Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 12:52 PM EDT

PDB ID	:	5IM6
Title	:	Crystal structure of designed two-component self-assembling icosahedral cage I32-28
Authors	:	Liu, Y.A.; Cascio, D.; Sawaya, M.R.; Bale, J.B.; Collazo, M.J.; Thomas, C.; Sheffler, W.; King, N.P.; Baker, D.; Yeates, T.O.
Deposited on	:	2016-03-05
Resolution	:	5.59 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

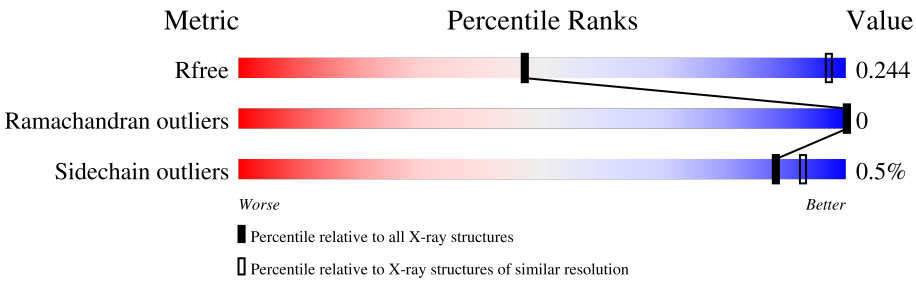
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 5.59 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1001 (7.32-3.84)
Ramachandran outliers	138981	1016 (7.32-3.82)
Sidechain outliers	138945	1192 (7.36-3.80)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	157	96%
1	B	157	96%
1	C	157	96%
1	D	157	96%
1	E	157	96%
1	F	157	96%
1	G	157	96%
1	H	157	96%

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Mol	Chain	Length	Quality of chain
1	I	157	96%
1	J	157	96%
1	K	157	96%
1	L	157	96%
1	M	157	96%
1	N	157	96%
1	O	157	96%
1	P	157	96%
1	Q	157	96%
1	R	157	96%
1	S	157	96%
1	T	157	96%
2	U	165	90% 10%
2	V	165	90% 10%
2	W	165	90% 10%
2	X	165	90% 10%
2	Y	165	90% 10%
2	Z	165	90% 10%
2	a	165	90% 10%
2	b	165	90% 10%
2	c	165	90% 10%
2	d	165	90% 10%
2	e	165	90% 10%
2	f	165	90% 10%
2	g	165	90% 10%

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Mol	Chain	Length	Quality of chain
2	h	165	90% 10%
2	i	165	90% 10%
2	j	165	90% 10%
2	k	165	90% 10%
2	l	165	90% 10%
2	m	165	90% 10%
2	n	165	90% 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 44220 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 Designed self-assembling icosahedral cage I32-28 trimeric subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	152	1134	719	203	209	3	0	0	0
1	B	152	1134	719	203	209	3	0	0	0
1	C	152	1134	719	203	209	3	0	0	0
1	D	152	1134	719	203	209	3	0	0	0
1	E	152	1134	719	203	209	3	0	0	0
1	F	152	1134	719	203	209	3	0	0	0
1	G	152	1134	719	203	209	3	0	0	0
1	H	152	1134	719	203	209	3	0	0	0
1	I	152	1134	719	203	209	3	0	0	0
1	J	152	1134	719	203	209	3	0	0	0
1	K	152	1134	719	203	209	3	0	0	0
1	L	152	1134	719	203	209	3	0	0	0
1	M	152	1134	719	203	209	3	0	0	0
1	N	152	1134	719	203	209	3	0	0	0
1	O	152	1134	719	203	209	3	0	0	0
1	P	152	1134	719	203	209	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	152	1134	719	203	209	3	0	0	0
			Total	C	N	O	S			
1	R	152	1134	719	203	209	3	0	0	0
			Total	C	N	O	S			
1	S	152	1134	719	203	209	3	0	0	0
			Total	C	N	O	S			
1	T	152	1134	719	203	209	3	0	0	0

There are 260 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	expression tag	UNP Q2SZ09
A	28	GLY	-	expression tag	UNP Q2SZ09
A	86	GLU	ASP	engineered mutation	UNP Q2SZ09
A	87	ASP	ALA	engineered mutation	UNP Q2SZ09
A	90	LEU	ALA	engineered mutation	UNP Q2SZ09
A	93	ALA	ASP	engineered mutation	UNP Q2SZ09
A	94	LEU	GLY	engineered mutation	UNP Q2SZ09
A	97	VAL	ALA	engineered mutation	UNP Q2SZ09
A	136	LYS	VAL	engineered mutation	UNP Q2SZ09
A	146	ILE	ALA	engineered mutation	UNP Q2SZ09
A	149	ALA	ARG	engineered mutation	UNP Q2SZ09
A	150	ALA	ARG	engineered mutation	UNP Q2SZ09
A	154	LEU	ARG	engineered mutation	UNP Q2SZ09
B	27	MET	-	expression tag	UNP Q2SZ09
B	28	GLY	-	expression tag	UNP Q2SZ09
B	86	GLU	ASP	engineered mutation	UNP Q2SZ09
B	87	ASP	ALA	engineered mutation	UNP Q2SZ09
B	90	LEU	ALA	engineered mutation	UNP Q2SZ09
B	93	ALA	ASP	engineered mutation	UNP Q2SZ09
B	94	LEU	GLY	engineered mutation	UNP Q2SZ09
B	97	VAL	ALA	engineered mutation	UNP Q2SZ09
B	136	LYS	VAL	engineered mutation	UNP Q2SZ09
B	146	ILE	ALA	engineered mutation	UNP Q2SZ09
B	149	ALA	ARG	engineered mutation	UNP Q2SZ09
B	150	ALA	ARG	engineered mutation	UNP Q2SZ09
B	154	LEU	ARG	engineered mutation	UNP Q2SZ09
C	27	MET	-	expression tag	UNP Q2SZ09
C	28	GLY	-	expression tag	UNP Q2SZ09
C	86	GLU	ASP	engineered mutation	UNP Q2SZ09
C	87	ASP	ALA	engineered mutation	UNP Q2SZ09
C	90	LEU	ALA	engineered mutation	UNP Q2SZ09

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Chain	Residue	Modelled	Actual	Comment	Reference
C	93	ALA	ASP	engineered mutation	UNP Q2SZ09
C	94	LEU	GLY	engineered mutation	UNP Q2SZ09
C	97	VAL	ALA	engineered mutation	UNP Q2SZ09
C	136	LYS	VAL	engineered mutation	UNP Q2SZ09
C	146	ILE	ALA	engineered mutation	UNP Q2SZ09
C	149	ALA	ARG	engineered mutation	UNP Q2SZ09
C	150	ALA	ARG	engineered mutation	UNP Q2SZ09
C	154	LEU	ARG	engineered mutation	UNP Q2SZ09
D	27	MET	-	expression tag	UNP Q2SZ09
D	28	GLY	-	expression tag	UNP Q2SZ09
D	86	GLU	ASP	engineered mutation	UNP Q2SZ09
D	87	ASP	ALA	engineered mutation	UNP Q2SZ09
D	90	LEU	ALA	engineered mutation	UNP Q2SZ09
D	93	ALA	ASP	engineered mutation	UNP Q2SZ09
D	94	LEU	GLY	engineered mutation	UNP Q2SZ09
D	97	VAL	ALA	engineered mutation	UNP Q2SZ09
D	136	LYS	VAL	engineered mutation	UNP Q2SZ09
D	146	ILE	ALA	engineered mutation	UNP Q2SZ09
D	149	ALA	ARG	engineered mutation	UNP Q2SZ09
D	150	ALA	ARG	engineered mutation	UNP Q2SZ09
D	154	LEU	ARG	engineered mutation	UNP Q2SZ09
E	27	MET	-	expression tag	UNP Q2SZ09
E	28	GLY	-	expression tag	UNP Q2SZ09
E	86	GLU	ASP	engineered mutation	UNP Q2SZ09
E	87	ASP	ALA	engineered mutation	UNP Q2SZ09
E	90	LEU	ALA	engineered mutation	UNP Q2SZ09
E	93	ALA	ASP	engineered mutation	UNP Q2SZ09
E	94	LEU	GLY	engineered mutation	UNP Q2SZ09
E	97	VAL	ALA	engineered mutation	UNP Q2SZ09
E	136	LYS	VAL	engineered mutation	UNP Q2SZ09
E	146	ILE	ALA	engineered mutation	UNP Q2SZ09
E	149	ALA	ARG	engineered mutation	UNP Q2SZ09
E	150	ALA	ARG	engineered mutation	UNP Q2SZ09
E	154	LEU	ARG	engineered mutation	UNP Q2SZ09
F	27	MET	-	expression tag	UNP Q2SZ09
F	28	GLY	-	expression tag	UNP Q2SZ09
F	86	GLU	ASP	engineered mutation	UNP Q2SZ09
F	87	ASP	ALA	engineered mutation	UNP Q2SZ09
F	90	LEU	ALA	engineered mutation	UNP Q2SZ09
F	93	ALA	ASP	engineered mutation	UNP Q2SZ09
F	94	LEU	GLY	engineered mutation	UNP Q2SZ09
F	97	VAL	ALA	engineered mutation	UNP Q2SZ09

