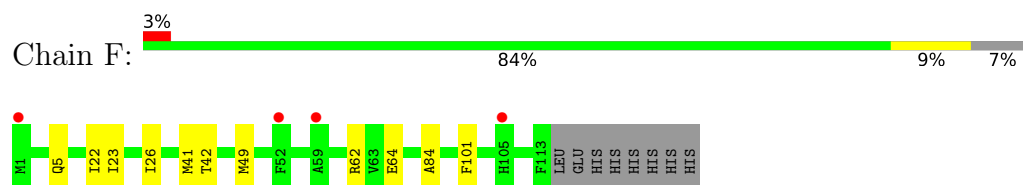
- Molecule 2: Macrophage migration inhibitory factor-like protein



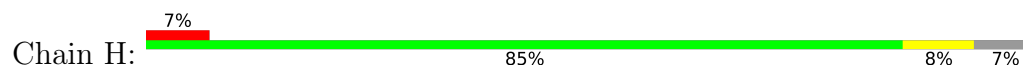
- Molecule 2: Macrophage migration inhibitory factor-like protein

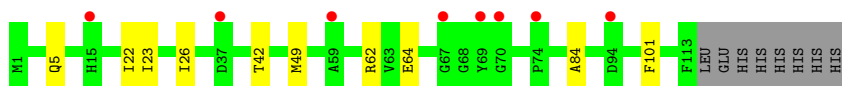


- Molecule 2: Macrophage migration inhibitory factor-like protein

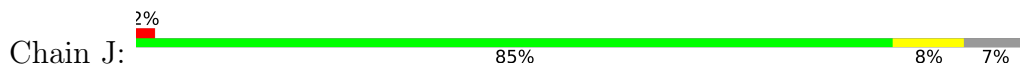


- Molecule 2: Macrophage migration inhibitory factor-like protein

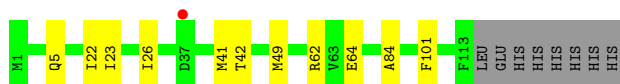
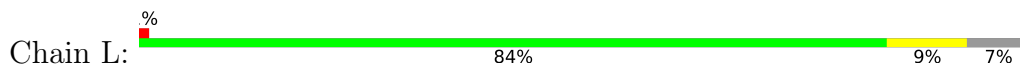




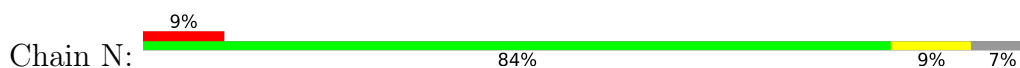
- Molecule 2: Macrophage migration inhibitory factor-like protein



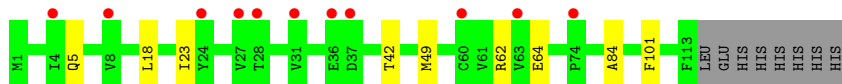
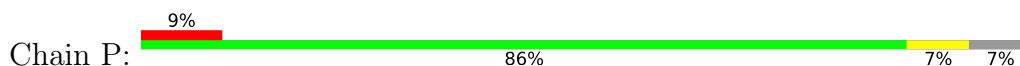
- Molecule 2: Macrophage migration inhibitory factor-like protein



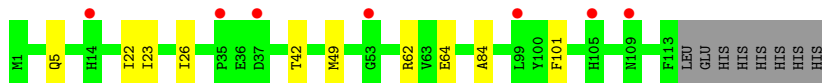
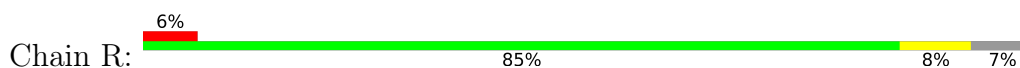
- Molecule 2: Macrophage migration inhibitory factor-like protein



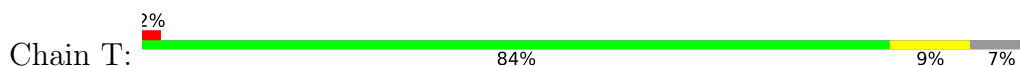
- Molecule 2: Macrophage migration inhibitory factor-like protein



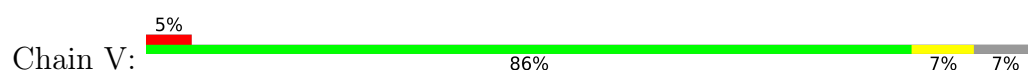
- Molecule 2: Macrophage migration inhibitory factor-like protein



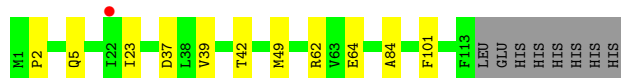
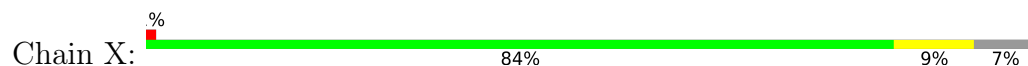
- Molecule 2: Macrophage migration inhibitory factor-like protein



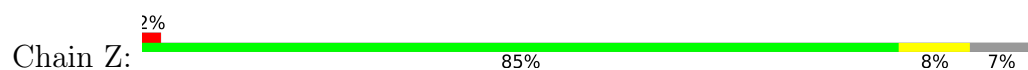
- Molecule 2: Macrophage migration inhibitory factor-like protein



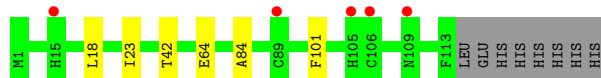
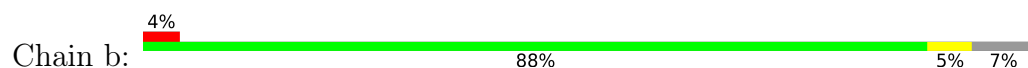
- Molecule 2: Macrophage migration inhibitory factor-like protein



