Full wwPDB X-ray Structure Validation Report (i)

Aug 1, 2016 – 04:36 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

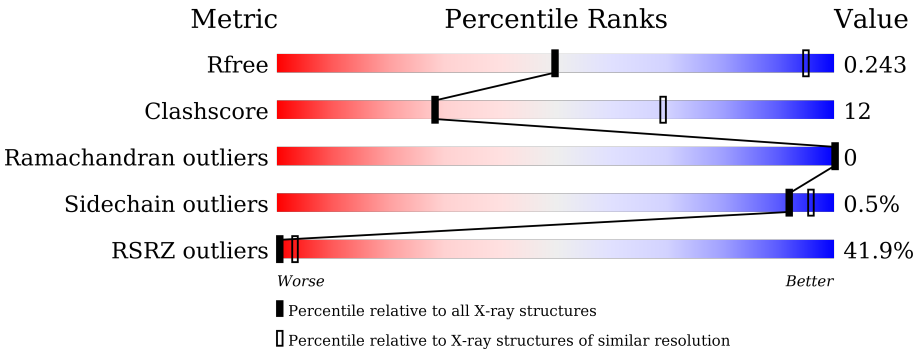
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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}	91344	1001 (7.50-3.64)
Clashscore	102246	1024 (7.40-3.70)
Ramachandran outliers	100387	1007 (7.50-3.66)
Sidechain outliers	100360	1021 (7.54-3.62)
RSRZ outliers	91569	1000 (7.50-3.64)

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. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	157	54% 83% 14% ·
1	B	157	38% 85% 11% ·
1	C	157	32% 85% 11% ·
1	D	157	51% 83% 14% ·
1	E	157	41% 84% 13% ·
1	F	157	55% 84% 13% ·

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Mol	Chain	Length	Quality of chain
1	G	157	44% 88% 9%
1	H	157	18% 89% 8%
1	I	157	40% 89% 8%
1	J	157	34% 88% 9%
1	K	157	46% 87% 10%
1	L	157	34% 89% 8%
1	M	157	34% 87% 10%
1	N	157	52% 87% 10%
1	O	157	46% 88% 9%
1	P	157	48% 88% 9%
1	Q	157	47% 88% 9%
1	R	157	17% 87% 10%
1	S	157	38% 89% 8%
1	T	157	35% 87% 10%
2	U	165	36% 75% 15% 10%
2	V	165	32% 74% 16% 10%
2	W	165	44% 70% 20% 10%
2	X	165	33% 75% 15% 10%
2	Y	165	38% 69% 21% 10%
2	Z	165	57% 75% 15% 10%
2	a	165	38% 90% 10%
2	b	165	16% 90% 10%
2	c	165	33% 90% 10%
2	d	165	53% 90% 10%
2	e	165	33% 90% 10%

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Mol	Chain	Length	Quality of chain
2	f	165	39% 90% 10%
2	g	165	44% 90% 10%
2	h	165	32% 90% 10%
2	i	165	36% 90% 10%
2	j	165	56% 90% 10%
2	k	165	32% 90% 10%
2	l	165	19% 90% 10%
2	m	165	39% 90% 10%
2	n	165	47% 90% 10%

2 Entry composition

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
1	A	152	Total	C	N	O	S	0	0	0
			1134	719	203	209	3			
1	B	152	Total	C	N	O	S	0	0	0
			1134	719	203	209	3			
1	C	152	Total	C	N	O	S	0	0	0
			1134	719	203	209	3			
1	D	152	Total	C	N	O	S	0	0	0
			1134	719	203	209	3			
1	E	152	Total	C	N	O	S	0	0	0
			1134	719	203	209	3			
1	F	152	Total	C	N	O	S	0	0	0
			1134	719	203	209	3			
1	G	152	Total	C	N	O	S	0	0	0
			1134	719	203	209	3			
1	H	152	Total	C	N	O	S	0	0	0
			1134	719	203	209	3			
1	I	152	Total	C	N	O	S	0	0	0
			1134	719	203	209	3			
1	J	152	Total	C	N	O	S	0	0	0
			1134	719	203	209	3			
1	K	152	Total	C	N	O	S	0	0	0
			1134	719	203	209	3			
1	L	152	Total	C	N	O	S	0	0	0
			1134	719	203	209	3			
1	M	152	Total	C	N	O	S	0	0	0
			1134	719	203	209	3			
1	N	152	Total	C	N	O	S	0	0	0
			1134	719	203	209	3			
1	O	152	Total	C	N	O	S	0	0	0
			1134	719	203	209	3			
1	P	152	Total	C	N	O	S	0	0	0
			1134	719	203	209	3			

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

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
2	U	148	Total	C	N	O	S	0	0	0
			1077	684	193	197	3			
2	V	148	Total	C	N	O	S	0	0	0
			1077	684	193	197	3			
2	W	148	Total	C	N	O	S	0	0	0
			1077	684	193	197	3			
2	X	148	Total	C	N	O	S	0	0	0
			1077	684	193	197	3			
2	Y	148	Total	C	N	O	S	0	0	0
			1077	684	193	197	3			
2	Z	148	Total	C	N	O	S	0	0	0
			1077	684	193	197	3			
2	a	148	Total	C	N	O	S	0	0	0
			1077	684	193	197	3			
2	b	148	Total	C	N	O	S	0	0	0
			1077	684	193	197	3			
2	c	148	Total	C	N	O	S	0	0	0
			1077	684	193	197	3			

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

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

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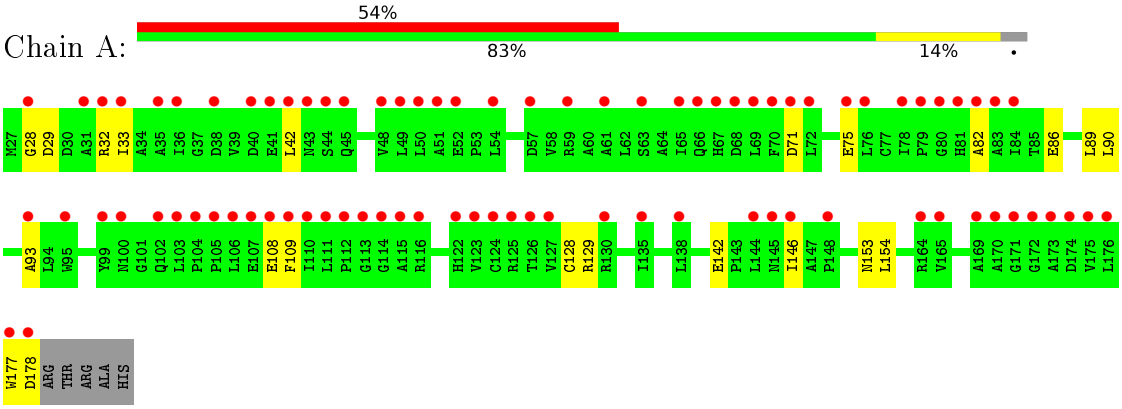
Chain	Residue	Modelled	Actual	Comment	Reference
n	159	GLU	-	expression tag	UNP Q9RSW5
n	160	HIS	-	expression tag	UNP Q9RSW5
n	161	HIS	-	expression tag	UNP Q9RSW5
n	162	HIS	-	expression tag	UNP Q9RSW5
n	163	HIS	-	expression tag	UNP Q9RSW5
n	164	HIS	-	expression tag	UNP Q9RSW5
n	165	HIS	-	expression tag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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA 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.

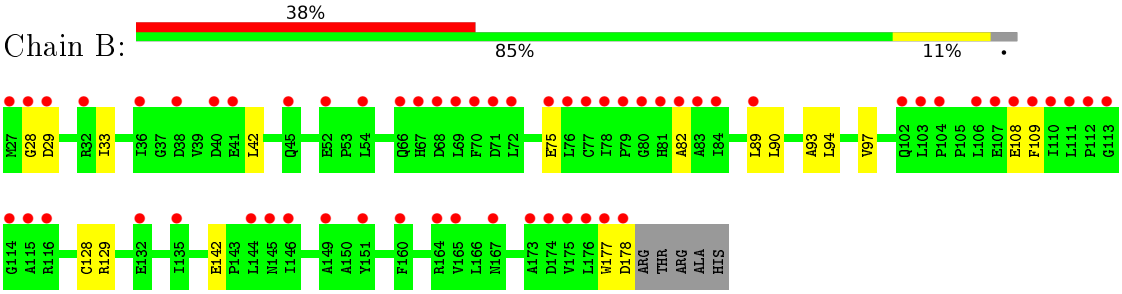
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain A:



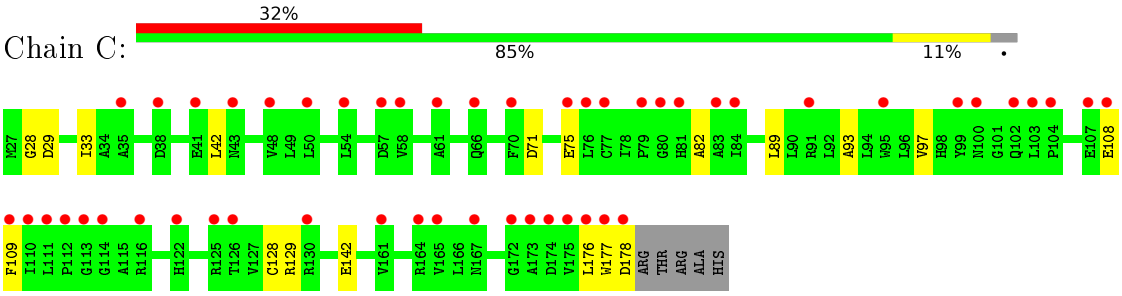
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain B:



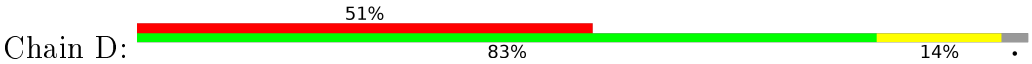
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

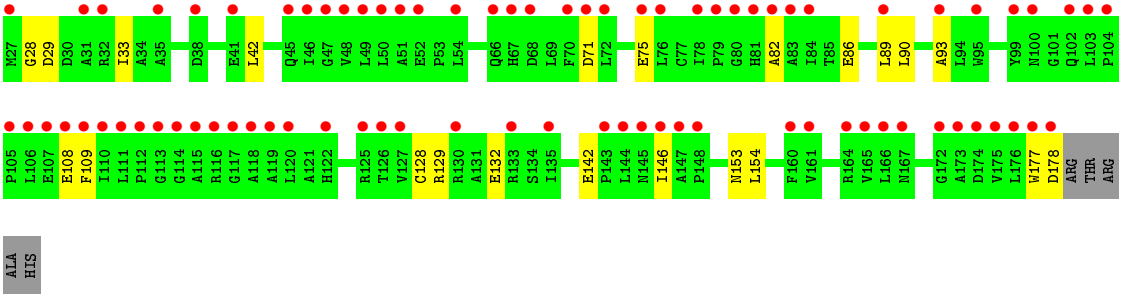
Chain C:



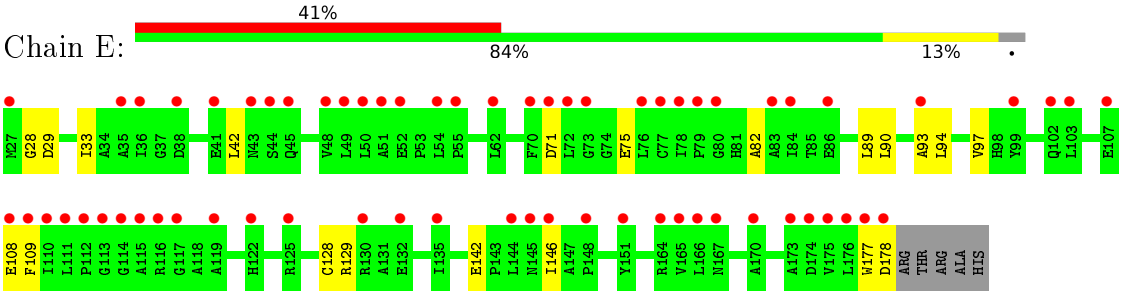
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain D:

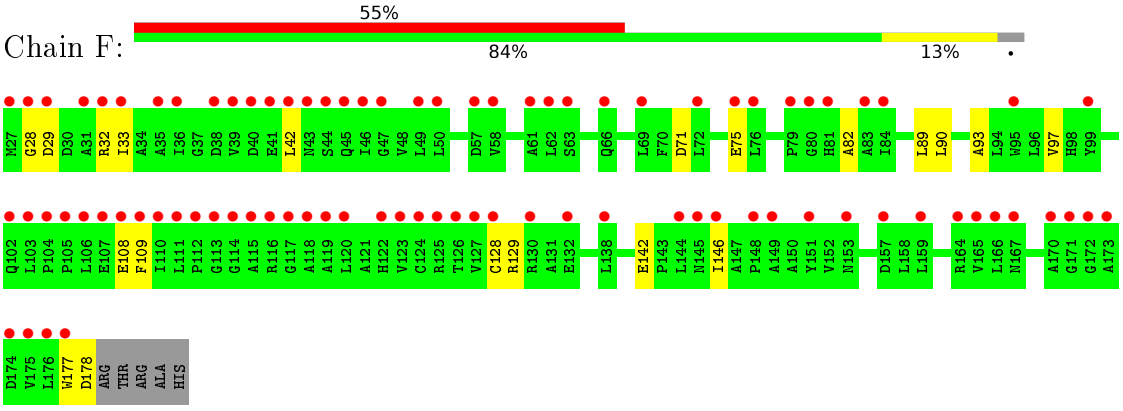




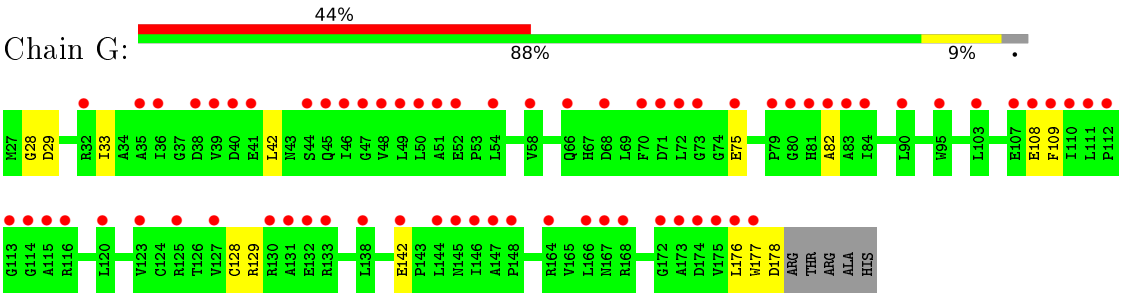
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit



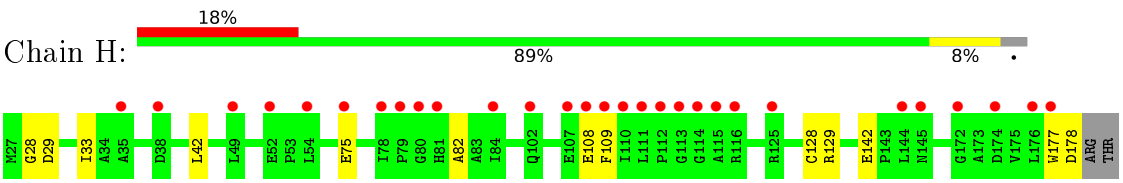
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit



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

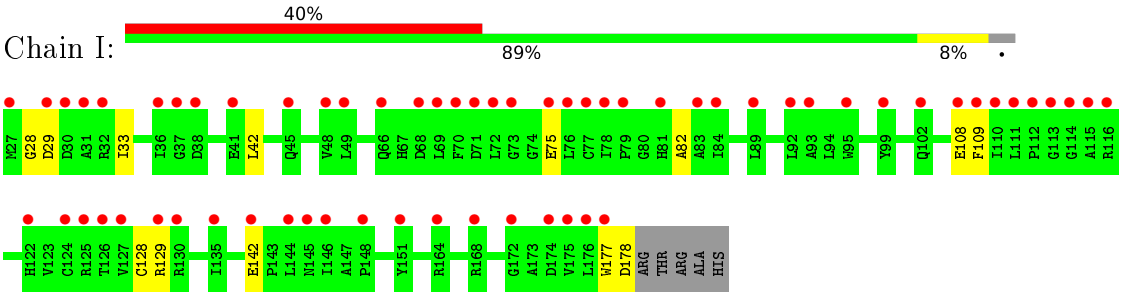


• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit



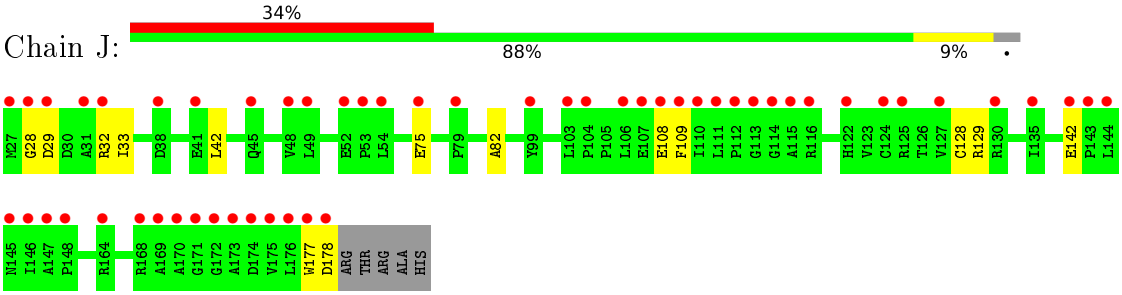
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain I:



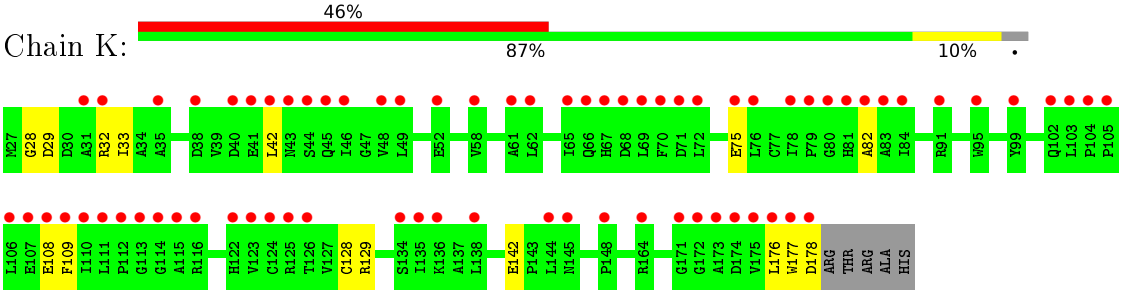
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain J:



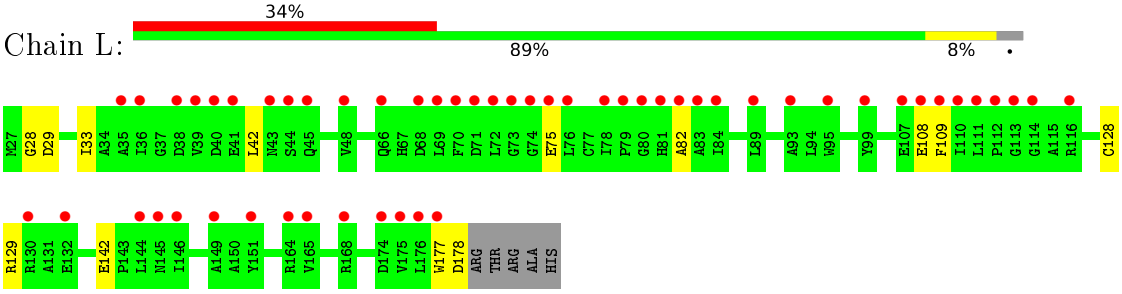
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain K:



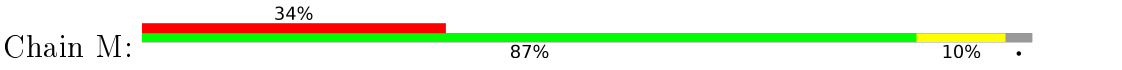
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

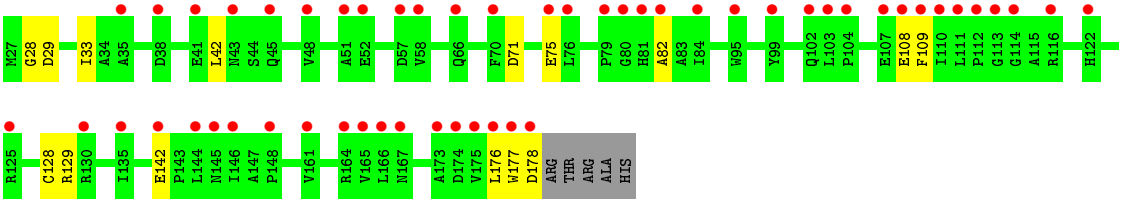
Chain L:



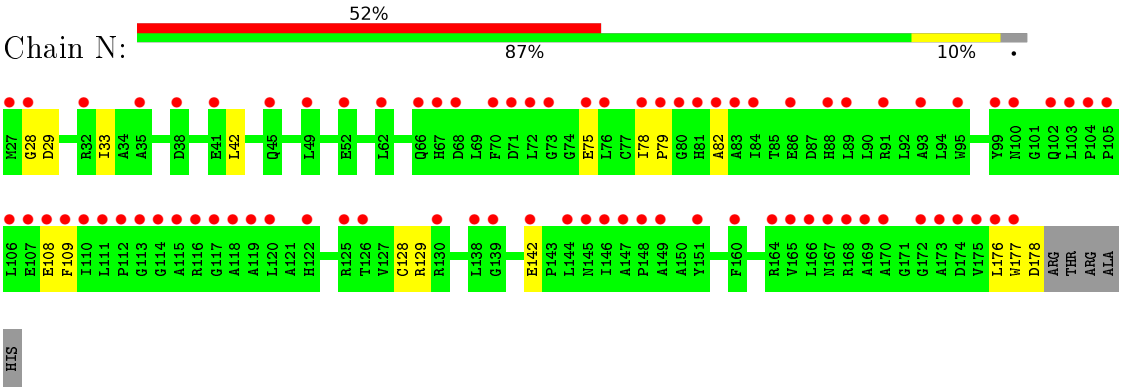
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

Chain M:

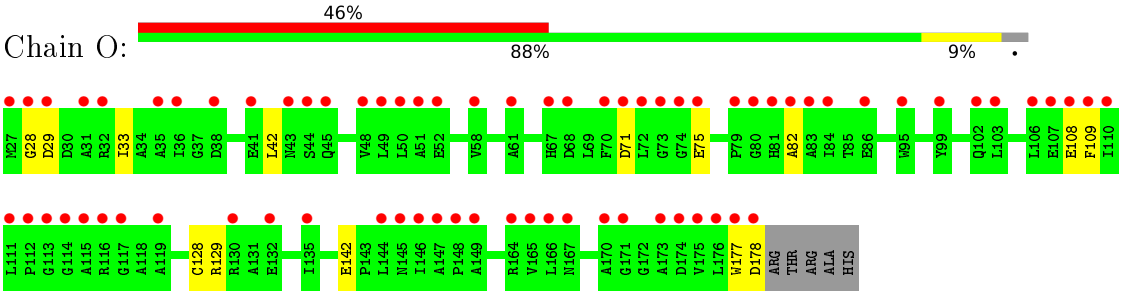




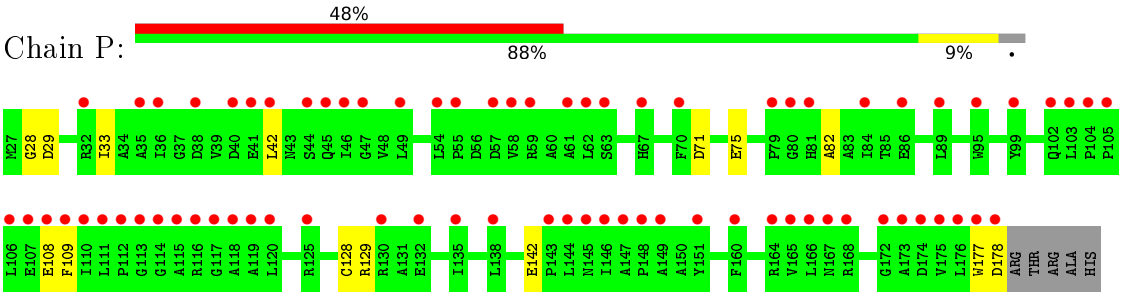
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit



