wwPDB X-ray Structure Validation Summary Report (i)

May 23, 2014 – 04:37 AM EDT

PDB ID	:	1VW5
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 validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

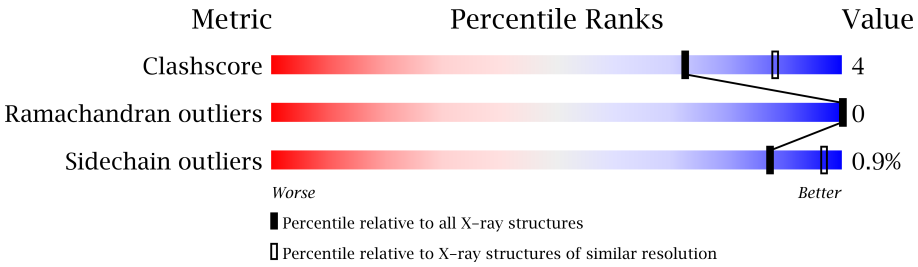
The following versions of software and data (see references) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	FAILED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22978

1 Overall quality at a glance

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))
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	158	
1	C	158	
1	E	158	
1	G	158	
1	I	158	
1	K	158	
1	M	158	
1	O	158	
1	Q	158	
1	S	158	
1	U	158	
1	W	158	
1	Y	158	
1	a	158	
1	c	158	
1	e	158	

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Mol	Chain	Length	Quality of chain
1	g	158	
1	i	158	
1	k	158	
1	m	158	
1	o	158	
1	q	158	
1	s	158	
1	u	158	
2	B	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	
2	V	121	
2	X	121	
2	Z	121	
2	b	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	
2	v	121	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 44468 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

There are 240 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
k	116	VAL	ALA	ENGINEERED MUTATION	UNP B0BGB0
m	49	ILE	LYS	ENGINEERED MUTATION	UNP B0BGB0

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Chain	Residue	Modelled	Actual	Comment	Reference
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
u	53	ALA	ASP	ENGINEERED MUTATION	UNP B0BGB0
u	56	ILE	GLN	ENGINEERED MUTATION	UNP B0BGB0

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

There are 384 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

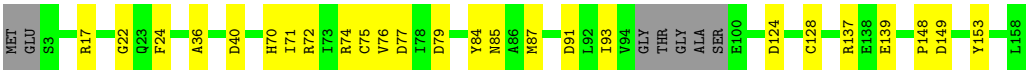
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS failed to run properly.

• Molecule 1: integron gene cassette protein

Chain A:

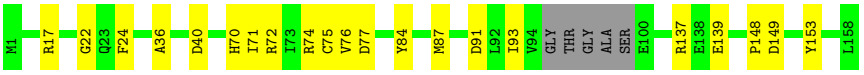


• Molecule 1: integron gene cassette protein

Chain C:

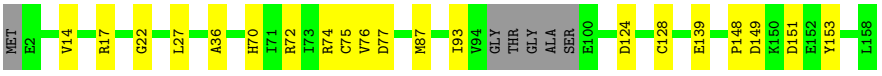
• Molecule 1: integron gene cassette protein

Chain E:



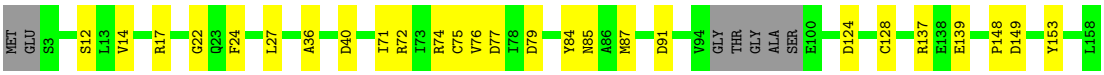
• Molecule 1: integron gene cassette protein

Chain G:



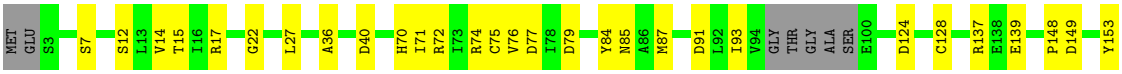
• Molecule 1: integron gene cassette protein

Chain I:



• Molecule 1: integron gene cassette protein

Chain K:

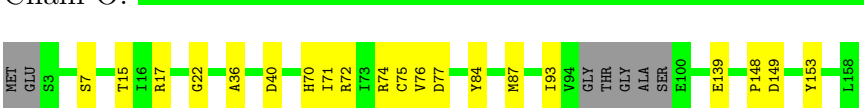


• Molecule 1: integron gene cassette protein

Chain M:

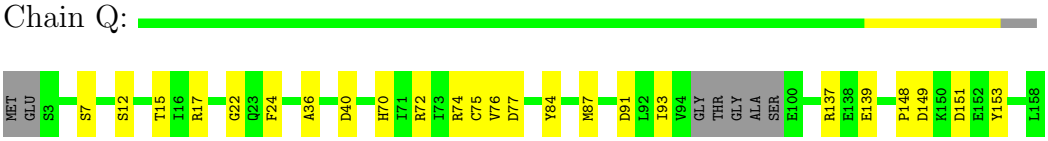
• Molecule 1: integron gene cassette protein

Chain O:



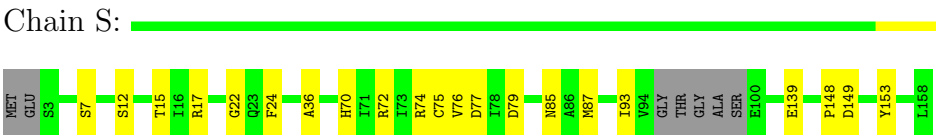
• Molecule 1: integron gene cassette protein

Chain Q:



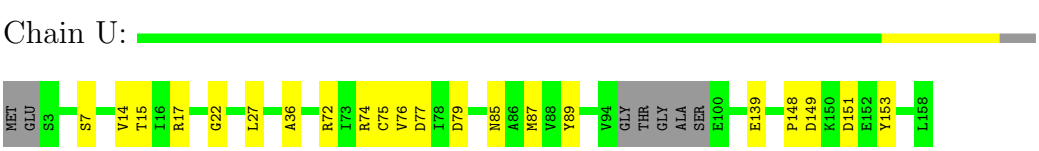
• Molecule 1: integron gene cassette protein

Chain S:



• Molecule 1: integron gene cassette protein

Chain U:

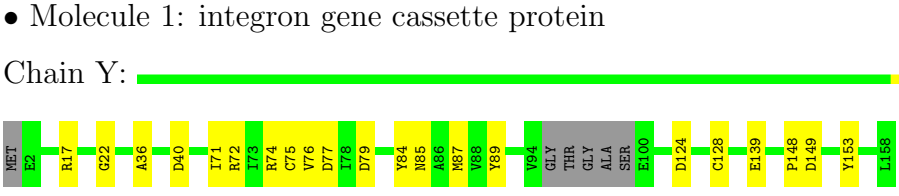


• Molecule 1: integron gene cassette protein

Chain W:

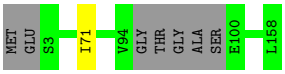
• Molecule 1: integron gene cassette protein

Chain Y:



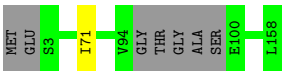
• Molecule 1: integron gene cassette protein

Chain a:



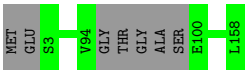
• Molecule 1: integron gene cassette protein

Chain c:



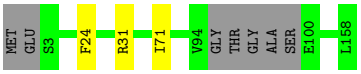
• Molecule 1: integron gene cassette protein

Chain e:



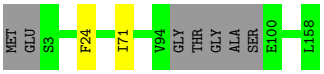
• Molecule 1: integron gene cassette protein

Chain g:



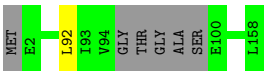
• Molecule 1: integron gene cassette protein

Chain i:



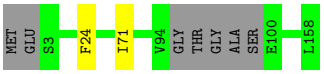
• Molecule 1: integron gene cassette protein

Chain k:



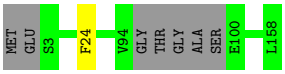
• Molecule 1: integron gene cassette protein

Chain m:



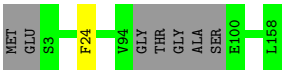
• Molecule 1: integron gene cassette protein

Chain o:



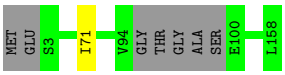
• Molecule 1: integron gene cassette protein

Chain q:



• Molecule 1: integron gene cassette protein

Chain s:



• Molecule 1: integron gene cassette protein

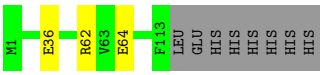
Chain u:

• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain B:

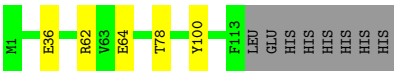
• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain D:



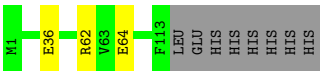
• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain F:



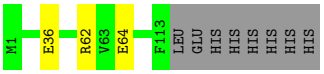
• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain H:



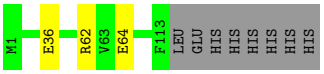
• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain J:



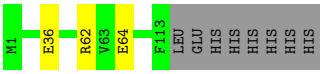
• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain L:



• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain N:



• Molecule 2: Macrophage migration inhibitory factor-like protein

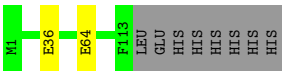
Chain P:

• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain R:

• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain T:

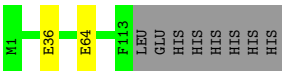


• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain V:

• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain X:



• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain Z:

• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain b:

• Molecule 2: Macrophage migration inhibitory factor-like protein

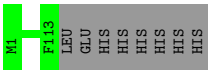
Chain d:

• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain f:

• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain h:



• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain j:

• Molecule 2: Macrophage migration inhibitory factor-like protein

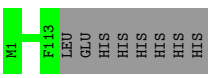
Chain l:

• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain n:

• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain p:



• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain r:

• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain t:

• Molecule 2: Macrophage migration inhibitory factor-like protein

Chain v:

4 Data and refinement statistics (i)

EDS failed to run properly - this section will therefore be incomplete.

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	Depositor
% Data completeness (in resolution range)	98.8 (94.21-3.50)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 3.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.262 , 0.298	Depositor
Wilson B-factor (Å^2)	90.6	Xtriage
Anisotropy	0.138	Xtriage
Estimated twinning fraction	0.328 for h,-k,-l	Xtriage
L-test for twinning	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 217956 reflections	Xtriage
Total number of atoms	44468	wwPDB-VP
Average B, all atoms (Å^2)	83.0	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.*

[1] Intensities estimated from amplitudes.

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	A	0.20	0/1062	0.35	0/1452
1	C	0.20	0/1071	0.35	0/1463
1	E	0.20	0/1072	0.35	0/1466
1	G	0.20	0/1078	0.35	0/1473
1	I	0.20	0/1068	0.35	0/1459
1	K	0.20	0/1071	0.35	0/1464
1	M	0.20	0/1067	0.34	0/1459
1	O	0.20	0/1062	0.35	0/1452
1	Q	0.20	0/1062	0.35	0/1452
1	S	0.20	0/1062	0.34	0/1452
1	U	0.20	0/1062	0.34	0/1452
1	W	0.20	0/1062	0.35	0/1452
1	Y	0.20	0/1067	0.35	0/1459
1	a	0.20	0/1062	0.35	0/1452
1	c	0.20	0/1057	0.35	0/1446
1	e	0.20	0/1075	0.35	0/1469
1	g	0.20	0/1068	0.36	0/1459
1	i	0.20	0/1062	0.36	0/1452
1	k	0.20	0/1073	0.37	0/1466
1	m	0.20	0/1062	0.35	0/1452
1	o	0.20	0/1062	0.35	0/1452
1	q	0.20	0/1062	0.34	0/1452
1	s	0.20	0/1062	0.34	0/1452
1	u	0.20	0/1067	0.35	0/1459
2	B	0.20	0/827	0.37	0/1138
2	D	0.20	0/826	0.38	0/1137
2	F	0.20	0/821	0.37	0/1130
2	H	0.20	0/824	0.37	0/1134
2	J	0.20	0/821	0.37	0/1130
2	L	0.20	0/836	0.37	0/1150
2	N	0.20	0/829	0.37	0/1141
2	P	0.20	0/833	0.37	0/1146
2	R	0.20	0/821	0.38	0/1130
2	T	0.20	0/821	0.38	0/1130

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
2	V	0.21	0/828	0.38	0/1139
2	X	0.20	0/824	0.37	0/1134
2	Z	0.20	0/828	0.37	0/1139
2	b	0.20	0/821	0.38	0/1130
2	d	0.20	0/821	0.37	0/1130
2	f	0.20	0/832	0.37	0/1145
2	h	0.20	0/821	0.37	0/1130
2	j	0.20	0/838	0.38	0/1153
2	l	0.20	0/821	0.37	0/1130
2	n	0.20	0/821	0.38	0/1130
2	p	0.20	0/821	0.38	0/1130
2	r	0.20	0/826	0.37	0/1137
2	t	0.21	0/828	0.38	0/1139
2	v	0.20	0/829	0.38	0/1141
All	All	0.20	0/45396	0.36	0/62239