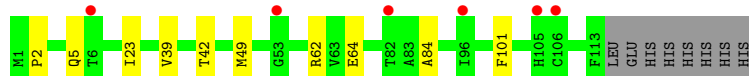
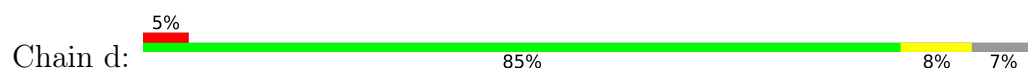
- Molecule 2: Macrophage migration inhibitory factor-like protein



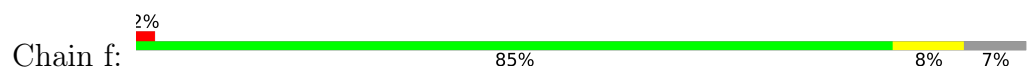
- Molecule 2: Macrophage migration inhibitory factor-like protein



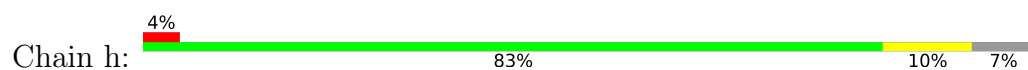
- Molecule 2: Macrophage migration inhibitory factor-like protein



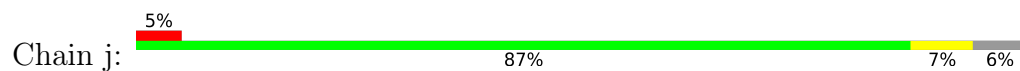
- Molecule 2: Macrophage migration inhibitory factor-like protein



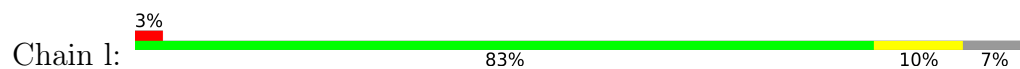
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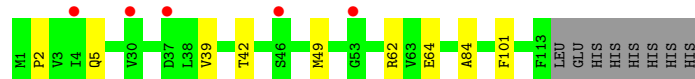
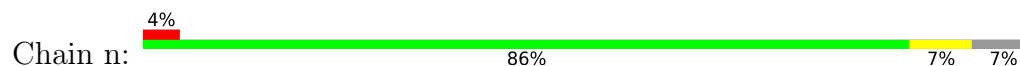
- Molecule 2: Macrophage migration inhibitory factor-like protein



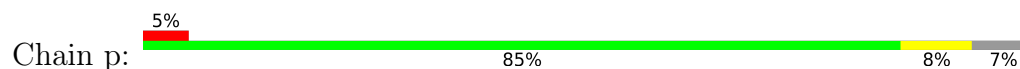
- Molecule 2: Macrophage migration inhibitory factor-like protein



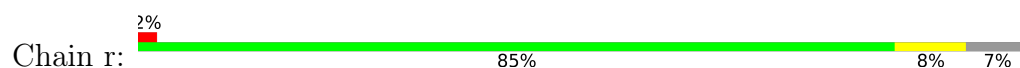
- Molecule 2: Macrophage migration inhibitory factor-like protein



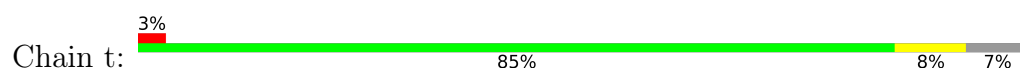
- Molecule 2: Macrophage migration inhibitory factor-like protein



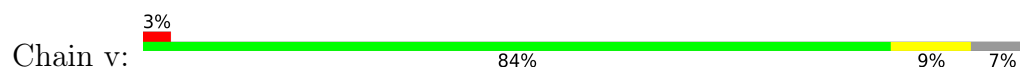
- Molecule 2: Macrophage migration inhibitory factor-like protein



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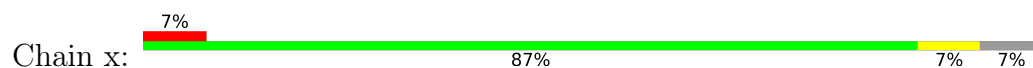


- Molecule 2: Macrophage migration inhibitory factor-like protein

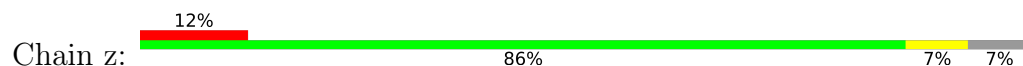




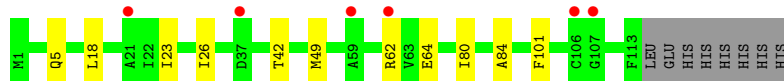
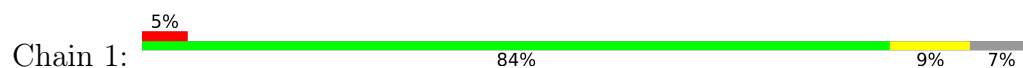
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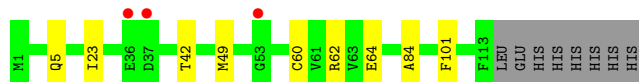
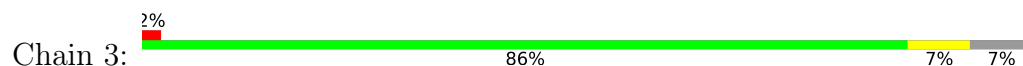
- Molecule 2: Macrophage migration inhibitory factor-like protein



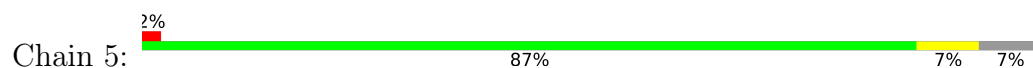
- Molecule 2: Macrophage migration inhibitory factor-like protein



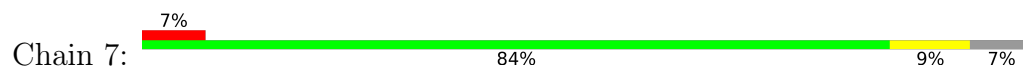
- Molecule 2: Macrophage migration inhibitory factor-like protein