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Chain	Residue	Modelled	Actual	Comment	Reference
F	136	LYS	VAL	engineered mutation	UNP Q2SZ09
F	146	ILE	ALA	engineered mutation	UNP Q2SZ09
F	149	ALA	ARG	engineered mutation	UNP Q2SZ09
F	150	ALA	ARG	engineered mutation	UNP Q2SZ09
F	154	LEU	ARG	engineered mutation	UNP Q2SZ09
G	27	MET	-	expression tag	UNP Q2SZ09
G	28	GLY	-	expression tag	UNP Q2SZ09
G	86	GLU	ASP	engineered mutation	UNP Q2SZ09
G	87	ASP	ALA	engineered mutation	UNP Q2SZ09
G	90	LEU	ALA	engineered mutation	UNP Q2SZ09
G	93	ALA	ASP	engineered mutation	UNP Q2SZ09
G	94	LEU	GLY	engineered mutation	UNP Q2SZ09
G	97	VAL	ALA	engineered mutation	UNP Q2SZ09
G	136	LYS	VAL	engineered mutation	UNP Q2SZ09
G	146	ILE	ALA	engineered mutation	UNP Q2SZ09
G	149	ALA	ARG	engineered mutation	UNP Q2SZ09
G	150	ALA	ARG	engineered mutation	UNP Q2SZ09
G	154	LEU	ARG	engineered mutation	UNP Q2SZ09
H	27	MET	-	expression tag	UNP Q2SZ09
H	28	GLY	-	expression tag	UNP Q2SZ09
H	86	GLU	ASP	engineered mutation	UNP Q2SZ09
H	87	ASP	ALA	engineered mutation	UNP Q2SZ09
H	90	LEU	ALA	engineered mutation	UNP Q2SZ09
H	93	ALA	ASP	engineered mutation	UNP Q2SZ09
H	94	LEU	GLY	engineered mutation	UNP Q2SZ09
H	97	VAL	ALA	engineered mutation	UNP Q2SZ09
H	136	LYS	VAL	engineered mutation	UNP Q2SZ09
H	146	ILE	ALA	engineered mutation	UNP Q2SZ09
H	149	ALA	ARG	engineered mutation	UNP Q2SZ09
H	150	ALA	ARG	engineered mutation	UNP Q2SZ09
H	154	LEU	ARG	engineered mutation	UNP Q2SZ09
I	27	MET	-	expression tag	UNP Q2SZ09
I	28	GLY	-	expression tag	UNP Q2SZ09
I	86	GLU	ASP	engineered mutation	UNP Q2SZ09
I	87	ASP	ALA	engineered mutation	UNP Q2SZ09
I	90	LEU	ALA	engineered mutation	UNP Q2SZ09
I	93	ALA	ASP	engineered mutation	UNP Q2SZ09
I	94	LEU	GLY	engineered mutation	UNP Q2SZ09
I	97	VAL	ALA	engineered mutation	UNP Q2SZ09
I	136	LYS	VAL	engineered mutation	UNP Q2SZ09
I	146	ILE	ALA	engineered mutation	UNP Q2SZ09
I	149	ALA	ARG	engineered mutation	UNP Q2SZ09

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Chain	Residue	Modelled	Actual	Comment	Reference
I	150	ALA	ARG	engineered mutation	UNP Q2SZ09
I	154	LEU	ARG	engineered mutation	UNP Q2SZ09
J	27	MET	-	expression tag	UNP Q2SZ09
J	28	GLY	-	expression tag	UNP Q2SZ09
J	86	GLU	ASP	engineered mutation	UNP Q2SZ09
J	87	ASP	ALA	engineered mutation	UNP Q2SZ09
J	90	LEU	ALA	engineered mutation	UNP Q2SZ09
J	93	ALA	ASP	engineered mutation	UNP Q2SZ09
J	94	LEU	GLY	engineered mutation	UNP Q2SZ09
J	97	VAL	ALA	engineered mutation	UNP Q2SZ09
J	136	LYS	VAL	engineered mutation	UNP Q2SZ09
J	146	ILE	ALA	engineered mutation	UNP Q2SZ09
J	149	ALA	ARG	engineered mutation	UNP Q2SZ09
J	150	ALA	ARG	engineered mutation	UNP Q2SZ09
J	154	LEU	ARG	engineered mutation	UNP Q2SZ09
K	27	MET	-	expression tag	UNP Q2SZ09
K	28	GLY	-	expression tag	UNP Q2SZ09
K	86	GLU	ASP	engineered mutation	UNP Q2SZ09
K	87	ASP	ALA	engineered mutation	UNP Q2SZ09
K	90	LEU	ALA	engineered mutation	UNP Q2SZ09
K	93	ALA	ASP	engineered mutation	UNP Q2SZ09
K	94	LEU	GLY	engineered mutation	UNP Q2SZ09
K	97	VAL	ALA	engineered mutation	UNP Q2SZ09
K	136	LYS	VAL	engineered mutation	UNP Q2SZ09
K	146	ILE	ALA	engineered mutation	UNP Q2SZ09
K	149	ALA	ARG	engineered mutation	UNP Q2SZ09
K	150	ALA	ARG	engineered mutation	UNP Q2SZ09
K	154	LEU	ARG	engineered mutation	UNP Q2SZ09
L	27	MET	-	expression tag	UNP Q2SZ09
L	28	GLY	-	expression tag	UNP Q2SZ09
L	86	GLU	ASP	engineered mutation	UNP Q2SZ09
L	87	ASP	ALA	engineered mutation	UNP Q2SZ09
L	90	LEU	ALA	engineered mutation	UNP Q2SZ09
L	93	ALA	ASP	engineered mutation	UNP Q2SZ09
L	94	LEU	GLY	engineered mutation	UNP Q2SZ09
L	97	VAL	ALA	engineered mutation	UNP Q2SZ09
L	136	LYS	VAL	engineered mutation	UNP Q2SZ09
L	146	ILE	ALA	engineered mutation	UNP Q2SZ09
L	149	ALA	ARG	engineered mutation	UNP Q2SZ09
L	150	ALA	ARG	engineered mutation	UNP Q2SZ09
L	154	LEU	ARG	engineered mutation	UNP Q2SZ09
M	27	MET	-	expression tag	UNP Q2SZ09