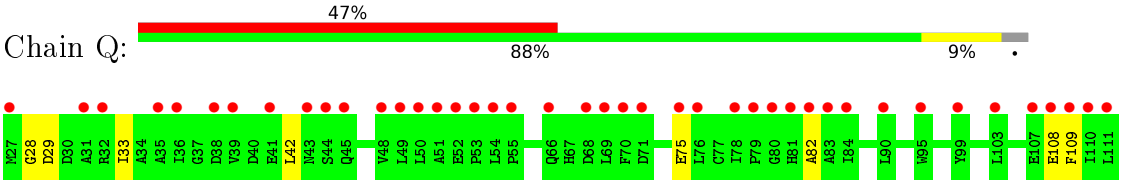
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

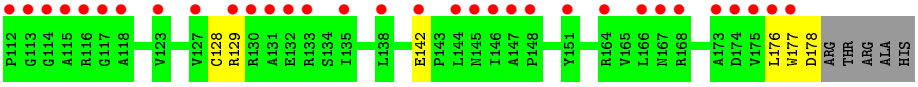


• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

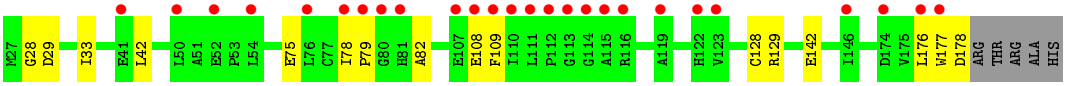


• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

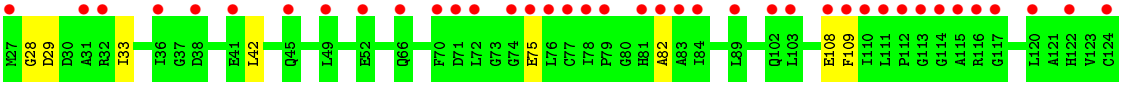


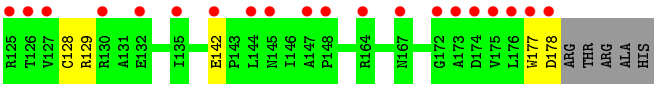


• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

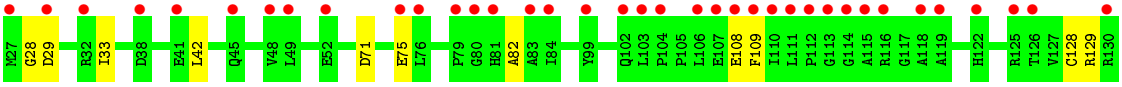


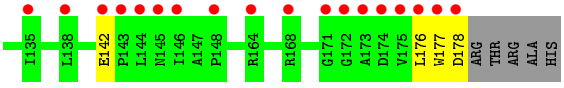
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit



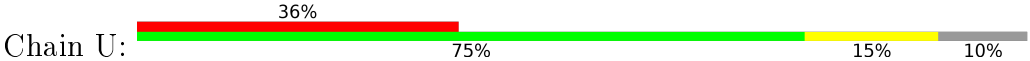


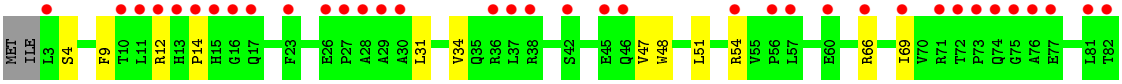
• Molecule 1: Designed self-assembling icosahedral cage I32-28 trimeric subunit

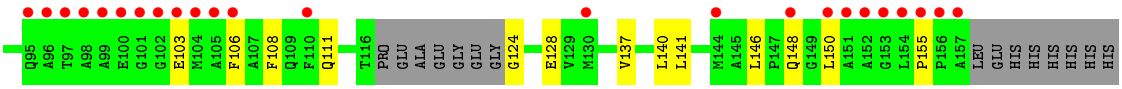




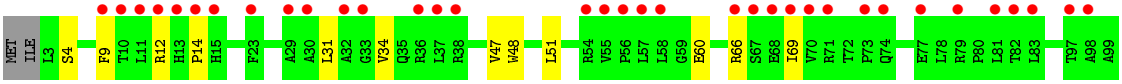
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

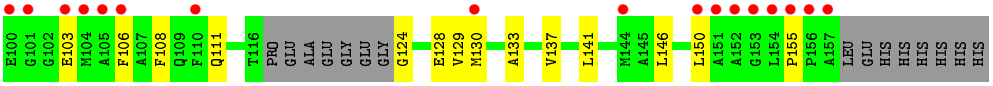






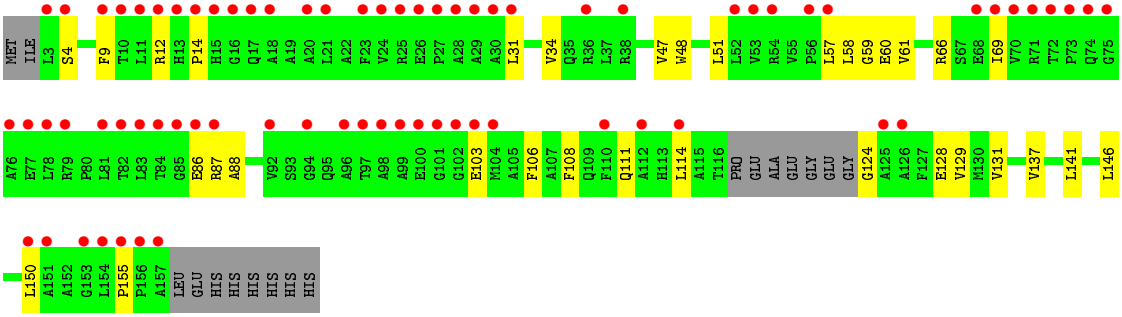
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit





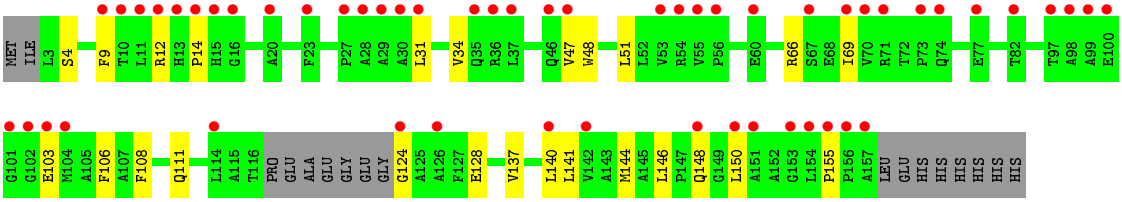
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain W:



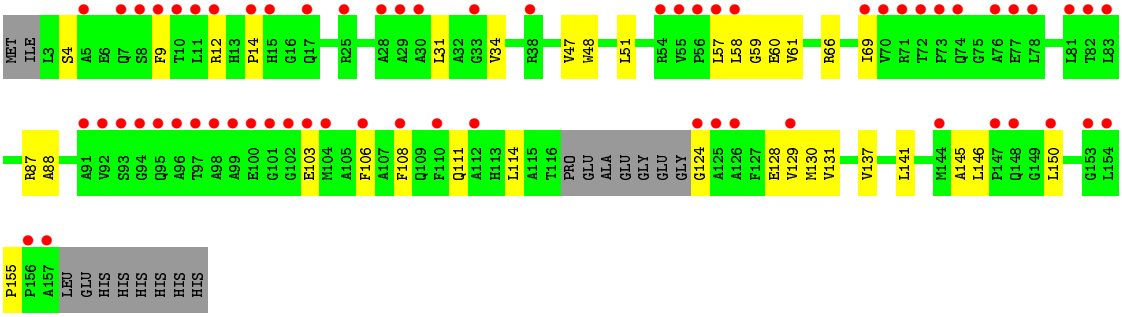
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain X:



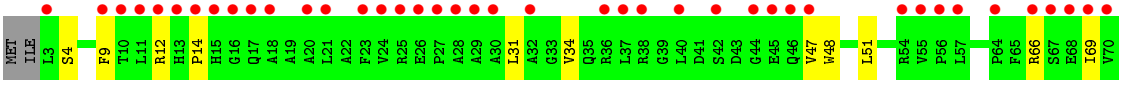
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

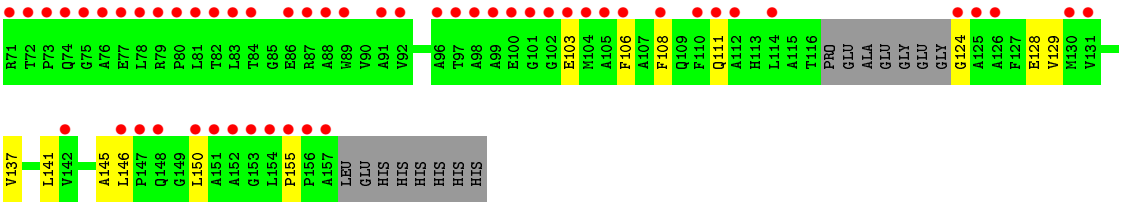
Chain Y:



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

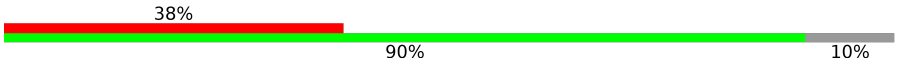
Chain Z:

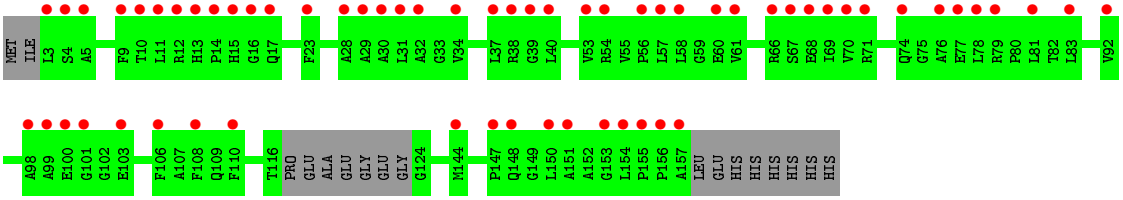




• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

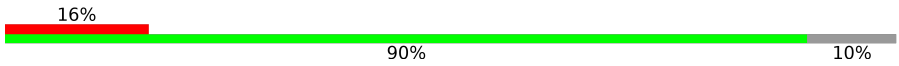
Chain a:

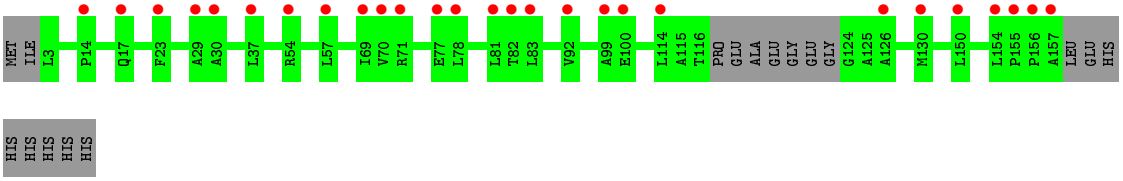




• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

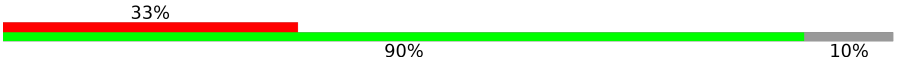
Chain b:

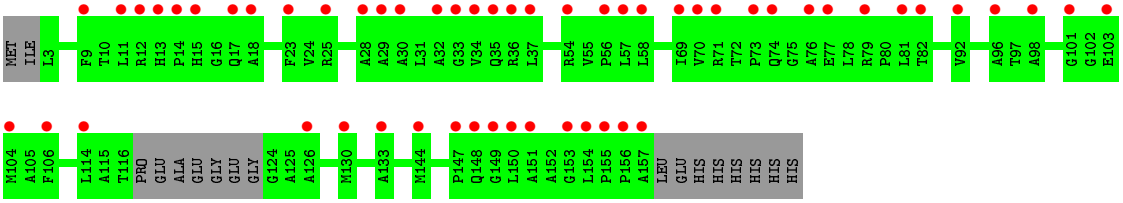




• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

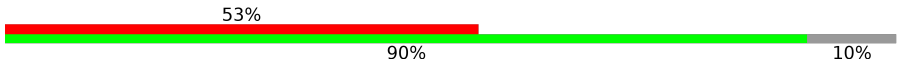
Chain c:

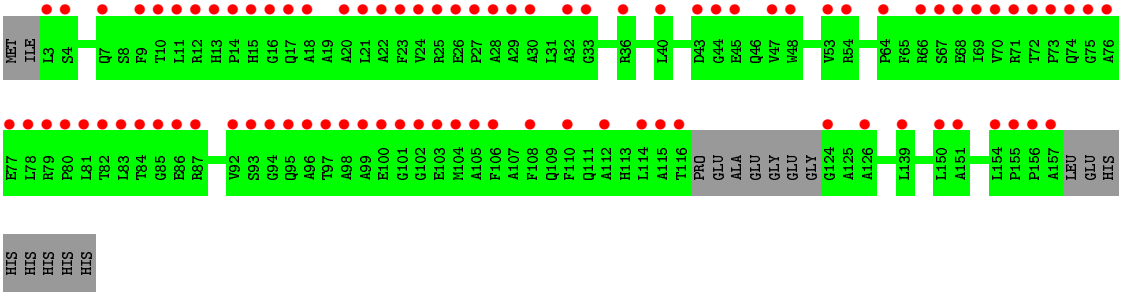




• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

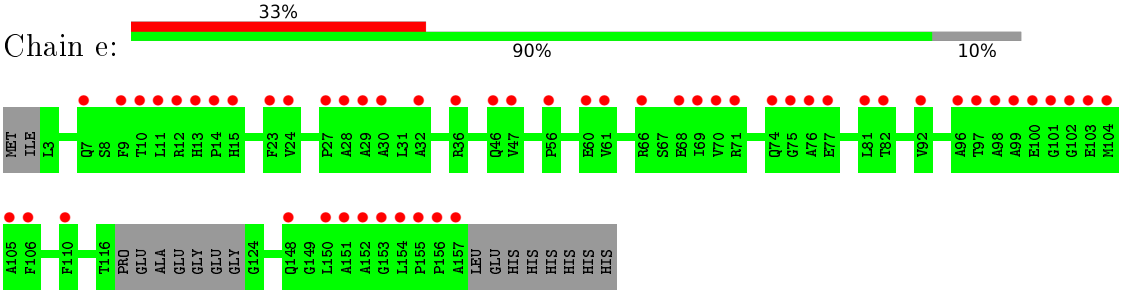
Chain d:





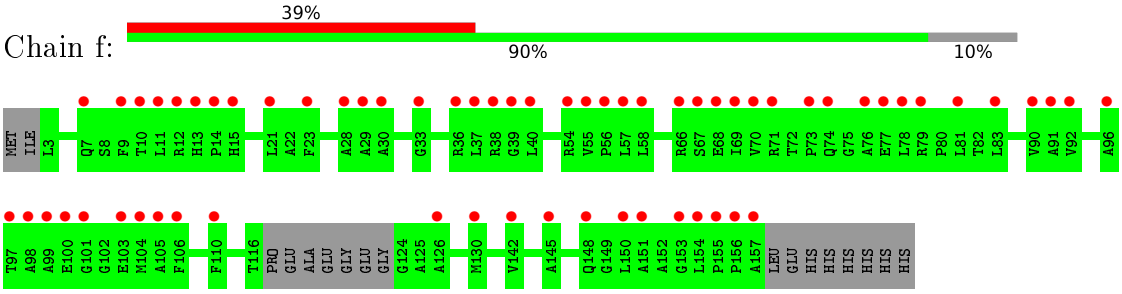
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain e:



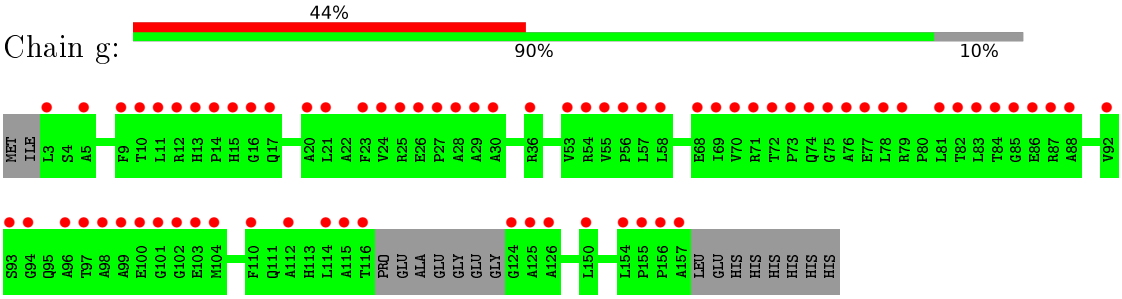
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain f:



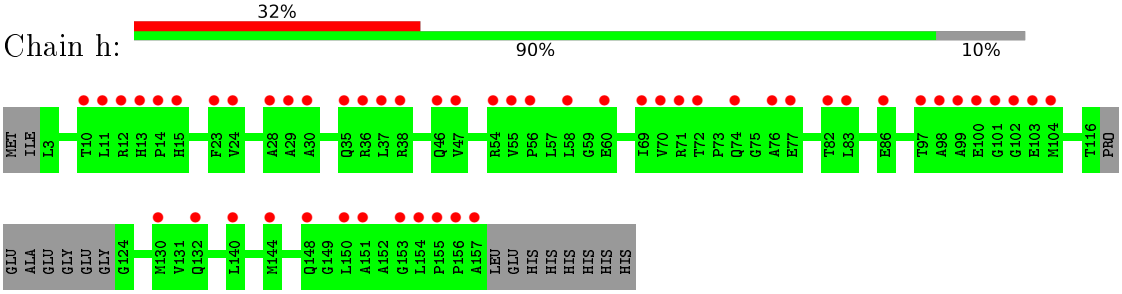
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

Chain g:



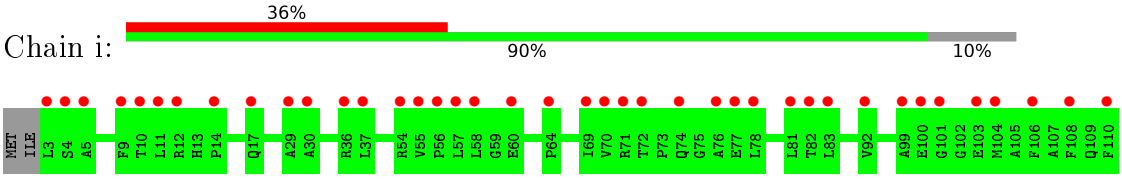
• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

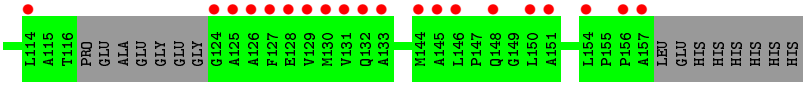
Chain h:



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

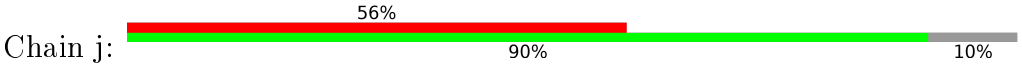
Chain i:

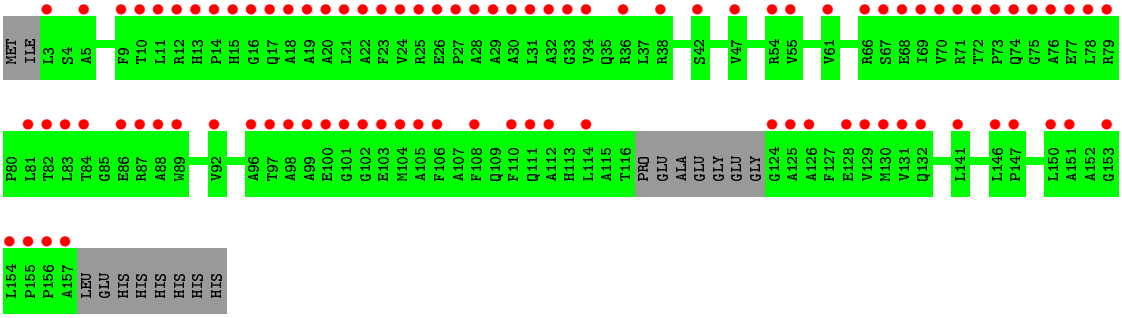




• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

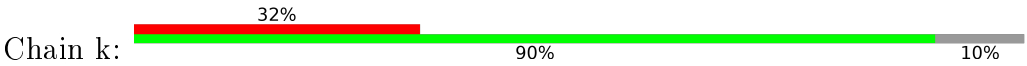
Chain j:

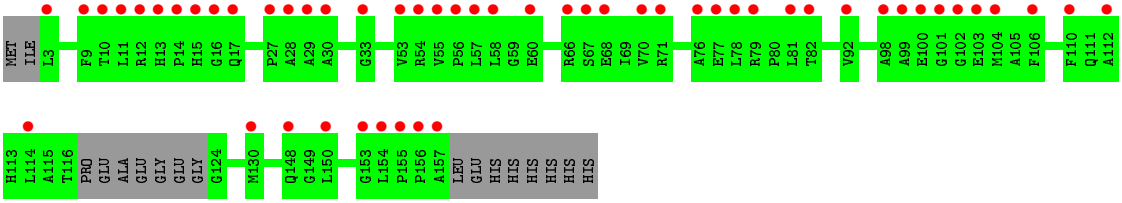




• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

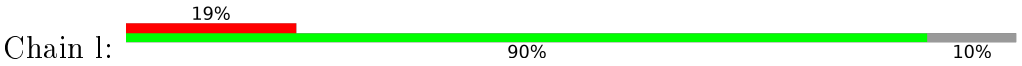
Chain k:

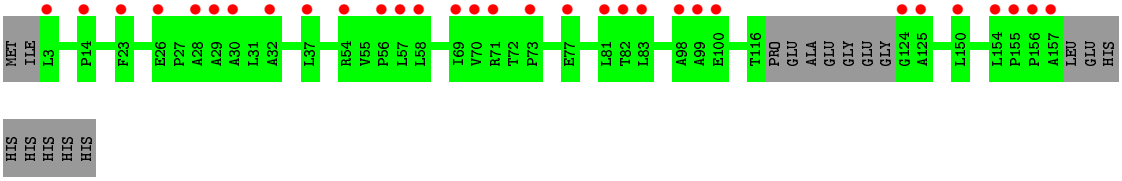




• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

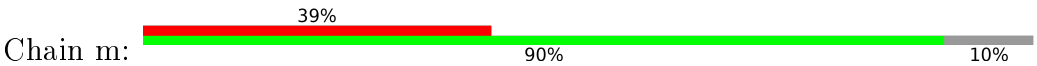
Chain l:

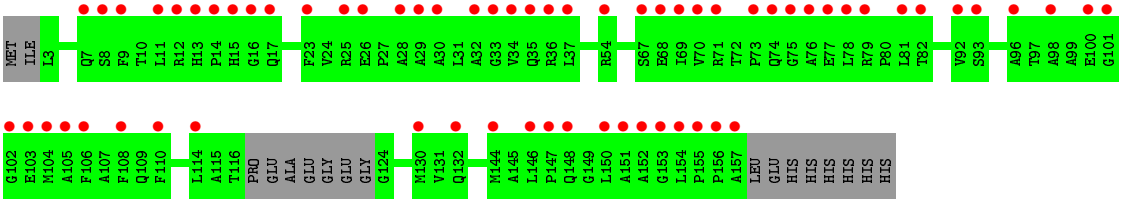




• Molecule 2: Designed self-assembling icosahedral cage I32-28 dimeric subunit

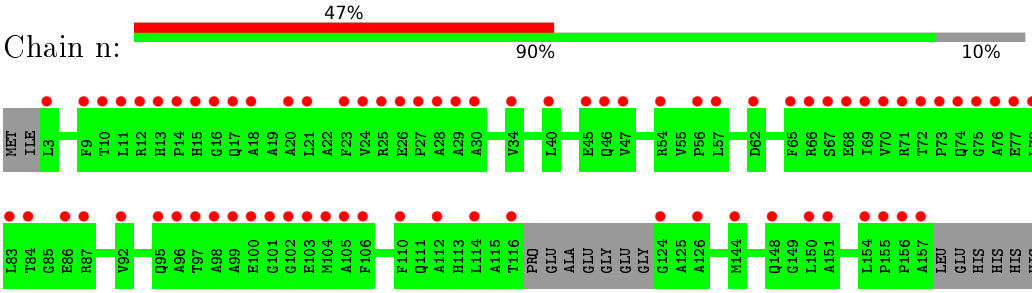
Chain m:





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

Chain n:


47%
90%
10%
MET ILE L3 F9 T10 L11 R12 H13 P14 H15 G16 Q17 A18 A19 A20 L21 A22 F23 V24 R25 E26 P27 A28 A29 A30 V34 I40 E45 Q46 V47 R54 V55 P56 L57 D62 F65 R66 S67 E68 I69 V70 R71 T72 P73 Q74 G75 A76 E77 L78 R79 P80 L81 T82
L83 T84 G85 E86 R87 V92 Q95 A96 T97 A98 A99 E100 G101 G102 E103 M104 A105 F106 F110 Q111 A112 H113 L114 A115 T116 PRO GLU ALA GLU GLY GLU GLY G124 A125 A126 M144 Q148 G149 L150 A151 L154 P155 P156 A157 LEU GLU HIS HIS HIS HIS HIS HIS

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 0.230 , 0.243	Depositor DCC
R_{free} test set	5385 reflections (10.01%)	DCC
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 , 443.0	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