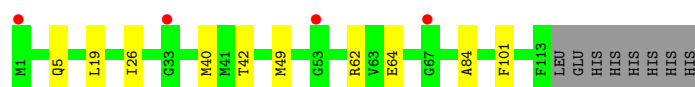
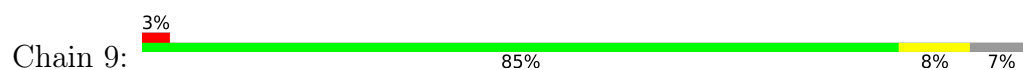
- Molecule 2: Macrophage migration inhibitory factor-like protein



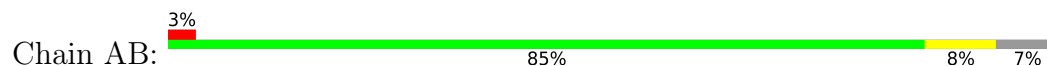
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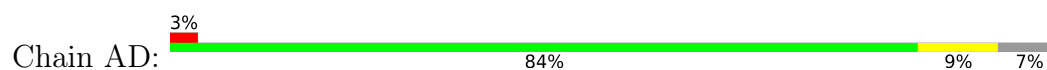
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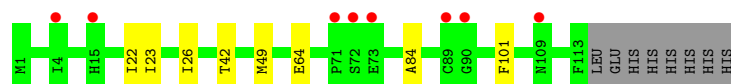
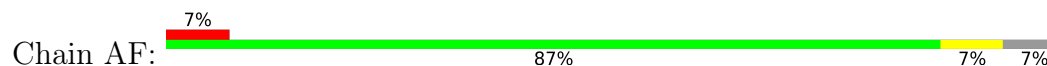
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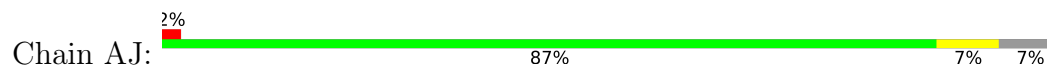
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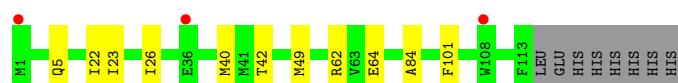
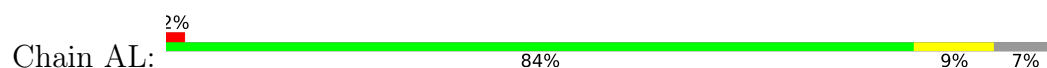
- Molecule 2: Macrophage migration inhibitory factor-like protein



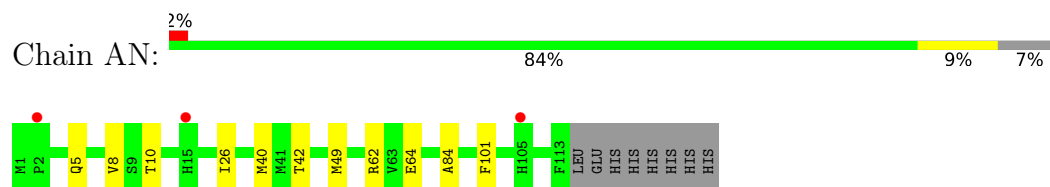
- Molecule 2: Macrophage migration inhibitory factor-like protein



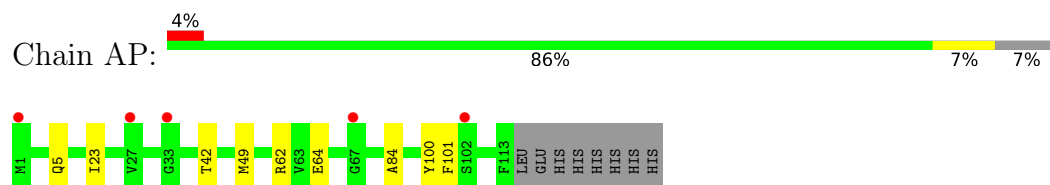
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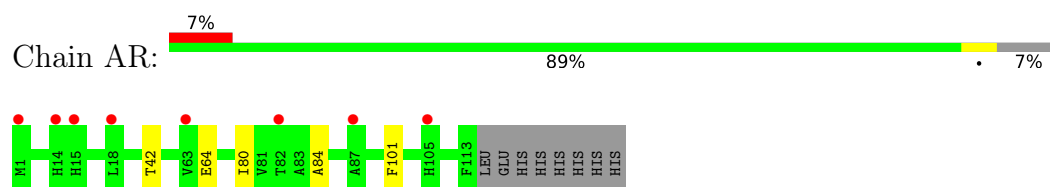
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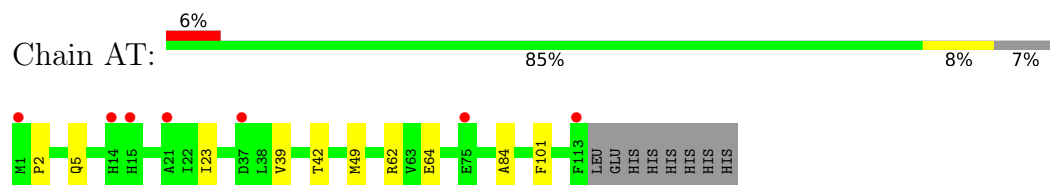
- Molecule 2: Macrophage migration inhibitory factor-like protein