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Chain	Residue	Modelled	Actual	Comment	Reference
M	28	GLY	-	expression tag	UNP Q2SZ09
M	86	GLU	ASP	engineered mutation	UNP Q2SZ09
M	87	ASP	ALA	engineered mutation	UNP Q2SZ09
M	90	LEU	ALA	engineered mutation	UNP Q2SZ09
M	93	ALA	ASP	engineered mutation	UNP Q2SZ09
M	94	LEU	GLY	engineered mutation	UNP Q2SZ09
M	97	VAL	ALA	engineered mutation	UNP Q2SZ09
M	136	LYS	VAL	engineered mutation	UNP Q2SZ09
M	146	ILE	ALA	engineered mutation	UNP Q2SZ09
M	149	ALA	ARG	engineered mutation	UNP Q2SZ09
M	150	ALA	ARG	engineered mutation	UNP Q2SZ09
M	154	LEU	ARG	engineered mutation	UNP Q2SZ09
N	27	MET	-	expression tag	UNP Q2SZ09
N	28	GLY	-	expression tag	UNP Q2SZ09
N	86	GLU	ASP	engineered mutation	UNP Q2SZ09
N	87	ASP	ALA	engineered mutation	UNP Q2SZ09
N	90	LEU	ALA	engineered mutation	UNP Q2SZ09
N	93	ALA	ASP	engineered mutation	UNP Q2SZ09
N	94	LEU	GLY	engineered mutation	UNP Q2SZ09
N	97	VAL	ALA	engineered mutation	UNP Q2SZ09
N	136	LYS	VAL	engineered mutation	UNP Q2SZ09
N	146	ILE	ALA	engineered mutation	UNP Q2SZ09
N	149	ALA	ARG	engineered mutation	UNP Q2SZ09
N	150	ALA	ARG	engineered mutation	UNP Q2SZ09
N	154	LEU	ARG	engineered mutation	UNP Q2SZ09
O	27	MET	-	expression tag	UNP Q2SZ09
O	28	GLY	-	expression tag	UNP Q2SZ09
O	86	GLU	ASP	engineered mutation	UNP Q2SZ09
O	87	ASP	ALA	engineered mutation	UNP Q2SZ09
O	90	LEU	ALA	engineered mutation	UNP Q2SZ09
O	93	ALA	ASP	engineered mutation	UNP Q2SZ09
O	94	LEU	GLY	engineered mutation	UNP Q2SZ09
O	97	VAL	ALA	engineered mutation	UNP Q2SZ09
O	136	LYS	VAL	engineered mutation	UNP Q2SZ09
O	146	ILE	ALA	engineered mutation	UNP Q2SZ09
O	149	ALA	ARG	engineered mutation	UNP Q2SZ09
O	150	ALA	ARG	engineered mutation	UNP Q2SZ09
O	154	LEU	ARG	engineered mutation	UNP Q2SZ09
P	27	MET	-	expression tag	UNP Q2SZ09
P	28	GLY	-	expression tag	UNP Q2SZ09
P	86	GLU	ASP	engineered mutation	UNP Q2SZ09
P	87	ASP	ALA	engineered mutation	UNP Q2SZ09

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Chain	Residue	Modelled	Actual	Comment	Reference
P	90	LEU	ALA	engineered mutation	UNP Q2SZ09
P	93	ALA	ASP	engineered mutation	UNP Q2SZ09
P	94	LEU	GLY	engineered mutation	UNP Q2SZ09
P	97	VAL	ALA	engineered mutation	UNP Q2SZ09
P	136	LYS	VAL	engineered mutation	UNP Q2SZ09
P	146	ILE	ALA	engineered mutation	UNP Q2SZ09
P	149	ALA	ARG	engineered mutation	UNP Q2SZ09
P	150	ALA	ARG	engineered mutation	UNP Q2SZ09
P	154	LEU	ARG	engineered mutation	UNP Q2SZ09
Q	27	MET	-	expression tag	UNP Q2SZ09
Q	28	GLY	-	expression tag	UNP Q2SZ09
Q	86	GLU	ASP	engineered mutation	UNP Q2SZ09
Q	87	ASP	ALA	engineered mutation	UNP Q2SZ09
Q	90	LEU	ALA	engineered mutation	UNP Q2SZ09
Q	93	ALA	ASP	engineered mutation	UNP Q2SZ09
Q	94	LEU	GLY	engineered mutation	UNP Q2SZ09
Q	97	VAL	ALA	engineered mutation	UNP Q2SZ09
Q	136	LYS	VAL	engineered mutation	UNP Q2SZ09
Q	146	ILE	ALA	engineered mutation	UNP Q2SZ09
Q	149	ALA	ARG	engineered mutation	UNP Q2SZ09
Q	150	ALA	ARG	engineered mutation	UNP Q2SZ09
Q	154	LEU	ARG	engineered mutation	UNP Q2SZ09
R	27	MET	-	expression tag	UNP Q2SZ09
R	28	GLY	-	expression tag	UNP Q2SZ09
R	86	GLU	ASP	engineered mutation	UNP Q2SZ09
R	87	ASP	ALA	engineered mutation	UNP Q2SZ09
R	90	LEU	ALA	engineered mutation	UNP Q2SZ09
R	93	ALA	ASP	engineered mutation	UNP Q2SZ09
R	94	LEU	GLY	engineered mutation	UNP Q2SZ09
R	97	VAL	ALA	engineered mutation	UNP Q2SZ09
R	136	LYS	VAL	engineered mutation	UNP Q2SZ09
R	146	ILE	ALA	engineered mutation	UNP Q2SZ09
R	149	ALA	ARG	engineered mutation	UNP Q2SZ09
R	150	ALA	ARG	engineered mutation	UNP Q2SZ09
R	154	LEU	ARG	engineered mutation	UNP Q2SZ09
S	27	MET	-	expression tag	UNP Q2SZ09
S	28	GLY	-	expression tag	UNP Q2SZ09
S	86	GLU	ASP	engineered mutation	UNP Q2SZ09
S	87	ASP	ALA	engineered mutation	UNP Q2SZ09
S	90	LEU	ALA	engineered mutation	UNP Q2SZ09
S	93	ALA	ASP	engineered mutation	UNP Q2SZ09
S	94	LEU	GLY	engineered mutation	UNP Q2SZ09

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Chain	Residue	Modelled	Actual	Comment	Reference
S	97	VAL	ALA	engineered mutation	UNP Q2SZ09
S	136	LYS	VAL	engineered mutation	UNP Q2SZ09
S	146	ILE	ALA	engineered mutation	UNP Q2SZ09
S	149	ALA	ARG	engineered mutation	UNP Q2SZ09
S	150	ALA	ARG	engineered mutation	UNP Q2SZ09
S	154	LEU	ARG	engineered mutation	UNP Q2SZ09
T	27	MET	-	expression tag	UNP Q2SZ09
T	28	GLY	-	expression tag	UNP Q2SZ09
T	86	GLU	ASP	engineered mutation	UNP Q2SZ09
T	87	ASP	ALA	engineered mutation	UNP Q2SZ09
T	90	LEU	ALA	engineered mutation	UNP Q2SZ09
T	93	ALA	ASP	engineered mutation	UNP Q2SZ09
T	94	LEU	GLY	engineered mutation	UNP Q2SZ09
T	97	VAL	ALA	engineered mutation	UNP Q2SZ09
T	136	LYS	VAL	engineered mutation	UNP Q2SZ09
T	146	ILE	ALA	engineered mutation	UNP Q2SZ09
T	149	ALA	ARG	engineered mutation	UNP Q2SZ09
T	150	ALA	ARG	engineered mutation	UNP Q2SZ09
T	154	LEU	ARG	engineered mutation	UNP Q2SZ09

- Molecule 2 is a protein called Designed self-assembling icosahedral cage I32-28 dimeric subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	U	148	1077	684	193	197	3	0	0	0
2	V	148	1077	684	193	197	3	0	0	0
2	W	148	1077	684	193	197	3	0	0	0
2	X	148	1077	684	193	197	3	0	0	0
2	Y	148	1077	684	193	197	3	0	0	0
2	Z	148	1077	684	193	197	3	0	0	0
2	a	148	1077	684	193	197	3	0	0	0
2	b	148	1077	684	193	197	3	0	0	0
2	c	148	1077	684	193	197	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	d	148	1077	684	193	197	3	0	0	0
2	e	148	1077	684	193	197	3	0	0	0
2	f	148	1077	684	193	197	3	0	0	0
2	g	148	1077	684	193	197	3	0	0	0
2	h	148	1077	684	193	197	3	0	0	0
2	i	148	1077	684	193	197	3	0	0	0
2	j	148	1077	684	193	197	3	0	0	0
2	k	148	1077	684	193	197	3	0	0	0
2	l	148	1077	684	193	197	3	0	0	0
2	m	148	1077	684	193	197	3	0	0	0
2	n	148	1077	684	193	197	3	0	0	0