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	0.34	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)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1134	0	1138	44	0
1	B	1134	0	1138	25	0
1	C	1134	0	1138	21	0
1	D	1134	0	1138	45	0
1	E	1134	0	1138	28	0
1	F	1134	0	1138	26	0
1	G	1134	0	1138	14	0
1	H	1134	0	1138	14	0
1	I	1134	0	1138	14	0
1	J	1134	0	1138	15	0
1	K	1134	0	1138	16	0
1	L	1134	0	1138	17	0
1	M	1134	0	1138	16	0
1	N	1134	0	1138	16	0
1	O	1134	0	1138	16	0
1	P	1134	0	1138	15	0
1	Q	1134	0	1138	14	0
1	R	1134	0	1138	15	0
1	S	1134	0	1138	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	1134	0	1138	16	0
2	U	1077	0	1078	43	0
2	V	1077	0	1078	24	0
2	W	1077	0	1078	55	0
2	X	1077	0	1078	41	0
2	Y	1077	0	1078	63	0
2	Z	1077	0	1078	23	0
2	a	1077	0	1078	0	0
2	b	1077	0	1078	0	0
2	c	1077	0	1078	0	0
2	d	1077	0	1078	0	0
2	e	1077	0	1078	0	0
2	f	1077	0	1078	0	0
2	g	1077	0	1078	0	0
2	h	1077	0	1078	0	0
2	i	1077	0	1078	0	0
2	j	1077	0	1078	0	0
2	k	1077	0	1078	0	0
2	l	1077	0	1078	0	0
2	m	1077	0	1078	0	0
2	n	1077	0	1078	0	0
All	All	44220	0	44320	512	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (512) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:LEU:CD1	2:X:141:LEU:HD21	1.53	1.39
1:A:89:LEU:CD1	2:U:141:LEU:HD21	1.59	1.31
1:A:89:LEU:HD13	2:U:141:LEU:HD21	1.19	1.14
2:W:57:LEU:HD13	2:Y:114:LEU:HD13	1.30	1.13
1:D:154:LEU:CD2	2:X:140:LEU:CD2	2.33	1.06
1:D:89:LEU:HD13	2:X:141:LEU:HD21	1.09	1.06
1:D:154:LEU:CD2	2:X:140:LEU:HD22	1.86	1.05
2:W:114:LEU:HD13	2:Y:57:LEU:HB3	1.37	1.01
1:D:154:LEU:HD21	2:X:140:LEU:HD22	1.42	1.01
1:D:154:LEU:HD21	2:X:140:LEU:CD2	1.91	1.01
1:D:93:ALA:HB2	2:X:137:VAL:CG2	1.91	0.99
1:E:97:VAL:HG12	2:Y:129:VAL:HG13	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:LEU:HD13	2:X:141:LEU:CD2	1.93	0.98
1:C:97:VAL:HG12	2:W:129:VAL:HG13	1.46	0.97
1:D:146:ILE:HG22	2:X:148:GLN:OE1	1.62	0.96
2:W:57:LEU:HD13	2:Y:114:LEU:CD1	1.97	0.94
1:D:93:ALA:CB	2:X:137:VAL:HG23	1.98	0.93
1:A:93:ALA:HB2	2:U:137:VAL:CG2	2.00	0.92
1:D:154:LEU:HG	2:X:140:LEU:CD2	2.03	0.89
1:D:93:ALA:CB	2:X:137:VAL:CG2	2.51	0.88
1:A:154:LEU:CD2	2:U:140:LEU:CD2	2.52	0.88
1:L:29:ASP:HB3	1:L:33:ILE:HD12	1.55	0.86
1:N:29:ASP:HB3	1:N:33:ILE:HD12	1.58	0.85
1:C:97:VAL:CG1	2:W:129:VAL:HG13	2.06	0.85
1:A:89:LEU:HD13	2:U:141:LEU:CD2	2.05	0.85
1:A:29:ASP:HB3	1:A:33:ILE:HD12	1.59	0.85
1:C:29:ASP:HB3	1:C:33:ILE:HD12	1.59	0.85
1:I:29:ASP:HB3	1:I:33:ILE:HD12	1.59	0.85
1:D:89:LEU:CD1	2:X:141:LEU:CD2	2.48	0.84
1:A:154:LEU:CD2	2:U:140:LEU:HD22	2.07	0.84
1:B:97:VAL:HG12	2:V:129:VAL:HG13	1.58	0.84
1:T:29:ASP:HB3	1:T:33:ILE:HD12	1.59	0.84
1:G:29:ASP:HB3	1:G:33:ILE:HD12	1.59	0.84
1:K:29:ASP:HB3	1:K:33:ILE:HD12	1.59	0.84
1:R:29:ASP:HB3	1:R:33:ILE:HD12	1.59	0.84
1:S:29:ASP:HB3	1:S:33:ILE:HD12	1.59	0.84
1:M:29:ASP:HB3	1:M:33:ILE:HD12	1.59	0.84
1:B:29:ASP:HB3	1:B:33:ILE:HD12	1.59	0.84
1:J:29:ASP:HB3	1:J:33:ILE:HD12	1.59	0.84
1:O:29:ASP:HB3	1:O:33:ILE:HD12	1.59	0.83
1:A:154:LEU:HD21	2:U:140:LEU:CD2	2.09	0.83
1:H:29:ASP:HB3	1:H:33:ILE:HD12	1.59	0.83
1:P:29:ASP:HB3	1:P:33:ILE:HD12	1.59	0.83
1:F:29:ASP:HB3	1:F:33:ILE:HD12	1.59	0.83
1:D:29:ASP:HB3	1:D:33:ILE:HD12	1.59	0.83
1:D:154:LEU:CG	2:X:140:LEU:CD2	2.56	0.83
1:E:29:ASP:HB3	1:E:33:ILE:HD12	1.59	0.82
1:Q:29:ASP:HB3	1:Q:33:ILE:HD12	1.59	0.82
1:A:89:LEU:HD11	2:U:141:LEU:HD21	1.61	0.81
1:A:154:LEU:HD21	2:U:140:LEU:HD22	1.61	0.81
1:L:29:ASP:HB3	1:L:33:ILE:CD1	2.10	0.81
2:W:114:LEU:HD13	2:Y:57:LEU:CB	2.11	0.81
1:D:93:ALA:HB2	2:X:137:VAL:HG22	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:97:VAL:HG12	2:Z:129:VAL:HG13	1.64	0.80
1:A:93:ALA:CB	2:U:137:VAL:HG23	2.11	0.79
1:E:97:VAL:CG1	2:Y:129:VAL:HG13	2.12	0.79
2:W:57:LEU:CD1	2:Y:114:LEU:HD13	2.11	0.78
1:D:153:ASN:OD1	2:X:140:LEU:HD11	1.84	0.78
2:W:57:LEU:O	2:Y:88:ALA:HB2	1.83	0.77
2:W:114:LEU:HB3	2:Y:57:LEU:HA	1.67	0.77
1:D:154:LEU:CG	2:X:140:LEU:HD23	2.16	0.76
1:A:93:ALA:CB	2:U:137:VAL:CG2	2.65	0.75
1:D:93:ALA:HB2	2:X:137:VAL:HG23	1.63	0.75
1:F:89:LEU:CD1	2:Z:141:LEU:HD21	2.17	0.75
1:A:93:ALA:HB2	2:U:137:VAL:HG23	1.67	0.75
1:E:89:LEU:CD1	2:Y:141:LEU:HD21	2.18	0.74
1:O:29:ASP:HB3	1:O:33:ILE:CD1	2.18	0.74
1:B:29:ASP:HB3	1:B:33:ILE:CD1	2.18	0.74
2:U:124:GLY:O	2:U:128:GLU:HG3	1.88	0.74
2:W:59:GLY:HA3	2:Y:87:ARG:HA	1.68	0.74
1:F:29:ASP:HB3	1:F:33:ILE:CD1	2.18	0.74
1:S:29:ASP:HB3	1:S:33:ILE:CD1	2.18	0.74
2:W:124:GLY:O	2:W:128:GLU:HG3	1.88	0.74
1:A:146:ILE:HG22	2:U:148:GLN:OE1	1.88	0.73
1:T:29:ASP:HB3	1:T:33:ILE:CD1	2.18	0.73
2:Y:124:GLY:O	2:Y:128:GLU:HG3	1.88	0.73
1:F:97:VAL:CG1	2:Z:129:VAL:HG13	2.19	0.73
1:N:29:ASP:HB3	1:N:33:ILE:CD1	2.18	0.73
1:E:29:ASP:HB3	1:E:33:ILE:CD1	2.18	0.73
1:K:29:ASP:HB3	1:K:33:ILE:CD1	2.19	0.73
1:Q:29:ASP:HB3	1:Q:33:ILE:CD1	2.18	0.73
1:R:29:ASP:HB3	1:R:33:ILE:CD1	2.18	0.73
1:M:29:ASP:HB3	1:M:33:ILE:CD1	2.18	0.73
1:I:29:ASP:HB3	1:I:33:ILE:CD1	2.18	0.72
2:V:124:GLY:O	2:V:128:GLU:HG3	1.88	0.72
1:H:29:ASP:HB3	1:H:33:ILE:CD1	2.18	0.72
1:J:29:ASP:HB3	1:J:33:ILE:CD1	2.18	0.72
2:Z:124:GLY:O	2:Z:128:GLU:HG3	1.88	0.72
1:D:29:ASP:HB3	1:D:33:ILE:CD1	2.18	0.72
1:G:29:ASP:HB3	1:G:33:ILE:CD1	2.18	0.72
1:P:29:ASP:HB3	1:P:33:ILE:CD1	2.18	0.72
2:X:124:GLY:O	2:X:128:GLU:HG3	1.88	0.72
1:A:29:ASP:HB3	1:A:33:ILE:CD1	2.18	0.72
1:C:29:ASP:HB3	1:C:33:ILE:CD1	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:HG	2:U:140:LEU:CD2	2.19	0.72
1:D:154:LEU:HG	2:X:140:LEU:HD21	1.72	0.71
1:D:154:LEU:HG	2:X:140:LEU:HD23	1.72	0.71
2:W:114:LEU:HD13	2:Y:57:LEU:HD13	1.73	0.71
2:W:114:LEU:CD1	2:Y:57:LEU:HD13	2.23	0.69
1:D:154:LEU:HD23	2:X:140:LEU:HD22	1.73	0.69
1:A:153:ASN:OD1	2:U:140:LEU:HD11	1.92	0.69
1:D:154:LEU:CD2	2:X:140:LEU:HD23	2.22	0.68
2:W:57:LEU:HB3	2:Y:114:LEU:HD13	1.76	0.68
1:L:29:ASP:O	1:L:33:ILE:HB	1.96	0.65
1:A:93:ALA:HB2	2:U:137:VAL:HG22	1.77	0.65
1:A:154:LEU:CG	2:U:140:LEU:CD2	2.76	0.64
1:B:97:VAL:CG1	2:V:129:VAL:HG13	2.27	0.64
1:B:97:VAL:HG11	2:V:129:VAL:HA	1.78	0.64
1:D:154:LEU:HD21	2:X:140:LEU:HD23	1.73	0.63
1:D:89:LEU:HD11	2:X:141:LEU:HD21	1.69	0.63
1:E:93:ALA:HB2	2:Y:137:VAL:HG23	1.80	0.63
2:W:86:GLU:O	2:Y:60:GLU:HG3	1.99	0.63
2:W:114:LEU:HD22	2:Y:57:LEU:O	1.99	0.62
1:B:93:ALA:HB2	2:V:137:VAL:HG23	1.80	0.62
1:A:154:LEU:HG	2:U:140:LEU:HD23	1.80	0.62
1:C:97:VAL:HG11	2:W:129:VAL:HA	1.80	0.62
1:A:154:LEU:CG	2:U:140:LEU:HD23	2.30	0.61
2:W:57:LEU:HD22	2:Y:114:LEU:HB3	1.82	0.61
2:W:61:VAL:HG22	2:Y:61:VAL:CG1	2.30	0.61
1:E:93:ALA:HB2	2:Y:137:VAL:CG2	2.31	0.61
2:W:61:VAL:HG11	2:Y:61:VAL:HG22	1.82	0.60
1:L:29:ASP:O	1:L:33:ILE:CB	2.50	0.60
2:W:131:VAL:HG11	2:Y:57:LEU:HB2	1.84	0.60
2:Y:9:PHE:CZ	2:Y:150:LEU:HD22	2.38	0.59
1:E:93:ALA:CB	2:Y:137:VAL:HG23	2.32	0.59
1:R:29:ASP:O	1:R:33:ILE:HB	2.03	0.59
2:X:9:PHE:CZ	2:X:150:LEU:HD22	2.38	0.59
2:W:57:LEU:HD22	2:Y:114:LEU:CB	2.32	0.59
1:P:29:ASP:O	1:P:33:ILE:HB	2.03	0.59
1:N:29:ASP:O	1:N:33:ILE:HB	2.02	0.59
1:O:29:ASP:O	1:O:33:ILE:HB	2.03	0.59
1:B:29:ASP:O	1:B:33:ILE:HB	2.02	0.59
1:J:29:ASP:O	1:J:33:ILE:HB	2.02	0.59
2:W:9:PHE:CZ	2:W:150:LEU:HD22	2.37	0.59
1:S:29:ASP:O	1:S:33:ILE:HB	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:29:ASP:O	1:H:33:ILE:HB	2.03	0.59
1:A:29:ASP:O	1:A:33:ILE:HB	2.02	0.58
1:A:86:GLU:CB	2:U:54:ARG:HH21	2.16	0.58
1:D:29:ASP:O	1:D:33:ILE:HB	2.03	0.58
1:E:29:ASP:O	1:E:33:ILE:HB	2.02	0.58
1:F:29:ASP:O	1:F:33:ILE:HB	2.03	0.58
2:U:9:PHE:CZ	2:U:150:LEU:HD22	2.37	0.58
1:C:29:ASP:O	1:C:33:ILE:HB	2.03	0.58
1:I:29:ASP:O	1:I:33:ILE:HB	2.03	0.58
2:Z:9:PHE:CZ	2:Z:150:LEU:HD22	2.38	0.58
2:V:9:PHE:CZ	2:V:150:LEU:HD22	2.38	0.58
1:K:29:ASP:O	1:K:33:ILE:HB	2.03	0.58
1:Q:29:ASP:O	1:Q:33:ILE:HB	2.03	0.58
1:A:154:LEU:HD21	2:U:140:LEU:HD23	1.86	0.58
1:T:29:ASP:O	1:T:33:ILE:HB	2.03	0.58
1:G:29:ASP:O	1:G:33:ILE:HB	2.03	0.58
1:O:177:TRP:CZ2	1:P:71:ASP:OD1	2.57	0.57
1:L:28:GLY:HA2	1:L:142:GLU:OE2	2.04	0.57
1:R:177:TRP:CG	1:R:178:ASP:N	2.73	0.57
1:D:177:TRP:CG	1:D:178:ASP:N	2.73	0.57
1:J:177:TRP:CG	1:J:178:ASP:N	2.73	0.57
1:K:177:TRP:CG	1:K:178:ASP:N	2.73	0.57
1:Q:177:TRP:CG	1:Q:178:ASP:N	2.73	0.57
1:S:177:TRP:CG	1:S:178:ASP:N	2.73	0.57