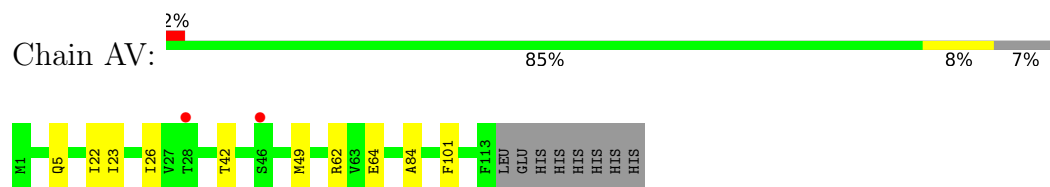
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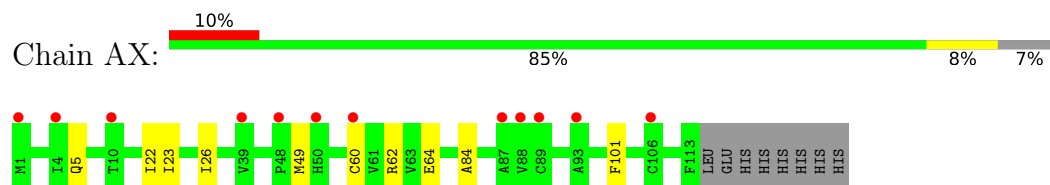
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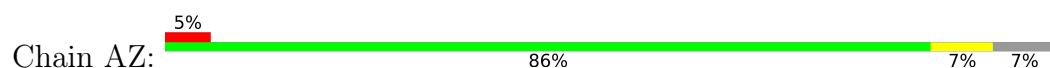
- Molecule 2: Macrophage migration inhibitory factor-like protein

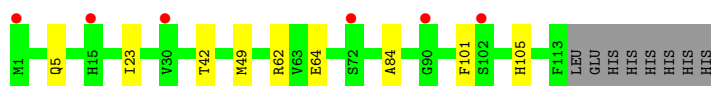


- Molecule 2: Macrophage migration inhibitory factor-like protein

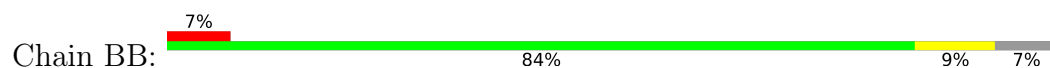


- Molecule 2: Macrophage migration inhibitory factor-like protein

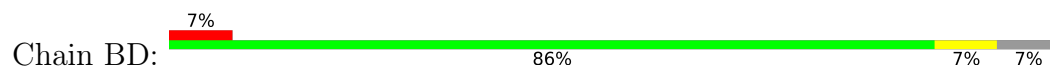




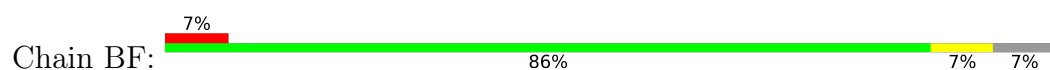
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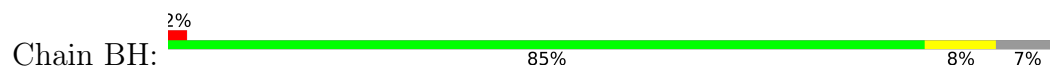
- Molecule 2: Macrophage migration inhibitory factor-like protein



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- Molecule 2: Macrophage migration inhibitory factor-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	124.91Å 189.25Å 376.83Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	94.21 – 3.50 94.21 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (94.21-3.50) 98.8 (94.21-3.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.262 , 0.298 0.266 , 0.301	Depositor DCC
R_{free} test set	21798 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	90.6	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 90.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.328 for h,-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	88858	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.89% 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 ⓘ

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	0	0.26	0/1062	0.69	0/1452
1	2	0.25	0/1066	0.69	0/1458
1	4	0.25	0/1062	0.68	0/1452
1	6	0.27	0/1066	0.69	0/1458
1	8	0.26	0/1066	0.70	1/1456 (0.1%)
1	A	0.26	0/1062	0.69	0/1452
1	AA	0.25	0/1073	0.68	0/1466
1	AC	0.25	0/1077	0.69	0/1471
1	AE	0.25	0/1062	0.68	0/1452
1	AG	0.26	0/1062	0.69	0/1452
1	AI	0.26	0/1062	0.69	0/1452
1	AK	0.25	0/1074	0.68	0/1467
1	AM	0.26	0/1075	0.68	0/1470
1	AO	0.26	0/1062	0.68	0/1452
1	AQ	0.26	0/1066	0.68	0/1457
1	AS	0.26	0/1062	0.69	0/1452
1	AU	0.25	0/1062	0.68	0/1452
1	AW	0.25	0/1062	0.68	0/1452
1	AY	0.26	0/1061	0.68	0/1451
1	BA	0.26	0/1062	0.69	0/1452
1	BC	0.26	0/1066	0.69	0/1458
1	BE	0.26	0/1062	0.69	0/1452
1	BG	0.25	0/1062	0.68	0/1452
1	C	0.25	0/1071	0.68	0/1463
1	E	0.25	0/1072	0.69	0/1466
1	G	0.26	0/1078	0.68	0/1473
1	I	0.26	0/1068	0.69	0/1459
1	K	0.25	0/1071	0.68	0/1464
1	M	0.25	0/1067	0.68	0/1459
1	O	0.26	0/1062	0.69	0/1452
1	Q	0.25	0/1062	0.69	0/1452
1	S	0.25	0/1062	0.68	0/1452
1	U	0.25	0/1062	0.68	0/1452
1	W	0.25	0/1062	0.68	0/1452

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Y	0.26	0/1067	0.69	0/1459
1	a	0.25	0/1062	0.68	0/1452
1	c	0.25	0/1057	0.69	0/1446
1	e	0.25	0/1075	0.67	0/1469
1	g	0.25	0/1068	0.68	0/1459
1	i	0.26	0/1062	0.69	0/1452
1	k	0.26	0/1073	0.69	0/1466
1	m	0.26	0/1062	0.70	0/1452
1	o	0.26	0/1062	0.69	0/1452
1	q	0.25	0/1062	0.68	0/1452
1	s	0.25	0/1062	0.68	0/1452
1	u	0.25	0/1067	0.68	0/1459
1	w	0.25	0/1061	0.68	0/1451
1	y	0.26	0/1057	0.69	0/1445
2	1	0.28	0/826	0.73	0/1137
2	3	0.28	0/821	0.73	0/1130
2	5	0.28	0/828	0.72	0/1139
2	7	0.29	0/821	0.74	0/1130
2	9	0.29	0/821	0.73	0/1130
2	AB	0.28	0/821	0.73	0/1130
2	AD	0.29	0/821	0.73	0/1130
2	AF	0.28	0/826	0.73	0/1137
2	AH	0.28	0/821	0.73	0/1130
2	AJ	0.29	0/821	0.75	0/1130
2	AL	0.28	0/821	0.72	0/1130
2	AN	0.29	0/823	0.72	0/1133
2	AP	0.28	0/831	0.73	0/1143
2	AR	0.28	0/824	0.73	0/1134
2	AT	0.28	0/828	0.75	0/1139
2	AV	0.28	0/826	0.73	0/1137
2	AX	0.28	0/821	0.73	0/1130
2	AZ	0.28	0/829	0.73	0/1141
2	B	0.28	0/827	0.73	0/1138
2	BB	0.28	0/821	0.73	0/1130
2	BD	0.29	0/821	0.74	0/1130
2	BF	0.28	0/821	0.73	0/1130
2	BH	0.28	0/821	0.73	0/1130
2	D	0.28	0/826	0.73	0/1137
2	F	0.28	0/821	0.73	0/1130
2	H	0.29	0/824	0.73	0/1134
2	J	0.28	0/821	0.74	0/1130
2	L	0.28	0/836	0.72	0/1150
2	N	0.28	0/829	0.72	0/1141