There are 360 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	35	GLN	ARG	engineered mutation	UNP Q9RSW5
U	36	ARG	PHE	engineered mutation	UNP Q9RSW5
U	54	ARG	THR	engineered mutation	UNP Q9RSW5
U	122	GLU	TRP	engineered mutation	UNP Q9RSW5
U	129	VAL	LYS	engineered mutation	UNP Q9RSW5
U	137	VAL	ARG	engineered mutation	UNP Q9RSW5
U	140	LEU	GLU	engineered mutation	UNP Q9RSW5
U	141	LEU	ARG	engineered mutation	UNP Q9RSW5
U	144	MET	LYS	engineered mutation	UNP Q9RSW5
U	148	GLN	GLU	engineered mutation	UNP Q9RSW5
U	158	LEU	-	expression tag	UNP Q9RSW5
U	159	GLU	-	expression tag	UNP Q9RSW5
U	160	HIS	-	expression tag	UNP Q9RSW5
U	161	HIS	-	expression tag	UNP Q9RSW5
U	162	HIS	-	expression tag	UNP Q9RSW5
U	163	HIS	-	expression tag	UNP Q9RSW5
U	164	HIS	-	expression tag	UNP Q9RSW5

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Chain	Residue	Modelled	Actual	Comment	Reference
U	165	HIS	-	expression tag	UNP Q9RSW5
V	35	GLN	ARG	engineered mutation	UNP Q9RSW5
V	36	ARG	PHE	engineered mutation	UNP Q9RSW5
V	54	ARG	THR	engineered mutation	UNP Q9RSW5
V	122	GLU	TRP	engineered mutation	UNP Q9RSW5
V	129	VAL	LYS	engineered mutation	UNP Q9RSW5
V	137	VAL	ARG	engineered mutation	UNP Q9RSW5
V	140	LEU	GLU	engineered mutation	UNP Q9RSW5
V	141	LEU	ARG	engineered mutation	UNP Q9RSW5
V	144	MET	LYS	engineered mutation	UNP Q9RSW5
V	148	GLN	GLU	engineered mutation	UNP Q9RSW5
V	158	LEU	-	expression tag	UNP Q9RSW5
V	159	GLU	-	expression tag	UNP Q9RSW5
V	160	HIS	-	expression tag	UNP Q9RSW5
V	161	HIS	-	expression tag	UNP Q9RSW5
V	162	HIS	-	expression tag	UNP Q9RSW5
V	163	HIS	-	expression tag	UNP Q9RSW5
V	164	HIS	-	expression tag	UNP Q9RSW5
V	165	HIS	-	expression tag	UNP Q9RSW5
W	35	GLN	ARG	engineered mutation	UNP Q9RSW5
W	36	ARG	PHE	engineered mutation	UNP Q9RSW5
W	54	ARG	THR	engineered mutation	UNP Q9RSW5
W	122	GLU	TRP	engineered mutation	UNP Q9RSW5
W	129	VAL	LYS	engineered mutation	UNP Q9RSW5
W	137	VAL	ARG	engineered mutation	UNP Q9RSW5
W	140	LEU	GLU	engineered mutation	UNP Q9RSW5
W	141	LEU	ARG	engineered mutation	UNP Q9RSW5
W	144	MET	LYS	engineered mutation	UNP Q9RSW5
W	148	GLN	GLU	engineered mutation	UNP Q9RSW5
W	158	LEU	-	expression tag	UNP Q9RSW5
W	159	GLU	-	expression tag	UNP Q9RSW5
W	160	HIS	-	expression tag	UNP Q9RSW5
W	161	HIS	-	expression tag	UNP Q9RSW5
W	162	HIS	-	expression tag	UNP Q9RSW5
W	163	HIS	-	expression tag	UNP Q9RSW5
W	164	HIS	-	expression tag	UNP Q9RSW5
W	165	HIS	-	expression tag	UNP Q9RSW5
X	35	GLN	ARG	engineered mutation	UNP Q9RSW5
X	36	ARG	PHE	engineered mutation	UNP Q9RSW5
X	54	ARG	THR	engineered mutation	UNP Q9RSW5
X	122	GLU	TRP	engineered mutation	UNP Q9RSW5
X	129	VAL	LYS	engineered mutation	UNP Q9RSW5

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Chain	Residue	Modelled	Actual	Comment	Reference
X	137	VAL	ARG	engineered mutation	UNP Q9RSW5
X	140	LEU	GLU	engineered mutation	UNP Q9RSW5
X	141	LEU	ARG	engineered mutation	UNP Q9RSW5
X	144	MET	LYS	engineered mutation	UNP Q9RSW5
X	148	GLN	GLU	engineered mutation	UNP Q9RSW5
X	158	LEU	-	expression tag	UNP Q9RSW5
X	159	GLU	-	expression tag	UNP Q9RSW5
X	160	HIS	-	expression tag	UNP Q9RSW5
X	161	HIS	-	expression tag	UNP Q9RSW5
X	162	HIS	-	expression tag	UNP Q9RSW5
X	163	HIS	-	expression tag	UNP Q9RSW5
X	164	HIS	-	expression tag	UNP Q9RSW5
X	165	HIS	-	expression tag	UNP Q9RSW5
Y	35	GLN	ARG	engineered mutation	UNP Q9RSW5
Y	36	ARG	PHE	engineered mutation	UNP Q9RSW5
Y	54	ARG	THR	engineered mutation	UNP Q9RSW5
Y	122	GLU	TRP	engineered mutation	UNP Q9RSW5
Y	129	VAL	LYS	engineered mutation	UNP Q9RSW5
Y	137	VAL	ARG	engineered mutation	UNP Q9RSW5
Y	140	LEU	GLU	engineered mutation	UNP Q9RSW5
Y	141	LEU	ARG	engineered mutation	UNP Q9RSW5
Y	144	MET	LYS	engineered mutation	UNP Q9RSW5
Y	148	GLN	GLU	engineered mutation	UNP Q9RSW5
Y	158	LEU	-	expression tag	UNP Q9RSW5
Y	159	GLU	-	expression tag	UNP Q9RSW5
Y	160	HIS	-	expression tag	UNP Q9RSW5
Y	161	HIS	-	expression tag	UNP Q9RSW5
Y	162	HIS	-	expression tag	UNP Q9RSW5
Y	163	HIS	-	expression tag	UNP Q9RSW5
Y	164	HIS	-	expression tag	UNP Q9RSW5
Y	165	HIS	-	expression tag	UNP Q9RSW5
Z	35	GLN	ARG	engineered mutation	UNP Q9RSW5
Z	36	ARG	PHE	engineered mutation	UNP Q9RSW5
Z	54	ARG	THR	engineered mutation	UNP Q9RSW5
Z	122	GLU	TRP	engineered mutation	UNP Q9RSW5
Z	129	VAL	LYS	engineered mutation	UNP Q9RSW5
Z	137	VAL	ARG	engineered mutation	UNP Q9RSW5
Z	140	LEU	GLU	engineered mutation	UNP Q9RSW5
Z	141	LEU	ARG	engineered mutation	UNP Q9RSW5
Z	144	MET	LYS	engineered mutation	UNP Q9RSW5
Z	148	GLN	GLU	engineered mutation	UNP Q9RSW5
Z	158	LEU	-	expression tag	UNP Q9RSW5