1:A:177:TRP:CG	1:A:178:ASP:N	2.73	0.57
1:F:177:TRP:CG	1:F:178:ASP:N	2.73	0.57
1:T:177:TRP:CG	1:T:178:ASP:N	2.73	0.57
1:L:177:TRP:CG	1:L:178:ASP:N	2.73	0.57
1:M:29:ASP:O	1:M:33:ILE:HB	2.03	0.57
1:B:177:TRP:CG	1:B:178:ASP:N	2.73	0.56
1:I:177:TRP:CG	1:I:178:ASP:N	2.73	0.56
1:E:177:TRP:CG	1:E:178:ASP:N	2.73	0.56
1:O:177:TRP:CG	1:O:178:ASP:N	2.73	0.56
1:G:177:TRP:CG	1:G:178:ASP:N	2.73	0.56
1:M:177:TRP:CG	1:M:178:ASP:N	2.73	0.56
1:N:177:TRP:CG	1:N:178:ASP:N	2.73	0.56
1:P:177:TRP:CG	1:P:178:ASP:N	2.73	0.56
2:W:114:LEU:HD13	2:Y:57:LEU:CG	2.35	0.56
1:B:93:ALA:CB	2:V:137:VAL:HG23	2.35	0.56
1:G:28:GLY:HA2	1:G:142:GLU:OE2	2.06	0.56
1:C:177:TRP:CG	1:C:178:ASP:N	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:177:TRP:CG	1:H:178:ASP:N	2.73	0.56
1:D:90:LEU:HA	2:X:137:VAL:HG21	1.88	0.55
1:B:93:ALA:HB2	2:V:137:VAL:CG2	2.36	0.55
1:A:177:TRP:CD2	1:A:178:ASP:N	2.75	0.55
1:B:28:GLY:HA2	1:B:142:GLU:OE2	2.06	0.55
1:C:28:GLY:HA2	1:C:142:GLU:OE2	2.07	0.55
1:E:28:GLY:HA2	1:E:142:GLU:OE2	2.07	0.55
1:F:28:GLY:HA2	1:F:142:GLU:OE2	2.07	0.55
1:D:28:GLY:HA2	1:D:142:GLU:OE2	2.07	0.55
1:K:28:GLY:HA2	1:K:142:GLU:OE2	2.06	0.55
1:Q:177:TRP:CD2	1:Q:178:ASP:N	2.75	0.55
1:B:177:TRP:CD2	1:B:178:ASP:N	2.75	0.55
1:D:177:TRP:CD2	1:D:178:ASP:N	2.75	0.55
1:G:177:TRP:CD2	1:G:178:ASP:N	2.75	0.55
1:N:28:GLY:HA2	1:N:142:GLU:OE2	2.06	0.55
1:P:28:GLY:HA2	1:P:142:GLU:OE2	2.06	0.55
1:A:28:GLY:HA2	1:A:142:GLU:OE2	2.07	0.55
1:I:28:GLY:HA2	1:I:142:GLU:OE2	2.06	0.55
1:E:94:LEU:HD21	2:Y:130:MET:SD	2.46	0.55
1:M:177:TRP:CD2	1:M:178:ASP:N	2.75	0.55
1:L:177:TRP:CD2	1:L:178:ASP:N	2.75	0.55
1:O:177:TRP:CD2	1:O:178:ASP:N	2.75	0.55
1:H:28:GLY:HA2	1:H:142:GLU:OE2	2.06	0.55
1:J:177:TRP:CD2	1:J:178:ASP:N	2.75	0.55
1:P:177:TRP:CD2	1:P:178:ASP:N	2.75	0.55
1:T:177:TRP:CD2	1:T:178:ASP:N	2.75	0.55
1:A:86:GLU:HB3	2:U:54:ARG:HH21	1.72	0.55
1:F:177:TRP:CD2	1:F:178:ASP:N	2.75	0.55
1:O:28:GLY:HA2	1:O:142:GLU:OE2	2.06	0.55
1:R:28:GLY:HA2	1:R:142:GLU:OE2	2.06	0.55
1:T:28:GLY:HA2	1:T:142:GLU:OE2	2.06	0.55
1:C:177:TRP:CD2	1:C:178:ASP:N	2.75	0.55
1:G:108:GLU:HG3	1:G:109:PHE:N	2.22	0.55
1:H:177:TRP:CD2	1:H:178:ASP:N	2.75	0.55
1:K:177:TRP:CD2	1:K:178:ASP:N	2.75	0.55
1:M:28:GLY:HA2	1:M:142:GLU:OE2	2.06	0.55
1:Q:28:GLY:HA2	1:Q:142:GLU:OE2	2.07	0.55
1:J:108:GLU:HG3	1:J:109:PHE:N	2.22	0.54
1:E:108:GLU:HG3	1:E:109:PHE:N	2.23	0.54
1:E:177:TRP:CD2	1:E:178:ASP:N	2.75	0.54
1:I:177:TRP:CD2	1:I:178:ASP:N	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:177:TRP:CD2	1:N:178:ASP:N	2.75	0.54
1:P:108:GLU:HG3	1:P:109:PHE:N	2.23	0.54
1:R:177:TRP:CD2	1:R:178:ASP:N	2.75	0.54
1:S:177:TRP:CD2	1:S:178:ASP:N	2.75	0.54
1:T:108:GLU:HG3	1:T:109:PHE:N	2.23	0.54
2:W:61:VAL:HG22	2:Y:61:VAL:HG11	1.88	0.54
1:S:28:GLY:HA2	1:S:142:GLU:OE2	2.07	0.54
1:H:108:GLU:HG3	1:H:109:PHE:N	2.22	0.54
1:N:108:GLU:HG3	1:N:109:PHE:N	2.23	0.54
1:K:108:GLU:HG3	1:K:109:PHE:N	2.23	0.54
1:M:108:GLU:HG3	1:M:109:PHE:N	2.23	0.54
1:Q:108:GLU:HG3	1:Q:109:PHE:N	2.22	0.54
1:J:28:GLY:HA2	1:J:142:GLU:OE2	2.07	0.54
1:O:108:GLU:HG3	1:O:109:PHE:N	2.23	0.54
1:S:108:GLU:HG3	1:S:109:PHE:N	2.23	0.54
1:B:89:LEU:CD1	2:V:141:LEU:HD21	2.39	0.53
1:L:108:GLU:HG3	1:L:109:PHE:N	2.23	0.53
1:A:108:GLU:HG3	1:A:109:PHE:N	2.22	0.53
1:F:108:GLU:HG3	1:F:109:PHE:N	2.23	0.53
2:W:87:ARG:HB3	2:Y:60:GLU:HB2	1.90	0.53
1:C:108:GLU:HG3	1:C:109:PHE:N	2.22	0.53
1:I:108:GLU:HG3	1:I:109:PHE:N	2.22	0.53
1:B:108:GLU:HG3	1:B:109:PHE:N	2.23	0.53
1:K:75:GLU:HG3	1:K:82:ALA:HA	1.91	0.53
1:L:75:GLU:HG3	1:L:82:ALA:HA	1.91	0.53
1:R:108:GLU:HG3	1:R:109:PHE:N	2.23	0.53
1:E:177:TRP:CZ2	1:F:71:ASP:OD1	2.62	0.53
1:C:75:GLU:HG3	1:C:82:ALA:HA	1.91	0.52
1:D:108:GLU:HG3	1:D:109:PHE:N	2.23	0.52
1:T:75:GLU:HG3	1:T:82:ALA:HA	1.91	0.52
2:W:114:LEU:HD13	2:Y:57:LEU:CD1	2.36	0.52
1:P:75:GLU:HG3	1:P:82:ALA:HA	1.91	0.52
2:W:114:LEU:CD1	2:Y:57:LEU:HD22	2.39	0.52
1:J:75:GLU:HG3	1:J:82:ALA:HA	1.91	0.52
1:R:75:GLU:HG3	1:R:82:ALA:HA	1.92	0.52
1:A:75:GLU:HG3	1:A:82:ALA:HA	1.91	0.52
1:E:75:GLU:HG3	1:E:82:ALA:HA	1.92	0.52
1:M:75:GLU:HG3	1:M:82:ALA:HA	1.92	0.52
1:B:75:GLU:HG3	1:B:82:ALA:HA	1.91	0.52
1:D:75:GLU:HG3	1:D:82:ALA:HA	1.92	0.51
1:F:75:GLU:HG3	1:F:82:ALA:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:75:GLU:HG3	1:N:82:ALA:HA	1.92	0.51
2:W:61:VAL:CG1	2:Y:61:VAL:HG22	2.40	0.51
2:U:106:PHE:CD1	2:U:150:LEU:HD21	2.46	0.51
2:W:106:PHE:CD1	2:W:150:LEU:HD21	2.46	0.51
1:S:75:GLU:HG3	1:S:82:ALA:HA	1.91	0.51
1:B:29:ASP:O	1:B:33:ILE:CB	2.59	0.51
1:E:29:ASP:O	1:E:33:ILE:CB	2.59	0.51
1:N:29:ASP:O	1:N:33:ILE:CB	2.59	0.51
1:O:75:GLU:HG3	1:O:82:ALA:HA	1.92	0.51
1:G:75:GLU:HG3	1:G:82:ALA:HA	1.92	0.51
1:H:75:GLU:HG3	1:H:82:ALA:HA	1.92	0.51
1:I:75:GLU:HG3	1:I:82:ALA:HA	1.92	0.51
1:R:29:ASP:O	1:R:33:ILE:CB	2.59	0.51
2:Y:106:PHE:CD1	2:Y:150:LEU:HD21	2.46	0.51
1:Q:75:GLU:HG3	1:Q:82:ALA:HA	1.91	0.51
1:F:93:ALA:HB2	2:Z:137:VAL:HG23	1.93	0.51
1:A:29:ASP:O	1:A:33:ILE:CB	2.59	0.50
1:D:29:ASP:O	1:D:33:ILE:CB	2.60	0.50
1:O:29:ASP:O	1:O:33:ILE:CB	2.59	0.50
1:F:29:ASP:O	1:F:33:ILE:CB	2.59	0.50
1:A:154:LEU:HG	2:U:140:LEU:HD21	1.93	0.50
1:G:29:ASP:O	1:G:33:ILE:CB	2.59	0.50
2:W:114:LEU:CD1	2:Y:57:LEU:HB3	2.26	0.50
1:M:29:ASP:O	1:M:33:ILE:CB	2.60	0.50
2:U:108:PHE:CD2	2:U:146:LEU:HD13	2.47	0.50
2:X:106:PHE:CZ	2:X:150:LEU:HD23	2.47	0.50
1:C:29:ASP:O	1:C:33:ILE:CB	2.59	0.50
1:H:29:ASP:O	1:H:33:ILE:CB	2.59	0.50
1:T:29:ASP:O	1:T:33:ILE:CB	2.59	0.50
2:W:108:PHE:CD2	2:W:146:LEU:HD13	2.47	0.50
2:X:106:PHE:CD1	2:X:150:LEU:HD21	2.46	0.50
2:Y:4:SER:OG	2:Y:111:GLN:OE1	2.30	0.50
2:Z:106:PHE:CD1	2:Z:150:LEU:HD21	2.46	0.50
1:I:29:ASP:O	1:I:33:ILE:CB	2.59	0.50
2:V:106:PHE:CZ	2:V:150:LEU:HD23	2.47	0.50
2:Z:106:PHE:CZ	2:Z:150:LEU:HD23	2.47	0.50
1:J:29:ASP:O	1:J:33:ILE:CB	2.59	0.50
2:U:4:SER:OG	2:U:111:GLN:OE1	2.30	0.50
2:V:106:PHE:CD1	2:V:150:LEU:HD21	2.46	0.50
2:V:108:PHE:CD2	2:V:146:LEU:HD13	2.47	0.50
2:Y:106:PHE:CZ	2:Y:150:LEU:HD23	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:ILE:HD13	2:Z:145:ALA:HB2	1.93	0.50
1:Q:29:ASP:O	1:Q:33:ILE:CB	2.59	0.50
2:Y:108:PHE:CD2	2:Y:146:LEU:HD13	2.47	0.50
1:L:29:ASP:HB3	1:L:33:ILE:HD11	1.91	0.49
1:P:29:ASP:O	1:P:33:ILE:CB	2.59	0.49
2:W:106:PHE:CZ	2:W:150:LEU:HD23	2.47	0.49
2:Z:108:PHE:CD2	2:Z:146:LEU:HD13	2.47	0.49
2:V:4:SER:OG	2:V:111:GLN:OE1	2.30	0.49
2:Y:12:ARG:HD2	2:Y:103:GLU:OE2	2.13	0.49
1:S:29:ASP:O	1:S:33:ILE:CB	2.60	0.49
2:X:108:PHE:CD2	2:X:146:LEU:HD13	2.47	0.49
2:V:12:ARG:HD2	2:V:103:GLU:OE2	2.13	0.49
2:Z:12:ARG:HD2	2:Z:103:GLU:OE2	2.13	0.49
2:Z:4:SER:OG	2:Z:111:GLN:OE1	2.30	0.49
2:X:4:SER:OG	2:X:111:GLN:OE1	2.30	0.49
2:W:87:ARG:HA	2:Y:59:GLY:HA3	1.95	0.49
2:W:4:SER:OG	2:W:111:GLN:OE1	2.30	0.49
1:K:29:ASP:O	1:K:33:ILE:CB	2.59	0.49
1:E:146:ILE:HD13	2:Y:145:ALA:HB2	1.95	0.49
2:W:12:ARG:HD2	2:W:103:GLU:OE2	2.13	0.49
1:E:97:VAL:HG11	2:Y:129:VAL:HA	1.94	0.49
2:Y:31:LEU:HA	2:Y:34:VAL:HG23	1.95	0.49
1:A:90:LEU:HA	2:U:137:VAL:HG21	1.95	0.48
2:Z:31:LEU:HA	2:Z:34:VAL:HG23	1.95	0.48
2:X:31:LEU:HA	2:X:34:VAL:HG23	1.95	0.48
1:A:154:LEU:HD23	2:U:140:LEU:HD22	1.90	0.48
2:U:31:LEU:HA	2:U:34:VAL:HG23	1.95	0.48
1:E:90:LEU:HA	2:Y:137:VAL:HG21	1.95	0.48
2:U:12:ARG:HD2	2:U:103:GLU:OE2	2.13	0.48
2:X:12:ARG:HD2	2:X:103:GLU:OE2	2.13	0.48
2:W:131:VAL:HG13	2:Y:58:LEU:HG	1.96	0.48
2:U:106:PHE:CZ	2:U:150:LEU:HD23	2.47	0.48
2:V:31:LEU:HA	2:V:34:VAL:HG23	1.95	0.48
2:W:61:VAL:HG22	2:Y:61:VAL:HG13	1.94	0.48
1:B:93:ALA:HB1	2:V:133:ALA:O	2.14	0.48
1:L:177:TRP:CE3	1:L:178:ASP:C	2.88	0.47
2:X:51:LEU:N	2:X:51:LEU:HD12	2.29	0.47
2:Y:51:LEU:HD12	2:Y:51:LEU:N	2.29	0.47
2:W:51:LEU:N	2:W:51:LEU:HD12	2.29	0.47
1:O:177:TRP:CE3	1:O:178:ASP:C	2.88	0.47
1:M:177:TRP:CE3	1:M:178:ASP:C	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:177:TRP:CE3	1:N:178:ASP:C	2.88	0.47
2:W:88:ALA:HB2	2:Y:57:LEU:O	2.15	0.47
1:B:29:ASP:O	1:B:33:ILE:N	2.43	0.47
1:E:177:TRP:CE3	1:E:178:ASP:C	2.88	0.47
2:U:51:LEU:N	2:U:51:LEU:HD12	2.29	0.47
1:I:177:TRP:CE3	1:I:178:ASP:C	2.88	0.47
1:P:177:TRP:CE3	1:P:178:ASP:C	2.88	0.47
1:B:177:TRP:CE3	1:B:178:ASP:C	2.88	0.47