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	P	0.28	0/833	0.72	0/1146
2	R	0.28	0/821	0.73	0/1130
2	T	0.29	0/821	0.73	0/1130
2	V	0.28	0/828	0.75	0/1139
2	X	0.28	0/824	0.72	0/1134
2	Z	0.28	0/828	0.72	0/1139
2	b	0.28	0/821	0.74	0/1130
2	d	0.28	0/821	0.73	0/1130
2	f	0.28	0/832	0.72	0/1145
2	h	0.28	0/821	0.73	0/1130
2	j	0.29	0/838	0.73	0/1153
2	l	0.29	0/821	0.73	0/1130
2	n	0.28	0/821	0.73	0/1130
2	p	0.28	0/821	0.73	0/1130
2	r	0.28	0/826	0.72	0/1137
2	t	0.29	0/828	0.76	0/1139
2	v	0.28	0/829	0.72	0/1141
2	x	0.28	0/821	0.74	0/1130
2	z	0.28	0/821	0.74	0/1130
All	All	0.27	0/90704	0.71	1/124361 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	8	62	THR	N-CA-C	-5.52	106.05	112.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	0	1044	0	863	21	0
1	2	1048	0	862	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4	1044	0	863	15	0
1	6	1048	0	861	21	0
1	8	1049	0	879	22	0
1	A	1044	0	863	18	0
1	AA	1055	0	876	16	0
1	AC	1059	0	882	21	0
1	AE	1044	0	863	19	0
1	AG	1044	0	863	16	0
1	AI	1044	0	863	15	0
1	AK	1056	0	878	17	0
1	AM	1057	0	883	20	0
1	AO	1044	0	863	17	0
1	AQ	1048	0	876	16	0
1	AS	1044	0	863	15	0
1	AU	1044	0	863	18	0
1	AW	1044	0	863	16	0
1	AY	1043	0	860	17	0
1	BA	1044	0	863	17	0
1	BC	1048	0	862	17	0
1	BE	1044	0	863	16	0
1	BG	1044	0	863	16	0
1	C	1053	0	876	15	0
1	E	1054	0	870	20	0
1	G	1059	0	883	18	0
1	I	1050	0	874	16	0
1	K	1053	0	883	18	0
1	M	1049	0	865	19	0
1	O	1044	0	863	20	0
1	Q	1044	0	863	15	0
1	S	1044	0	863	17	0
1	U	1044	0	863	19	0
1	W	1044	0	863	18	0
1	Y	1049	0	865	17	0
1	a	1044	0	863	19	0
1	c	1039	0	856	17	0
1	e	1057	0	889	16	0
1	g	1050	0	874	18	0
1	i	1044	0	863	16	0
1	k	1055	0	883	20	0
1	m	1044	0	863	15	0
1	o	1044	0	863	15	0
1	q	1044	0	863	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	s	1044	0	863	18	0
1	u	1049	0	865	15	0
1	w	1043	0	860	19	0
1	y	1039	0	861	17	0
2	1	805	0	742	9	0
2	3	801	0	739	7	0
2	5	807	0	746	6	0
2	7	801	0	739	8	0
2	9	801	0	739	8	0
2	AB	801	0	739	7	0
2	AD	801	0	739	8	0
2	AF	805	0	742	6	0
2	AH	801	0	739	6	0
2	AJ	801	0	739	6	0
2	AL	801	0	739	8	0
2	AN	803	0	746	8	0
2	AP	810	0	748	7	0
2	AR	804	0	741	4	0
2	AT	807	0	746	7	0
2	AV	805	0	742	7	0
2	AX	801	0	739	7	0
2	AZ	808	0	751	7	0
2	B	806	0	744	8	0
2	BB	801	0	739	9	0
2	BD	801	0	739	7	0
2	BF	801	0	739	7	0
2	BH	801	0	739	7	0
2	D	805	0	742	6	0
2	F	801	0	739	8	0
2	H	804	0	748	7	0
2	J	801	0	739	7	0
2	L	814	0	758	9	0
2	N	808	0	751	9	0
2	P	811	0	749	7	0
2	R	801	0	739	7	0
2	T	801	0	739	9	0
2	V	807	0	746	8	0
2	X	804	0	741	8	0
2	Z	807	0	746	8	0
2	b	801	0	739	6	0
2	d	801	0	739	7	0
2	f	811	0	760	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	h	801	0	739	8	0
2	j	816	0	751	6	0
2	l	801	0	739	9	0
2	n	801	0	739	6	0
2	p	801	0	739	7	0
2	r	805	0	742	9	0
2	t	807	0	746	8	0
2	v	808	0	751	8	0
2	x	801	0	739	6	0
2	z	801	0	739	7	0
All	All	88858	0	77289	959	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 6.