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	159	GLU	-	expression tag	UNP Q9RSW5
Z	160	HIS	-	expression tag	UNP Q9RSW5
Z	161	HIS	-	expression tag	UNP Q9RSW5
Z	162	HIS	-	expression tag	UNP Q9RSW5
Z	163	HIS	-	expression tag	UNP Q9RSW5
Z	164	HIS	-	expression tag	UNP Q9RSW5
Z	165	HIS	-	expression tag	UNP Q9RSW5
a	35	GLN	ARG	engineered mutation	UNP Q9RSW5
a	36	ARG	PHE	engineered mutation	UNP Q9RSW5
a	54	ARG	THR	engineered mutation	UNP Q9RSW5
a	122	GLU	TRP	engineered mutation	UNP Q9RSW5
a	129	VAL	LYS	engineered mutation	UNP Q9RSW5
a	137	VAL	ARG	engineered mutation	UNP Q9RSW5
a	140	LEU	GLU	engineered mutation	UNP Q9RSW5
a	141	LEU	ARG	engineered mutation	UNP Q9RSW5
a	144	MET	LYS	engineered mutation	UNP Q9RSW5
a	148	GLN	GLU	engineered mutation	UNP Q9RSW5
a	158	LEU	-	expression tag	UNP Q9RSW5
a	159	GLU	-	expression tag	UNP Q9RSW5
a	160	HIS	-	expression tag	UNP Q9RSW5
a	161	HIS	-	expression tag	UNP Q9RSW5
a	162	HIS	-	expression tag	UNP Q9RSW5
a	163	HIS	-	expression tag	UNP Q9RSW5
a	164	HIS	-	expression tag	UNP Q9RSW5
a	165	HIS	-	expression tag	UNP Q9RSW5
b	35	GLN	ARG	engineered mutation	UNP Q9RSW5
b	36	ARG	PHE	engineered mutation	UNP Q9RSW5
b	54	ARG	THR	engineered mutation	UNP Q9RSW5
b	122	GLU	TRP	engineered mutation	UNP Q9RSW5
b	129	VAL	LYS	engineered mutation	UNP Q9RSW5
b	137	VAL	ARG	engineered mutation	UNP Q9RSW5
b	140	LEU	GLU	engineered mutation	UNP Q9RSW5
b	141	LEU	ARG	engineered mutation	UNP Q9RSW5
b	144	MET	LYS	engineered mutation	UNP Q9RSW5
b	148	GLN	GLU	engineered mutation	UNP Q9RSW5
b	158	LEU	-	expression tag	UNP Q9RSW5
b	159	GLU	-	expression tag	UNP Q9RSW5
b	160	HIS	-	expression tag	UNP Q9RSW5
b	161	HIS	-	expression tag	UNP Q9RSW5
b	162	HIS	-	expression tag	UNP Q9RSW5
b	163	HIS	-	expression tag	UNP Q9RSW5
b	164	HIS	-	expression tag	UNP Q9RSW5

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Chain	Residue	Modelled	Actual	Comment	Reference
b	165	HIS	-	expression tag	UNP Q9RSW5
c	35	GLN	ARG	engineered mutation	UNP Q9RSW5
c	36	ARG	PHE	engineered mutation	UNP Q9RSW5
c	54	ARG	THR	engineered mutation	UNP Q9RSW5
c	122	GLU	TRP	engineered mutation	UNP Q9RSW5
c	129	VAL	LYS	engineered mutation	UNP Q9RSW5
c	137	VAL	ARG	engineered mutation	UNP Q9RSW5
c	140	LEU	GLU	engineered mutation	UNP Q9RSW5
c	141	LEU	ARG	engineered mutation	UNP Q9RSW5
c	144	MET	LYS	engineered mutation	UNP Q9RSW5
c	148	GLN	GLU	engineered mutation	UNP Q9RSW5
c	158	LEU	-	expression tag	UNP Q9RSW5
c	159	GLU	-	expression tag	UNP Q9RSW5
c	160	HIS	-	expression tag	UNP Q9RSW5
c	161	HIS	-	expression tag	UNP Q9RSW5
c	162	HIS	-	expression tag	UNP Q9RSW5
c	163	HIS	-	expression tag	UNP Q9RSW5
c	164	HIS	-	expression tag	UNP Q9RSW5
c	165	HIS	-	expression tag	UNP Q9RSW5
d	35	GLN	ARG	engineered mutation	UNP Q9RSW5
d	36	ARG	PHE	engineered mutation	UNP Q9RSW5
d	54	ARG	THR	engineered mutation	UNP Q9RSW5
d	122	GLU	TRP	engineered mutation	UNP Q9RSW5
d	129	VAL	LYS	engineered mutation	UNP Q9RSW5
d	137	VAL	ARG	engineered mutation	UNP Q9RSW5
d	140	LEU	GLU	engineered mutation	UNP Q9RSW5
d	141	LEU	ARG	engineered mutation	UNP Q9RSW5
d	144	MET	LYS	engineered mutation	UNP Q9RSW5
d	148	GLN	GLU	engineered mutation	UNP Q9RSW5
d	158	LEU	-	expression tag	UNP Q9RSW5
d	159	GLU	-	expression tag	UNP Q9RSW5
d	160	HIS	-	expression tag	UNP Q9RSW5
d	161	HIS	-	expression tag	UNP Q9RSW5
d	162	HIS	-	expression tag	UNP Q9RSW5
d	163	HIS	-	expression tag	UNP Q9RSW5
d	164	HIS	-	expression tag	UNP Q9RSW5
d	165	HIS	-	expression tag	UNP Q9RSW5
e	35	GLN	ARG	engineered mutation	UNP Q9RSW5
e	36	ARG	PHE	engineered mutation	UNP Q9RSW5
e	54	ARG	THR	engineered mutation	UNP Q9RSW5
e	122	GLU	TRP	engineered mutation	UNP Q9RSW5
e	129	VAL	LYS	engineered mutation	UNP Q9RSW5

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Chain	Residue	Modelled	Actual	Comment	Reference
e	137	VAL	ARG	engineered mutation	UNP Q9RSW5
e	140	LEU	GLU	engineered mutation	UNP Q9RSW5
e	141	LEU	ARG	engineered mutation	UNP Q9RSW5
e	144	MET	LYS	engineered mutation	UNP Q9RSW5
e	148	GLN	GLU	engineered mutation	UNP Q9RSW5
e	158	LEU	-	expression tag	UNP Q9RSW5
e	159	GLU	-	expression tag	UNP Q9RSW5
e	160	HIS	-	expression tag	UNP Q9RSW5
e	161	HIS	-	expression tag	UNP Q9RSW5
e	162	HIS	-	expression tag	UNP Q9RSW5
e	163	HIS	-	expression tag	UNP Q9RSW5
e	164	HIS	-	expression tag	UNP Q9RSW5
e	165	HIS	-	expression tag	UNP Q9RSW5
f	35	GLN	ARG	engineered mutation	UNP Q9RSW5
f	36	ARG	PHE	engineered mutation	UNP Q9RSW5
f	54	ARG	THR	engineered mutation	UNP Q9RSW5
f	122	GLU	TRP	engineered mutation	UNP Q9RSW5
f	129	VAL	LYS	engineered mutation	UNP Q9RSW5
f	137	VAL	ARG	engineered mutation	UNP Q9RSW5
f	140	LEU	GLU	engineered mutation	UNP Q9RSW5
f	141	LEU	ARG	engineered mutation	UNP Q9RSW5
f	144	MET	LYS	engineered mutation	UNP Q9RSW5
f	148	GLN	GLU	engineered mutation	UNP Q9RSW5
f	158	LEU	-	expression tag	UNP Q9RSW5
f	159	GLU	-	expression tag	UNP Q9RSW5
f	160	HIS	-	expression tag	UNP Q9RSW5
f	161	HIS	-	expression tag	UNP Q9RSW5
f	162	HIS	-	expression tag	UNP Q9RSW5
f	163	HIS	-	expression tag	UNP Q9RSW5
f	164	HIS	-	expression tag	UNP Q9RSW5
f	165	HIS	-	expression tag	UNP Q9RSW5
g	35	GLN	ARG	engineered mutation	UNP Q9RSW5
g	36	ARG	PHE	engineered mutation	UNP Q9RSW5
g	54	ARG	THR	engineered mutation	UNP Q9RSW5
g	122	GLU	TRP	engineered mutation	UNP Q9RSW5
g	129	VAL	LYS	engineered mutation	UNP Q9RSW5
g	137	VAL	ARG	engineered mutation	UNP Q9RSW5
g	140	LEU	GLU	engineered mutation	UNP Q9RSW5
g	141	LEU	ARG	engineered mutation	UNP Q9RSW5
g	144	MET	LYS	engineered mutation	UNP Q9RSW5
g	148	GLN	GLU	engineered mutation	UNP Q9RSW5
g	158	LEU	-	expression tag	UNP Q9RSW5