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1044	0	0	14	0
1	C	1053	0	1	12	0
1	E	1054	0	6	13	0
1	G	1059	0	1	14	0
1	I	1050	0	0	15	0
1	K	1053	0	0	18	0
1	M	1049	0	1	15	0
1	O	1044	0	0	12	0
1	Q	1044	0	0	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S	1044	0	0	13	0
1	U	1044	0	0	15	0
1	W	1044	0	0	9	0
1	Y	1049	0	1	12	0
1	a	1044	0	0	0	0
1	c	1039	0	0	0	0
1	e	1057	0	0	0	0
1	g	1050	0	0	0	0
1	i	1044	0	0	0	0
1	k	1055	0	1	0	0
1	m	1044	0	0	0	0
1	o	1044	0	0	0	0
1	q	1044	0	0	0	0
1	s	1044	0	0	0	0
1	u	1049	0	1	0	0
2	B	806	0	0	4	0
2	D	805	0	0	3	0
2	F	801	0	0	5	0
2	H	804	0	0	4	0
2	J	801	0	0	3	0
2	L	814	0	0	4	0
2	N	808	0	0	5	0
2	P	811	0	0	5	0
2	R	801	0	0	4	0
2	T	801	0	0	3	0
2	V	807	0	0	6	0
2	X	804	0	0	2	0
2	Z	807	0	0	4	0
2	b	801	0	0	0	0
2	d	801	0	0	0	0
2	f	811	0	0	0	0
2	h	801	0	0	0	0
2	j	816	0	1	0	0
2	l	801	0	0	0	0
2	n	801	0	0	0	0
2	p	801	0	0	0	0
2	r	805	0	0	0	0
2	t	807	0	0	0	0
2	v	808	0	0	0	0
All	All	44468	0	13	188	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

The worst 5 of 188 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:22:GLY:O	1:C:72:ARG:NH2	2.47	0.70
1:A:22:GLY:O	1:A:72:ARG:NH2	2.29	0.65
1:O:22:GLY:O	1:O:72:ARG:NH2	2.36	0.64
1:E:22:GLY:O	1:E:72:ARG:NH2	2.32	0.63
1:I:22:GLY:O	1:I:72:ARG:NH2	2.33	0.62

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	6201/6696 (93%)	6033 (97%)	168 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	86/137 (63%)	84 (98%)	2 (2%)	63 92
1	C	87/137 (64%)	85 (98%)	2 (2%)	63 92
1	E	86/137 (63%)	84 (98%)	2 (2%)	63 92
1	G	88/137 (64%)	88 (100%)	0	100 100
1	I	87/137 (64%)	85 (98%)	2 (2%)	63 92
1	K	89/137 (65%)	88 (99%)	1 (1%)	84 96
1	M	86/137 (63%)	85 (99%)	1 (1%)	82 96
1	O	86/137 (63%)	85 (99%)	1 (1%)	82 96
1	Q	86/137 (63%)	85 (99%)	1 (1%)	82 96
1	S	86/137 (63%)	85 (99%)	1 (1%)	82 96
1	U	86/137 (63%)	86 (100%)	0	100 100
1	W	86/137 (63%)	85 (99%)	1 (1%)	82 96
1	Y	86/137 (63%)	85 (99%)	1 (1%)	82 96
1	a	86/137 (63%)	85 (99%)	1 (1%)	82 96
1	c	84/137 (61%)	83 (99%)	1 (1%)	82 96
1	e	90/137 (66%)	90 (100%)	0	100 100
1	g	87/137 (64%)	84 (97%)	3 (3%)	49 88
1	i	86/137 (63%)	84 (98%)	2 (2%)	63 92
1	k	88/137 (64%)	87 (99%)	1 (1%)	84 96
1	m	86/137 (63%)	84 (98%)	2 (2%)	63 92
1	o	86/137 (63%)	85 (99%)	1 (1%)	82 96
1	q	86/137 (63%)	85 (99%)	1 (1%)	82 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	s	86/137 (63%)	85 (99%)	1 (1%)	82 96
1	u	86/137 (63%)	85 (99%)	1 (1%)	82 96
2	B	75/106 (71%)	74 (99%)	1 (1%)	80 96
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%)	75 (99%)	1 (1%)	80 96
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%)	74 (99%)	1 (1%)	80 96
2	X	75/106 (71%)	75 (100%)	0	100 100
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%)	80 96
2	v	76/106 (72%)	76 (100%)	0	100 100
All	All	3874/5832 (66%)	3841 (99%)	33 (1%)	87 97

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	71	ILE
1	Y	71	ILE

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Mol	Chain	Res	Type
1	q	24	PHE
1	Q	24	PHE
1	S	24	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers

EDS failed to run properly - this section will therefore be empty.