The worst 5 of 959 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)
2:Z:64:GLU:HG2	2:Z:101:PHE:HB2	1.63	0.81
2:AX:64:GLU:HG2	2:AX:101:PHE:HB2	1.64	0.80
2:B:64:GLU:HG2	2:B:101:PHE:HB2	1.65	0.78
2:AT:64:GLU:HG2	2:AT:101:PHE:HB2	1.66	0.77
2:J:64:GLU:HG2	2:J:101:PHE:HB2	1.64	0.77

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	2	148/158 (94%)	144 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	6	148/158 (94%)	144 (97%)	4 (3%)	0	100	100
1	8	144/158 (91%)	141 (98%)	3 (2%)	0	100	100
1	A	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	AA	148/158 (94%)	144 (97%)	4 (3%)	0	100	100
1	AC	148/158 (94%)	144 (97%)	4 (3%)	0	100	100
1	AE	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	AG	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	AI	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	AK	148/158 (94%)	144 (97%)	4 (3%)	0	100	100
1	AM	148/158 (94%)	144 (97%)	4 (3%)	0	100	100
1	AO	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	AQ	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	AS	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	AU	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	AW	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	AY	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	BA	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	BC	148/158 (94%)	144 (97%)	4 (3%)	0	100	100
1	BE	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	BG	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	C	148/158 (94%)	144 (97%)	4 (3%)	0	100	100
1	E	149/158 (94%)	145 (97%)	4 (3%)	0	100	100
1	G	148/158 (94%)	144 (97%)	4 (3%)	0	100	100
1	I	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	K	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	M	148/158 (94%)	144 (97%)	4 (3%)	0	100	100
1	O	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	Q	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	S	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	U	147/158 (93%)	143 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	Y	148/158 (94%)	144 (97%)	4 (3%)	0	100	100
1	a	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	c	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	e	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	g	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	i	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	k	148/158 (94%)	144 (97%)	4 (3%)	0	100	100
1	m	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	o	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	q	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	s	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	u	148/158 (94%)	144 (97%)	4 (3%)	0	100	100
1	w	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
1	y	146/158 (92%)	142 (97%)	4 (3%)	0	100	100
2	1	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	3	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	5	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	7	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	9	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	AB	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	AD	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	AF	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	AH	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	AJ	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	AL	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	AN	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	AP	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	AR	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	AT	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	AV	111/121 (92%)	108 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AX	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	AZ	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	B	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	BB	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	BD	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	BF	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	BH	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	D	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	F	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	H	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	J	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	L	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	N	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	P	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	R	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	T	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	V	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	X	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	Z	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	b	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	d	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	f	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	h	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	j	112/121 (93%)	109 (97%)	3 (3%)	0	100	100
2	l	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	n	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	p	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	r	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	t	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	v	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
2	x	111/121 (92%)	108 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	z	111/121 (92%)	108 (97%)	3 (3%)	0	100	100
All	All	12396/13392 (93%)	12061 (97%)	335 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	0	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	2	85/137 (62%)	82 (96%)	3 (4%)	32	57
1	4	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	6	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	8	89/137 (65%)	86 (97%)	3 (3%)	32	57
1	A	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	AA	87/137 (64%)	84 (97%)	3 (3%)	32	57
1	AC	88/137 (64%)	83 (94%)	5 (6%)	18	45
1	AE	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	AG	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	AI	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	AK	88/137 (64%)	85 (97%)	3 (3%)	32	57
1	AM	89/137 (65%)	86 (97%)	3 (3%)	32	57
1	AO	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	AQ	87/137 (64%)	84 (97%)	3 (3%)	32	57
1	AS	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	AU	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	AW	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	AY	85/137 (62%)	82 (96%)	3 (4%)	32	57
1	BA	86/137 (63%)	83 (96%)	3 (4%)	32	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BC	85/137 (62%)	82 (96%)	3 (4%)	32	57
1	BE	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	BG	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	C	87/137 (64%)	83 (95%)	4 (5%)	24	50
1	E	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	G	88/137 (64%)	85 (97%)	3 (3%)	32	57
1	I	87/137 (64%)	84 (97%)	3 (3%)	32	57
1	K	89/137 (65%)	86 (97%)	3 (3%)	32	57
1	M	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	O	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	Q	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	S	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	U	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	W	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	Y	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	a	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	c	84/137 (61%)	81 (96%)	3 (4%)	31	57
1	e	90/137 (66%)	87 (97%)	3 (3%)	33	58
1	g	87/137 (64%)	84 (97%)	3 (3%)	32	57
1	i	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	k	88/137 (64%)	84 (96%)	4 (4%)	24	50
1	m	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	o	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	q	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	s	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	u	86/137 (63%)	83 (96%)	3 (4%)	32	57
1	w	85/137 (62%)	82 (96%)	3 (4%)	32	57
1	y	86/137 (63%)	83 (96%)	3 (4%)	32	57
2	1	75/106 (71%)	75 (100%)	0	100	100
2	3	74/106 (70%)	74 (100%)	0	100	100
2	5	75/106 (71%)	75 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	7	74/106 (70%)	74 (100%)	0	100	100
2	9	74/106 (70%)	74 (100%)	0	100	100
2	AB	74/106 (70%)	74 (100%)	0	100	100
2	AD	74/106 (70%)	74 (100%)	0	100	100
2	AF	75/106 (71%)	75 (100%)	0	100	100
2	AH	74/106 (70%)	74 (100%)	0	100	100
2	AJ	74/106 (70%)	74 (100%)	0	100	100
2	AL	74/106 (70%)	74 (100%)	0	100	100
2	AN	75/106 (71%)	75 (100%)	0	100	100
2	AP	76/106 (72%)	76 (100%)	0	100	100
2	AR	75/106 (71%)	75 (100%)	0	100	100
2	AT	75/106 (71%)	75 (100%)	0	100	100
2	AV	75/106 (71%)	75 (100%)	0	100	100
2	AX	74/106 (70%)	74 (100%)	0	100	100
2	AZ	76/106 (72%)	76 (100%)	0	100	100
2	B	75/106 (71%)	74 (99%)	1 (1%)	61	72
2	BB	74/106 (70%)	74 (100%)	0	100	100
2	BD	74/106 (70%)	74 (100%)	0	100	100
2	BF	74/106 (70%)	74 (100%)	0	100	100
2	BH	74/106 (70%)	74 (100%)	0	100	100
2	D	75/106 (71%)	75 (100%)	0	100	100
2	F	74/106 (70%)	74 (100%)	0	100	100
2	H	75/106 (71%)	75 (100%)	0	100	100
2	J	74/106 (70%)	74 (100%)	0	100	100
2	L	77/106 (73%)	77 (100%)	0	100	100
2	N	76/106 (72%)	76 (100%)	0	100	100
2	P	76/106 (72%)	76 (100%)	0	100	100
2	R	74/106 (70%)	74 (100%)	0	100	100
2	T	74/106 (70%)	74 (100%)	0	100	100
2	V	75/106 (71%)	75 (100%)	0	100	100
2	X	75/106 (71%)	75 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Z	75/106 (71%)	75 (100%)	0	100	100
2	b	74/106 (70%)	74 (100%)	0	100	100
2	d	74/106 (70%)	74 (100%)	0	100	100
2	f	77/106 (73%)	77 (100%)	0	100	100
2	h	74/106 (70%)	74 (100%)	0	100	100
2	j	76/106 (72%)	76 (100%)	0	100	100
2	l	74/106 (70%)	74 (100%)	0	100	100
2	n	74/106 (70%)	74 (100%)	0	100	100
2	p	74/106 (70%)	74 (100%)	0	100	100
2	r	75/106 (71%)	75 (100%)	0	100	100
2	t	75/106 (71%)	74 (99%)	1 (1%)	61	72
2	v	76/106 (72%)	76 (100%)	0	100	100
2	x	74/106 (70%)	74 (100%)	0	100	100
2	z	74/106 (70%)	74 (100%)	0	100	100
All	All	7733/11664 (66%)	7583 (98%)	150 (2%)	50	68