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Chain	Residue	Modelled	Actual	Comment	Reference
g	159	GLU	-	expression tag	UNP Q9RSW5
g	160	HIS	-	expression tag	UNP Q9RSW5
g	161	HIS	-	expression tag	UNP Q9RSW5
g	162	HIS	-	expression tag	UNP Q9RSW5
g	163	HIS	-	expression tag	UNP Q9RSW5
g	164	HIS	-	expression tag	UNP Q9RSW5
g	165	HIS	-	expression tag	UNP Q9RSW5
h	35	GLN	ARG	engineered mutation	UNP Q9RSW5
h	36	ARG	PHE	engineered mutation	UNP Q9RSW5
h	54	ARG	THR	engineered mutation	UNP Q9RSW5
h	122	GLU	TRP	engineered mutation	UNP Q9RSW5
h	129	VAL	LYS	engineered mutation	UNP Q9RSW5
h	137	VAL	ARG	engineered mutation	UNP Q9RSW5
h	140	LEU	GLU	engineered mutation	UNP Q9RSW5
h	141	LEU	ARG	engineered mutation	UNP Q9RSW5
h	144	MET	LYS	engineered mutation	UNP Q9RSW5
h	148	GLN	GLU	engineered mutation	UNP Q9RSW5
h	158	LEU	-	expression tag	UNP Q9RSW5
h	159	GLU	-	expression tag	UNP Q9RSW5
h	160	HIS	-	expression tag	UNP Q9RSW5
h	161	HIS	-	expression tag	UNP Q9RSW5
h	162	HIS	-	expression tag	UNP Q9RSW5
h	163	HIS	-	expression tag	UNP Q9RSW5
h	164	HIS	-	expression tag	UNP Q9RSW5
h	165	HIS	-	expression tag	UNP Q9RSW5
i	35	GLN	ARG	engineered mutation	UNP Q9RSW5
i	36	ARG	PHE	engineered mutation	UNP Q9RSW5
i	54	ARG	THR	engineered mutation	UNP Q9RSW5
i	122	GLU	TRP	engineered mutation	UNP Q9RSW5
i	129	VAL	LYS	engineered mutation	UNP Q9RSW5
i	137	VAL	ARG	engineered mutation	UNP Q9RSW5
i	140	LEU	GLU	engineered mutation	UNP Q9RSW5
i	141	LEU	ARG	engineered mutation	UNP Q9RSW5
i	144	MET	LYS	engineered mutation	UNP Q9RSW5
i	148	GLN	GLU	engineered mutation	UNP Q9RSW5
i	158	LEU	-	expression tag	UNP Q9RSW5
i	159	GLU	-	expression tag	UNP Q9RSW5
i	160	HIS	-	expression tag	UNP Q9RSW5
i	161	HIS	-	expression tag	UNP Q9RSW5
i	162	HIS	-	expression tag	UNP Q9RSW5
i	163	HIS	-	expression tag	UNP Q9RSW5
i	164	HIS	-	expression tag	UNP Q9RSW5

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Chain	Residue	Modelled	Actual	Comment	Reference
i	165	HIS	-	expression tag	UNP Q9RSW5
j	35	GLN	ARG	engineered mutation	UNP Q9RSW5
j	36	ARG	PHE	engineered mutation	UNP Q9RSW5
j	54	ARG	THR	engineered mutation	UNP Q9RSW5
j	122	GLU	TRP	engineered mutation	UNP Q9RSW5
j	129	VAL	LYS	engineered mutation	UNP Q9RSW5
j	137	VAL	ARG	engineered mutation	UNP Q9RSW5
j	140	LEU	GLU	engineered mutation	UNP Q9RSW5
j	141	LEU	ARG	engineered mutation	UNP Q9RSW5
j	144	MET	LYS	engineered mutation	UNP Q9RSW5
j	148	GLN	GLU	engineered mutation	UNP Q9RSW5
j	158	LEU	-	expression tag	UNP Q9RSW5
j	159	GLU	-	expression tag	UNP Q9RSW5
j	160	HIS	-	expression tag	UNP Q9RSW5
j	161	HIS	-	expression tag	UNP Q9RSW5
j	162	HIS	-	expression tag	UNP Q9RSW5
j	163	HIS	-	expression tag	UNP Q9RSW5
j	164	HIS	-	expression tag	UNP Q9RSW5
j	165	HIS	-	expression tag	UNP Q9RSW5
k	35	GLN	ARG	engineered mutation	UNP Q9RSW5
k	36	ARG	PHE	engineered mutation	UNP Q9RSW5
k	54	ARG	THR	engineered mutation	UNP Q9RSW5
k	122	GLU	TRP	engineered mutation	UNP Q9RSW5
k	129	VAL	LYS	engineered mutation	UNP Q9RSW5
k	137	VAL	ARG	engineered mutation	UNP Q9RSW5
k	140	LEU	GLU	engineered mutation	UNP Q9RSW5
k	141	LEU	ARG	engineered mutation	UNP Q9RSW5
k	144	MET	LYS	engineered mutation	UNP Q9RSW5
k	148	GLN	GLU	engineered mutation	UNP Q9RSW5
k	158	LEU	-	expression tag	UNP Q9RSW5
k	159	GLU	-	expression tag	UNP Q9RSW5
k	160	HIS	-	expression tag	UNP Q9RSW5
k	161	HIS	-	expression tag	UNP Q9RSW5
k	162	HIS	-	expression tag	UNP Q9RSW5
k	163	HIS	-	expression tag	UNP Q9RSW5
k	164	HIS	-	expression tag	UNP Q9RSW5
k	165	HIS	-	expression tag	UNP Q9RSW5
l	35	GLN	ARG	engineered mutation	UNP Q9RSW5
l	36	ARG	PHE	engineered mutation	UNP Q9RSW5
l	54	ARG	THR	engineered mutation	UNP Q9RSW5
l	122	GLU	TRP	engineered mutation	UNP Q9RSW5
l	129	VAL	LYS	engineered mutation	UNP Q9RSW5

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Chain	Residue	Modelled	Actual	Comment	Reference
l	137	VAL	ARG	engineered mutation	UNP Q9RSW5
l	140	LEU	GLU	engineered mutation	UNP Q9RSW5
l	141	LEU	ARG	engineered mutation	UNP Q9RSW5
l	144	MET	LYS	engineered mutation	UNP Q9RSW5
l	148	GLN	GLU	engineered mutation	UNP Q9RSW5
l	158	LEU	-	expression tag	UNP Q9RSW5
l	159	GLU	-	expression tag	UNP Q9RSW5
l	160	HIS	-	expression tag	UNP Q9RSW5
l	161	HIS	-	expression tag	UNP Q9RSW5
l	162	HIS	-	expression tag	UNP Q9RSW5
l	163	HIS	-	expression tag	UNP Q9RSW5
l	164	HIS	-	expression tag	UNP Q9RSW5
l	165	HIS	-	expression tag	UNP Q9RSW5
m	35	GLN	ARG	engineered mutation	UNP Q9RSW5
m	36	ARG	PHE	engineered mutation	UNP Q9RSW5
m	54	ARG	THR	engineered mutation	UNP Q9RSW5
m	122	GLU	TRP	engineered mutation	UNP Q9RSW5
m	129	VAL	LYS	engineered mutation	UNP Q9RSW5
m	137	VAL	ARG	engineered mutation	UNP Q9RSW5
m	140	LEU	GLU	engineered mutation	UNP Q9RSW5
m	141	LEU	ARG	engineered mutation	UNP Q9RSW5
m	144	MET	LYS	engineered mutation	UNP Q9RSW5
m	148	GLN	GLU	engineered mutation	UNP Q9RSW5
m	158	LEU	-	expression tag	UNP Q9RSW5
m	159	GLU	-	expression tag	UNP Q9RSW5
m	160	HIS	-	expression tag	UNP Q9RSW5
m	161	HIS	-	expression tag	UNP Q9RSW5
m	162	HIS	-	expression tag	UNP Q9RSW5
m	163	HIS	-	expression tag	UNP Q9RSW5
m	164	HIS	-	expression tag	UNP Q9RSW5
m	165	HIS	-	expression tag	UNP Q9RSW5
n	35	GLN	ARG	engineered mutation	UNP Q9RSW5
n	36	ARG	PHE	engineered mutation	UNP Q9RSW5
n	54	ARG	THR	engineered mutation	UNP Q9RSW5
n	122	GLU	TRP	engineered mutation	UNP Q9RSW5
n	129	VAL	LYS	engineered mutation	UNP Q9RSW5
n	137	VAL	ARG	engineered mutation	UNP Q9RSW5
n	140	LEU	GLU	engineered mutation	UNP Q9RSW5
n	141	LEU	ARG	engineered mutation	UNP Q9RSW5
n	144	MET	LYS	engineered mutation	UNP Q9RSW5
n	148	GLN	GLU	engineered mutation	UNP Q9RSW5
n	158	LEU	-	expression tag	UNP Q9RSW5

Continued on next page...

Continued from previous page...

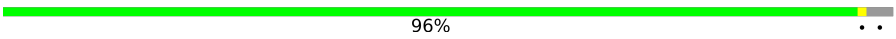
Chain	Residue	Modelled	Actual	Comment	Reference
n	159	GLU	-	expression tag	UNP Q9RSW5
n	160	HIS	-	expression tag	UNP Q9RSW5
n	161	HIS	-	expression tag	UNP Q9RSW5
n	162	HIS	-	expression tag	UNP Q9RSW5
n	163	HIS	-	expression tag	UNP Q9RSW5
n	164	HIS	-	expression tag	UNP Q9RSW5
n	165	HIS	-	expression tag	UNP Q9RSW5

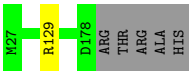
3 Residue-property plots (i)

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

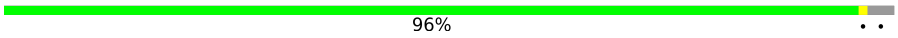
Chain A:

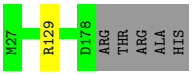




• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

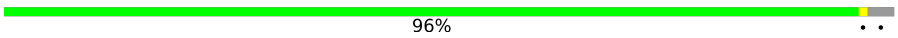
Chain B:

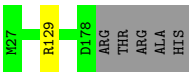




• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

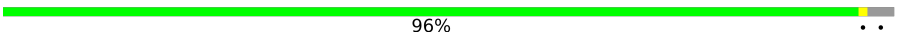
Chain C:

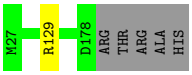




• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

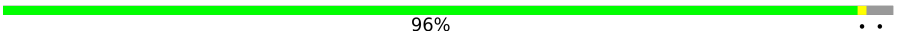
Chain D:

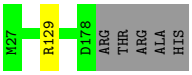




• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

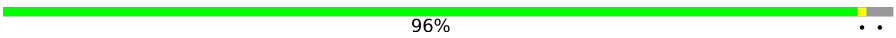
Chain E:

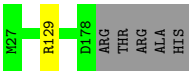




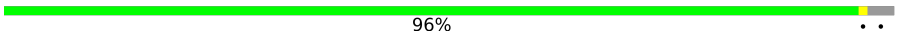
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

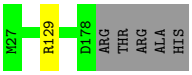
Chain F:



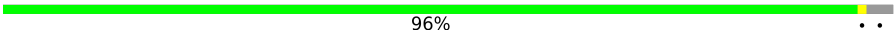


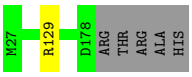
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain G: 

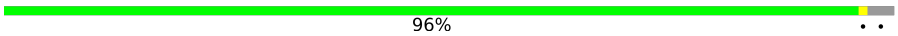


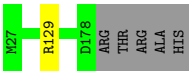
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain H: 

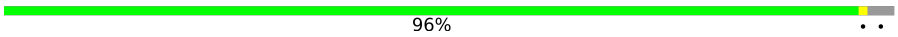


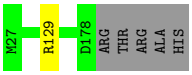
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain I: 

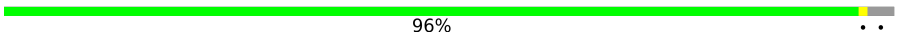


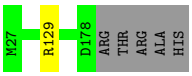
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain J: 

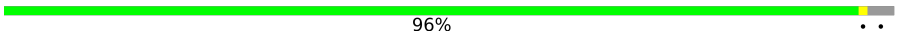


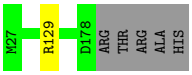
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain K: 

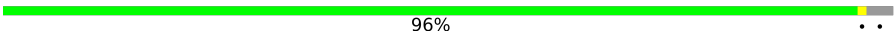


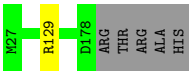
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain L: 



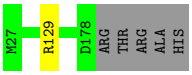
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain M: 



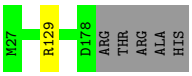
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain N: 96%



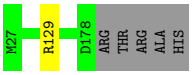
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain O: 96%



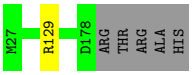
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain P: 96%



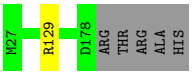
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain Q: 96%



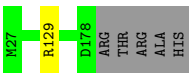
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain R: 96%



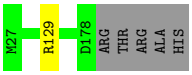
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain S: 96%



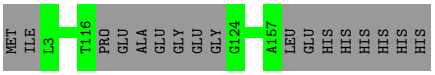
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain T: 96%



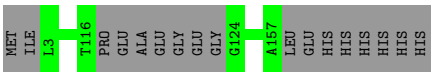
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain U:



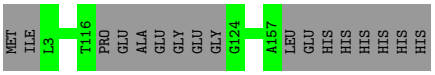
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain V:



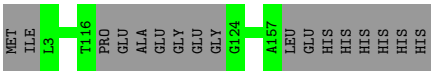
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain W:



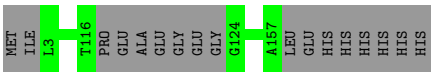
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain X:



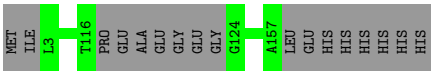
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain Y:



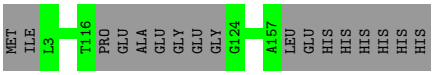
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain Z:



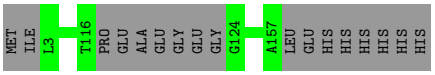
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain a:



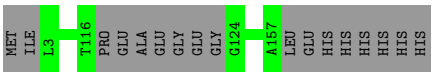
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain b:



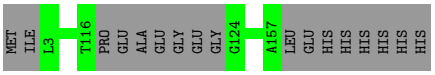
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain c:



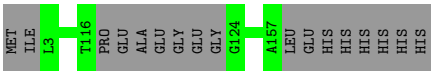
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain d:



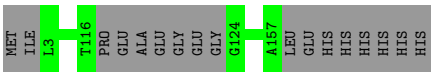
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain e:



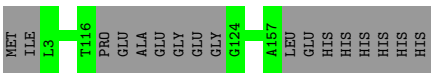
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain f:



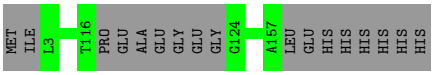
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain g:



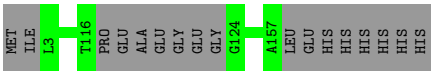
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain h:



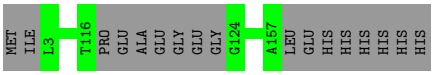
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain i:



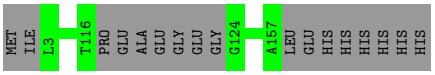
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain j:



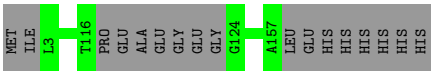
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain k:



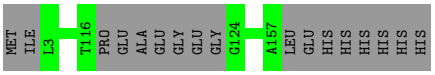
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain l:



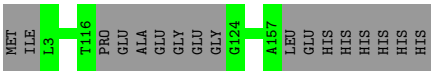
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain m:



• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain n:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	284.17Å 284.17Å 640.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	213.20 – 5.59 213.49 – 5.59	Depositor EDS
% Data completeness (in resolution range)	90.0 (213.20-5.59) 90.2 (213.49-5.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 5.42Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.226 , 0.240 0.232 , 0.244	Depositor DCC
R_{free} test set	5407 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å^2)	317.4	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 443.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.440 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	44220	wwPDB-VP
Average B, all atoms (Å^2)	327.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.34	0/1155	0.51	0/1577
1	B	0.35	0/1155	0.51	0/1577
1	C	0.34	0/1155	0.50	0/1577
1	D	0.34	0/1155	0.51	0/1577
1	E	0.34	0/1155	0.50	0/1577
1	F	0.34	0/1155	0.50	0/1577
1	G	0.34	0/1155	0.51	0/1577
1	H	0.34	0/1155	0.50	0/1577
1	I	0.34	0/1155	0.50	0/1577
1	J	0.34	0/1155	0.51	0/1577
1	K	0.35	0/1155	0.51	0/1577
1	L	0.35	0/1155	0.50	0/1577
1	M	0.35	0/1155	0.51	0/1577
1	N	0.34	0/1155	0.51	0/1577
1	O	0.35	0/1155	0.50	0/1577
1	P	0.34	0/1155	0.50	0/1577
1	Q	0.35	0/1155	0.51	0/1577
1	R	0.34	0/1155	0.51	0/1577
1	S	0.34	0/1155	0.51	0/1577
1	T	0.34	0/1155	0.51	0/1577
2	U	0.62	0/1097	0.54	0/1494
2	V	0.62	0/1097	0.55	0/1494
2	W	0.62	0/1097	0.55	0/1494
2	X	0.62	0/1097	0.55	0/1494
2	Y	0.62	0/1097	0.55	0/1494
2	Z	0.62	0/1097	0.55	0/1494
2	a	0.63	0/1097	0.55	0/1494
2	b	0.62	0/1097	0.55	0/1494
2	c	0.62	0/1097	0.54	0/1494
2	d	0.62	0/1097	0.55	0/1494
2	e	0.62	0/1097	0.55	0/1494
2	f	0.62	0/1097	0.55	0/1494
2	g	0.62	0/1097	0.55	0/1494
2	h	0.62	0/1097	0.55	0/1494

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	i	0.62	0/1097	0.55	0/1494
2	j	0.62	0/1097	0.55	0/1494
2	k	0.62	0/1097	0.55	0/1494
2	l	0.62	0/1097	0.55	0/1494
2	m	0.62	0/1097	0.55	0/1494
2	n	0.62	0/1097	0.55	0/1494
All	All	0.50	0/45040	0.53	0/61420

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
1	B	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
1	C	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
1	D	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
1	E	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
1	F	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
1	G	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
1	H	150/157 (96%)	149 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
1	J	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
1	K	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
1	L	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
1	M	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
1	N	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
1	O	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
1	P	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
1	Q	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
1	R	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
1	S	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
1	T	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
2	U	144/165 (87%)	142 (99%)	2 (1%)	0	100	100
2	V	144/165 (87%)	142 (99%)	2 (1%)	0	100	100
2	W	144/165 (87%)	142 (99%)	2 (1%)	0	100	100
2	X	144/165 (87%)	142 (99%)	2 (1%)	0	100	100
2	Y	144/165 (87%)	142 (99%)	2 (1%)	0	100	100
2	Z	144/165 (87%)	142 (99%)	2 (1%)	0	100	100
2	a	144/165 (87%)	142 (99%)	2 (1%)	0	100	100
2	b	144/165 (87%)	142 (99%)	2 (1%)	0	100	100
2	c	144/165 (87%)	142 (99%)	2 (1%)	0	100	100
2	d	144/165 (87%)	142 (99%)	2 (1%)	0	100	100
2	e	144/165 (87%)	142 (99%)	2 (1%)	0	100	100
2	f	144/165 (87%)	142 (99%)	2 (1%)	0	100	100
2	g	144/165 (87%)	142 (99%)	2 (1%)	0	100	100
2	h	144/165 (87%)	142 (99%)	2 (1%)	0	100	100
2	i	144/165 (87%)	142 (99%)	2 (1%)	0	100	100
2	j	144/165 (87%)	142 (99%)	2 (1%)	0	100	100
2	k	144/165 (87%)	142 (99%)	2 (1%)	0	100	100
2	l	144/165 (87%)	142 (99%)	2 (1%)	0	100	100
2	m	144/165 (87%)	142 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	n	144/165 (87%)	142 (99%)	2 (1%)	0	100	100
All	All	5880/6440 (91%)	5820 (99%)	60 (1%)	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	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	B	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	C	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	D	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	E	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	F	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	G	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	H	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	I	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	J	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	K	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	L	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	M	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	N	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	O	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	P	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	Q	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	R	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	S	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	T	114/119 (96%)	113 (99%)	1 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	U	102/118 (86%)	102 (100%)	0	100	100
2	V	102/118 (86%)	102 (100%)	0	100	100
2	W	102/118 (86%)	102 (100%)	0	100	100
2	X	102/118 (86%)	102 (100%)	0	100	100
2	Y	102/118 (86%)	102 (100%)	0	100	100
2	Z	102/118 (86%)	102 (100%)	0	100	100
2	a	102/118 (86%)	102 (100%)	0	100	100
2	b	102/118 (86%)	102 (100%)	0	100	100
2	c	102/118 (86%)	102 (100%)	0	100	100
2	d	102/118 (86%)	102 (100%)	0	100	100
2	e	102/118 (86%)	102 (100%)	0	100	100
2	f	102/118 (86%)	102 (100%)	0	100	100
2	g	102/118 (86%)	102 (100%)	0	100	100
2	h	102/118 (86%)	102 (100%)	0	100	100
2	i	102/118 (86%)	102 (100%)	0	100	100
2	j	102/118 (86%)	102 (100%)	0	100	100
2	k	102/118 (86%)	102 (100%)	0	100	100
2	l	102/118 (86%)	102 (100%)	0	100	100
2	m	102/118 (86%)	102 (100%)	0	100	100
2	n	102/118 (86%)	102 (100%)	0	100	100
All	All	4320/4740 (91%)	4300 (100%)	20 (0%)	88	93

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ARG
1	B	129	ARG
1	C	129	ARG
1	D	129	ARG
1	E	129	ARG
1	F	129	ARG
1	G	129	ARG
1	H	129	ARG
1	I	129	ARG
1	J	129	ARG

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Mol	Chain	Res	Type
1	K	129	ARG
1	L	129	ARG
1	M	129	ARG
1	N	129	ARG
1	O	129	ARG
1	P	129	ARG
1	Q	129	ARG
1	R	129	ARG
1	S	129	ARG
1	T	129	ARG

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.