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AK	72	ARG
1	BC	73	ILE
1	AM	73	ILE
1	AU	72	ARG
1	e	71	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
2	AL	112	ASN
1	AE	5	ASN
2	AX	112	ASN
1	AA	5	ASN
1	o	5	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](#)

There are no ligands in this entry.

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	0	151/158 (95%)	0.88	8 (5%) 32 18	87, 119, 159, 172	0
1	2	152/158 (96%)	0.75	8 (5%) 32 18	51, 91, 122, 137	0
1	4	151/158 (95%)	0.68	6 (3%) 42 23	60, 89, 126, 137	0
1	6	152/158 (96%)	0.77	8 (5%) 32 18	60, 102, 137, 153	0
1	8	150/158 (94%)	0.52	5 (3%) 49 28	44, 74, 108, 125	0
1	A	151/158 (95%)	0.54	4 (2%) 57 33	49, 70, 114, 134	0
1	AA	152/158 (96%)	0.55	6 (3%) 43 23	42, 69, 96, 104	0
1	AC	152/158 (96%)	0.40	4 (2%) 57 33	39, 69, 97, 124	0
1	AE	151/158 (95%)	0.88	12 (7%) 18 12	85, 99, 132, 151	0
1	AG	151/158 (95%)	0.91	14 (9%) 14 9	91, 114, 147, 167	0
1	AI	151/158 (95%)	0.92	14 (9%) 14 9	84, 115, 137, 162	0
1	AK	152/158 (96%)	0.46	4 (2%) 57 33	37, 66, 104, 133	0
1	AM	152/158 (96%)	0.65	11 (7%) 21 14	46, 74, 111, 142	0
1	AO	151/158 (95%)	0.58	5 (3%) 49 28	47, 75, 109, 125	0
1	AQ	151/158 (95%)	0.93	13 (8%) 16 11	80, 113, 148, 183	0
1	AS	151/158 (95%)	0.79	9 (5%) 27 16	77, 112, 135, 158	0
1	AU	151/158 (95%)	0.88	9 (5%) 27 16	88, 105, 128, 151	0
1	AW	151/158 (95%)	0.80	10 (6%) 24 15	86, 117, 151, 160	0
1	AY	151/158 (95%)	1.02	19 (12%) 8 6	81, 122, 147, 204	0
1	BA	151/158 (95%)	0.94	12 (7%) 18 12	83, 120, 152, 167	0
1	BC	152/158 (96%)	0.81	8 (5%) 32 18	68, 106, 128, 170	0
1	BE	151/158 (95%)	0.87	16 (10%) 11 8	68, 94, 129, 148	0
1	BG	151/158 (95%)	0.82	10 (6%) 24 15	65, 90, 131, 142	0
1	C	152/158 (96%)	0.73	9 (5%) 28 16	53, 88, 118, 141	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	153/158 (96%)	0.58	6 (3%) 43 23	44, 77, 110, 127	0
1	G	152/158 (96%)	0.51	7 (4%) 37 20	50, 66, 89, 105	0
1	I	151/158 (95%)	0.58	8 (5%) 32 18	51, 78, 102, 136	0
1	K	151/158 (95%)	0.45	4 (2%) 57 33	43, 64, 92, 106	0
1	M	152/158 (96%)	0.85	11 (7%) 21 14	70, 95, 123, 155	0
1	O	151/158 (95%)	0.95	15 (9%) 13 8	111, 129, 147, 160	0
1	Q	151/158 (95%)	0.99	14 (9%) 14 9	82, 119, 167, 177	0
1	S	151/158 (95%)	0.71	7 (4%) 37 20	55, 86, 122, 136	0
1	U	151/158 (95%)	0.73	7 (4%) 37 20	67, 92, 118, 131	0
1	W	151/158 (95%)	0.57	8 (5%) 32 18	53, 79, 104, 128	0
1	Y	152/158 (96%)	0.47	2 (1%) 75 50	47, 73, 108, 124	0
1	a	151/158 (95%)	0.68	8 (5%) 32 18	53, 81, 107, 121	0
1	c	151/158 (95%)	0.55	6 (3%) 42 23	49, 77, 103, 122	0
1	e	151/158 (95%)	0.51	5 (3%) 49 28	44, 69, 98, 111	0
1	g	151/158 (95%)	0.57	6 (3%) 42 23	47, 76, 101, 128	0
1	i	151/158 (95%)	0.43	3 (1%) 65 39	43, 61, 89, 106	0
1	k	152/158 (96%)	0.82	10 (6%) 24 15	61, 96, 124, 161	0
1	m	151/158 (95%)	0.89	13 (8%) 16 11	89, 126, 151, 165	0
1	o	151/158 (95%)	1.04	19 (12%) 8 6	92, 122, 155, 177	0
1	q	151/158 (95%)	0.74	9 (5%) 27 16	56, 88, 122, 154	0
1	s	151/158 (95%)	0.73	8 (5%) 32 18	69, 86, 109, 143	0
1	u	152/158 (96%)	0.61	4 (2%) 57 33	43, 80, 108, 120	0
1	w	151/158 (95%)	1.07	18 (11%) 9 6	82, 119, 157, 172	0
1	y	150/158 (94%)	0.83	9 (6%) 27 16	87, 118, 141, 148	0
2	1	113/121 (93%)	0.59	6 (5%) 32 18	73, 99, 131, 133	0
2	3	113/121 (93%)	0.48	3 (2%) 56 33	43, 72, 107, 139	0
2	5	113/121 (93%)	0.71	2 (1%) 67 42	64, 91, 116, 132	0
2	7	113/121 (93%)	0.84	8 (7%) 22 14	80, 104, 129, 145	0
2	9	113/121 (93%)	0.30	4 (3%) 47 26	51, 70, 95, 118	0
2	AB	113/121 (93%)	0.57	4 (3%) 47 26	55, 83, 119, 138	0
2	AD	113/121 (93%)	0.45	4 (3%) 47 26	58, 77, 102, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	AF	113/121 (93%)	0.83	8 (7%) 22 14	59, 91, 118, 130	0
2	AH	113/121 (93%)	0.88	10 (8%) 15 10	68, 99, 119, 130	0
2	AJ	113/121 (93%)	0.61	3 (2%) 56 33	69, 88, 111, 128	0
2	AL	113/121 (93%)	0.47	3 (2%) 56 33	60, 81, 117, 131	0
2	AN	113/121 (93%)	0.37	3 (2%) 56 33	52, 71, 92, 111	0
2	AP	113/121 (93%)	0.49	5 (4%) 39 21	58, 83, 105, 115	0
2	AR	113/121 (93%)	0.83	8 (7%) 22 14	72, 95, 118, 138	0
2	AT	113/121 (93%)	0.64	7 (6%) 26 16	66, 90, 117, 124	0
2	AV	113/121 (93%)	0.50	2 (1%) 67 42	65, 85, 102, 109	0
2	AX	113/121 (93%)	0.91	12 (10%) 11 8	75, 100, 128, 140	0
2	AZ	113/121 (93%)	0.84	6 (5%) 32 18	68, 100, 120, 134	0
2	B	113/121 (93%)	0.34	3 (2%) 56 33	54, 75, 97, 112	0
2	BB	113/121 (93%)	0.74	8 (7%) 22 14	71, 97, 120, 133	0
2	BD	113/121 (93%)	0.81	8 (7%) 22 14	73, 96, 120, 140	0
2	BF	113/121 (93%)	0.51	8 (7%) 22 14	47, 72, 117, 129	0
2	BH	113/121 (93%)	0.65	2 (1%) 67 42	63, 90, 113, 125	0
2	D	113/121 (93%)	0.56	6 (5%) 32 18	50, 69, 91, 110	0
2	F	113/121 (93%)	0.49	4 (3%) 47 26	61, 84, 110, 133	0
2	H	113/121 (93%)	0.51	8 (7%) 22 14	51, 71, 89, 108	0
2	J	113/121 (93%)	0.59	3 (2%) 56 33	53, 80, 103, 115	0
2	L	113/121 (93%)	0.29	1 (0%) 81 58	42, 66, 84, 101	0
2	N	113/121 (93%)	0.69	11 (9%) 13 9	55, 81, 106, 114	0
2	P	113/121 (93%)	0.81	11 (9%) 13 9	78, 96, 114, 124	0
2	R	113/121 (93%)	0.80	7 (6%) 26 16	69, 93, 120, 132	0
2	T	113/121 (93%)	0.35	3 (2%) 56 33	47, 71, 93, 111	0
2	V	113/121 (93%)	0.39	6 (5%) 32 18	51, 74, 96, 116	0
2	X	113/121 (93%)	0.43	1 (0%) 81 58	57, 76, 97, 116	0
2	Z	113/121 (93%)	0.38	3 (2%) 56 33	57, 75, 109, 129	0
2	b	113/121 (93%)	0.60	5 (4%) 39 21	52, 72, 97, 114	0
2	d	113/121 (93%)	0.76	6 (5%) 32 18	54, 89, 119, 151	0
2	f	113/121 (93%)	0.44	2 (1%) 67 42	51, 69, 94, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	h	113/121 (93%)	0.45	5 (4%) 39 21	56, 75, 105, 116	0
2	j	114/121 (94%)	0.38	6 (5%) 32 18	42, 61, 84, 101	0
2	l	113/121 (93%)	0.52	4 (3%) 47 26	53, 72, 96, 105	0
2	n	113/121 (93%)	0.73	5 (4%) 39 21	65, 94, 115, 127	0
2	p	113/121 (93%)	0.51	6 (5%) 32 18	67, 91, 106, 122	0
2	r	113/121 (93%)	0.33	2 (1%) 67 42	54, 67, 92, 107	0
2	t	113/121 (93%)	0.34	4 (3%) 47 26	47, 70, 94, 105	0
2	v	113/121 (93%)	0.48	4 (3%) 47 26	57, 79, 103, 132	0
2	x	113/121 (93%)	0.72	8 (7%) 22 14	69, 92, 114, 118	0
2	z	113/121 (93%)	1.02	15 (13%) 7 6	80, 103, 127, 150	0
All	All	12686/13392 (94%)	0.67	694 (5%) 30 18	37, 88, 131, 204	0

The worst 5 of 694 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BC	151	ASP	5.1
1	A	152	GLU	4.9
2	P	31	VAL	4.6
2	d	96	ILE	4.6
1	o	152	GLU	4.6

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.