1:K:177:TRP:CE3	1:K:178:ASP:C	2.88	0.47
1:G:177:TRP:CE3	1:G:178:ASP:C	2.88	0.47
1:R:177:TRP:CE3	1:R:178:ASP:C	2.88	0.47
1:T:177:TRP:CE3	1:T:178:ASP:C	2.88	0.47
1:D:177:TRP:CZ2	1:E:71:ASP:OD1	2.68	0.47
1:F:177:TRP:CE3	1:F:178:ASP:C	2.88	0.47
1:Q:177:TRP:CE3	1:Q:178:ASP:C	2.88	0.47
2:Z:51:LEU:N	2:Z:51:LEU:HD12	2.29	0.47
1:C:177:TRP:CE3	1:C:178:ASP:C	2.88	0.46
1:D:177:TRP:CE3	1:D:178:ASP:C	2.88	0.46
2:W:31:LEU:HA	2:W:34:VAL:HG23	1.95	0.46
1:S:177:TRP:CE3	1:S:178:ASP:C	2.88	0.46
1:A:177:TRP:CE3	1:A:178:ASP:C	2.88	0.46
1:H:177:TRP:CE3	1:H:178:ASP:C	2.88	0.46
1:J:177:TRP:CE3	1:J:178:ASP:C	2.88	0.46
2:V:51:LEU:N	2:V:51:LEU:HD12	2.29	0.46
1:K:28:GLY:CA	1:K:142:GLU:OE2	2.64	0.46
1:N:28:GLY:CA	1:N:142:GLU:OE2	2.64	0.46
1:F:90:LEU:HA	2:Z:137:VAL:HG21	1.96	0.46
1:J:29:ASP:O	1:J:33:ILE:N	2.43	0.46
1:M:28:GLY:CA	1:M:142:GLU:OE2	2.64	0.46
2:W:9:PHE:CE2	2:W:150:LEU:HD22	2.51	0.46
2:Y:9:PHE:CE2	2:Y:150:LEU:HD22	2.51	0.46
1:F:93:ALA:HB2	2:Z:137:VAL:CG2	2.46	0.46
1:D:28:GLY:CA	1:D:142:GLU:OE2	2.64	0.46
1:G:28:GLY:CA	1:G:142:GLU:OE2	2.64	0.46
1:L:29:ASP:O	1:L:33:ILE:CG1	2.63	0.46
1:O:28:GLY:CA	1:O:142:GLU:OE2	2.64	0.46
1:S:28:GLY:CA	1:S:142:GLU:OE2	2.64	0.46
1:A:28:GLY:CA	1:A:142:GLU:OE2	2.64	0.45
1:F:28:GLY:CA	1:F:142:GLU:OE2	2.64	0.45
1:B:28:GLY:CA	1:B:142:GLU:OE2	2.64	0.45
1:H:28:GLY:CA	1:H:142:GLU:OE2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:28:GLY:CA	1:J:142:GLU:OE2	2.64	0.45
2:U:9:PHE:CE2	2:U:150:LEU:HD22	2.51	0.45
2:W:57:LEU:HB2	2:Y:131:VAL:HG11	1.99	0.45
1:F:29:ASP:O	1:F:33:ILE:N	2.43	0.45
1:N:177:TRP:CZ2	1:O:71:ASP:OD1	2.69	0.45
1:D:86:GLU:O	2:V:60:GLU:HG3	132.65	0.45
2:W:58:LEU:HA	2:Y:88:ALA:HB2	1.98	0.45
1:I:28:GLY:CA	1:I:142:GLU:OE2	2.64	0.45
1:L:29:ASP:O	1:L:33:ILE:N	2.38	0.45
1:T:28:GLY:CA	1:T:142:GLU:OE2	2.64	0.45
1:L:28:GLY:CA	1:L:142:GLU:OE2	2.65	0.45
1:R:28:GLY:CA	1:R:142:GLU:OE2	2.64	0.45
1:P:28:GLY:CA	1:P:142:GLU:OE2	2.64	0.45
2:Z:9:PHE:CE2	2:Z:150:LEU:HD22	2.51	0.45
1:C:28:GLY:CA	1:C:142:GLU:OE2	2.64	0.45
1:D:177:TRP:CZ3	1:D:178:ASP:O	2.70	0.45
1:B:177:TRP:CZ3	1:B:178:ASP:O	2.70	0.44
1:E:28:GLY:CA	1:E:142:GLU:OE2	2.64	0.44
1:J:177:TRP:CZ3	1:J:178:ASP:O	2.71	0.44
1:O:29:ASP:O	1:O:33:ILE:N	2.43	0.44
1:A:154:LEU:CD2	2:U:140:LEU:HD23	2.35	0.44
1:I:29:ASP:O	1:I:33:ILE:N	2.43	0.44
1:P:29:ASP:O	1:P:33:ILE:N	2.43	0.44
1:N:177:TRP:CZ3	1:N:178:ASP:O	2.70	0.44
1:O:177:TRP:CZ3	1:O:178:ASP:O	2.70	0.44
2:U:14:PRO:HG2	2:U:155:PRO:O	2.18	0.44
2:X:9:PHE:CE2	2:X:150:LEU:HD22	2.51	0.44
1:E:177:TRP:CZ3	1:E:178:ASP:O	2.70	0.44
1:F:93:ALA:CB	2:Z:137:VAL:HG23	2.48	0.44
2:V:9:PHE:CE2	2:V:150:LEU:HD22	2.51	0.44
1:I:177:TRP:CZ3	1:I:178:ASP:O	2.70	0.44
1:R:177:TRP:CZ3	1:R:178:ASP:O	2.71	0.44
2:W:14:PRO:HG2	2:W:155:PRO:O	2.18	0.44
1:G:177:TRP:CZ3	1:G:178:ASP:O	2.71	0.44
2:V:47:VAL:HG23	2:V:69:ILE:HD11	2.00	0.44
1:H:29:ASP:O	1:H:33:ILE:N	2.43	0.44
1:M:177:TRP:CZ3	1:M:178:ASP:O	2.71	0.44
2:Y:14:PRO:HG2	2:Y:155:PRO:O	2.18	0.44
1:A:177:TRP:CZ3	1:A:178:ASP:O	2.71	0.44
1:E:42:LEU:HD22	1:E:128:CYS:HA	2.00	0.43
2:X:47:VAL:HG23	2:X:69:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:TRP:CZ3	1:F:178:ASP:O	2.71	0.43
1:H:177:TRP:CZ3	1:H:178:ASP:O	2.70	0.43
1:K:42:LEU:HD22	1:K:128:CYS:HA	2.00	0.43
1:L:177:TRP:CZ3	1:L:178:ASP:O	2.70	0.43
1:P:177:TRP:CZ3	1:P:178:ASP:O	2.70	0.43
1:C:177:TRP:CZ3	1:C:178:ASP:O	2.71	0.43
1:C:89:LEU:CD1	2:W:141:LEU:HD21	2.48	0.43
1:Q:28:GLY:CA	1:Q:142:GLU:OE2	2.64	0.43
2:W:114:LEU:HB3	2:Y:57:LEU:CA	2.44	0.43
1:D:71:ASP:OD1	1:F:177:TRP:CZ2	2.72	0.43
1:K:177:TRP:CZ3	1:K:178:ASP:O	2.70	0.43
1:N:42:LEU:HD22	1:N:128:CYS:HA	2.01	0.43
1:S:42:LEU:HD22	1:S:128:CYS:HA	2.01	0.43
1:T:177:TRP:CZ3	1:T:178:ASP:O	2.71	0.43
1:T:42:LEU:HD22	1:T:128:CYS:HA	2.01	0.43
1:A:86:GLU:HB2	2:U:54:ARG:HH21	1.82	0.43
1:D:93:ALA:HB3	2:X:137:VAL:CG2	2.46	0.43
1:E:29:ASP:O	1:E:33:ILE:N	2.43	0.43
1:Q:177:TRP:CZ3	1:Q:178:ASP:O	2.71	0.43
2:W:47:VAL:HG23	2:W:69:ILE:HD11	2.00	0.43
1:D:132:GLU:OE2	2:X:144:MET:HE1	2.18	0.43
2:Z:14:PRO:HG2	2:Z:155:PRO:O	2.18	0.43
1:Q:42:LEU:HD22	1:Q:128:CYS:HA	2.01	0.43
2:Z:48:TRP:HB3	2:Z:66:ARG:HG3	2.01	0.43
1:C:42:LEU:HD22	1:C:128:CYS:HA	2.01	0.43
1:I:42:LEU:HD22	1:I:128:CYS:HA	2.01	0.43
1:P:42:LEU:HD22	1:P:128:CYS:HA	2.00	0.43
2:X:48:TRP:HB3	2:X:66:ARG:HG3	2.01	0.43
2:Y:47:VAL:HG23	2:Y:69:ILE:HD11	2.00	0.43
1:F:42:LEU:HD22	1:F:128:CYS:HA	2.00	0.43
1:L:42:LEU:HD22	1:L:128:CYS:HA	2.01	0.43
2:V:14:PRO:HG2	2:V:155:PRO:O	2.18	0.43
1:H:42:LEU:HD22	1:H:128:CYS:HA	2.01	0.43
1:J:42:LEU:HD22	1:J:128:CYS:HA	2.01	0.43
1:S:177:TRP:CZ3	1:S:178:ASP:O	2.71	0.43
1:B:177:TRP:CZ2	1:C:71:ASP:OD1	2.72	0.43
1:D:42:LEU:HD22	1:D:128:CYS:HA	2.00	0.43
2:U:47:VAL:HG23	2:U:69:ILE:HD11	2.00	0.43
2:X:14:PRO:HG2	2:X:155:PRO:O	2.18	0.43
2:Z:47:VAL:HG23	2:Z:69:ILE:HD11	2.00	0.43
1:E:89:LEU:HD13	2:Y:141:LEU:HD21	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:LEU:HD22	1:G:128:CYS:HA	2.01	0.42
1:B:94:LEU:HD21	2:V:130:MET:SD	2.59	0.42
1:A:42:LEU:HD22	1:A:128:CYS:HA	2.01	0.42
1:A:29:ASP:O	1:A:33:ILE:N	2.43	0.42
1:M:42:LEU:HD22	1:M:128:CYS:HA	2.01	0.42
2:W:60:GLU:H	2:Y:87:ARG:HB3	1.84	0.42
1:E:97:VAL:CG1	2:Y:129:VAL:CG1	2.92	0.42
2:W:57:LEU:CB	2:Y:114:LEU:HD13	2.47	0.42
1:C:93:ALA:HB2	2:W:137:VAL:HG23	2.01	0.42
1:K:29:ASP:O	1:K:33:ILE:N	2.43	0.42
1:L:177:TRP:CZ2	1:M:71:ASP:OD1	2.73	0.42
2:U:48:TRP:HB3	2:U:66:ARG:HG3	2.01	0.42
2:Y:48:TRP:HB3	2:Y:66:ARG:HG3	2.01	0.42
1:B:42:LEU:HD22	1:B:128:CYS:HA	2.01	0.42
1:O:42:LEU:HD22	1:O:128:CYS:HA	2.01	0.42
1:R:78:ILE:HA	1:R:79:PRO:HD2	1.94	0.42
2:W:58:LEU:HA	2:Y:88:ALA:CB	2.49	0.42
1:N:78:ILE:HA	1:N:79:PRO:HD2	1.94	0.42
1:S:29:ASP:O	1:S:33:ILE:N	2.43	0.42
2:W:48:TRP:HB3	2:W:66:ARG:HG3	2.01	0.42
2:W:57:LEU:CD2	2:Y:114:LEU:HB3	2.48	0.42
1:B:90:LEU:HA	2:V:137:VAL:HG21	2.02	0.41
1:A:28:GLY:O	1:A:32:ARG:N	2.40	0.41
1:K:28:GLY:O	1:K:32:ARG:N	2.40	0.41
1:T:29:ASP:O	1:T:33:ILE:N	2.43	0.41
1:M:29:ASP:O	1:M:33:ILE:N	2.43	0.41
2:V:48:TRP:HB3	2:V:66:ARG:HG3	2.01	0.41
1:A:71:ASP:OD1	1:C:177:TRP:CZ2	2.73	0.41
1:R:42:LEU:HD22	1:R:128:CYS:HA	2.01	0.41
2:Z:9:PHE:HZ	2:Z:150:LEU:HD22	1.85	0.41
1:J:28:GLY:O	1:J:32:ARG:N	2.40	0.41
1:S:177:TRP:CZ2	1:T:71:ASP:OD1	2.74	0.41
1:F:89:LEU:HD13	2:Z:141:LEU:HD21	2.00	0.41
1:F:28:GLY:O	1:F:32:ARG:N	2.40	0.41
2:U:9:PHE:HZ	2:U:150:LEU:HD22	1.85	0.41
1:C:108:GLU:HB3	1:C:176:LEU:HD22	2.03	0.41
1:N:108:GLU:HB3	1:N:176:LEU:HD22	2.03	0.41
1:G:108:GLU:HB3	1:G:176:LEU:HD22	2.03	0.40
2:W:57:LEU:HA	2:Y:114:LEU:HB3	2.02	0.40
1:K:108:GLU:HB3	1:K:176:LEU:HD22	2.04	0.40
1:T:108:GLU:HB3	1:T:176:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:108:GLU:HB3	1:M:176:LEU:HD22	2.04	0.40
2:U:106:PHE:CE1	2:U:150:LEU:HD21	2.57	0.40
1:D:89:LEU:HD12	2:X:141:LEU:HD21	1.76	0.40
2:Y:9:PHE:HZ	2:Y:150:LEU:HD22	1.85	0.40
1:A:89:LEU:CD1	2:U:141:LEU:CD2	2.56	0.40
1:D:29:ASP:O	1:D:33:ILE:N	2.43	0.40
1:Q:108:GLU:HB3	1:Q:176:LEU:HD22	2.04	0.40
1:R:108:GLU:HB3	1:R:176:LEU:HD22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	84	93
1	B	114/119 (96%)	113 (99%)	1 (1%)	84	93
1	C	114/119 (96%)	113 (99%)	1 (1%)	84	93
1	D	114/119 (96%)	113 (99%)	1 (1%)	84	93
1	E	114/119 (96%)	113 (99%)	1 (1%)	84	93
1	F	114/119 (96%)	113 (99%)	1 (1%)	84	93
1	G	114/119 (96%)	113 (99%)	1 (1%)	84	93
1	H	114/119 (96%)	113 (99%)	1 (1%)	84	93
1	I	114/119 (96%)	113 (99%)	1 (1%)	84	93
1	J	114/119 (96%)	113 (99%)	1 (1%)	84	93
1	K	114/119 (96%)	113 (99%)	1 (1%)	84	93
1	L	114/119 (96%)	113 (99%)	1 (1%)	84	93
1	M	114/119 (96%)	113 (99%)	1 (1%)	84	93
1	N	114/119 (96%)	113 (99%)	1 (1%)	84	93
1	O	114/119 (96%)	113 (99%)	1 (1%)	84	93
1	P	114/119 (96%)	113 (99%)	1 (1%)	84	93
1	Q	114/119 (96%)	113 (99%)	1 (1%)	84	93
1	R	114/119 (96%)	113 (99%)	1 (1%)	84	93
1	S	114/119 (96%)	113 (99%)	1 (1%)	84	93
1	T	114/119 (96%)	113 (99%)	1 (1%)	84	93
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	92	96

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
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

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Mol	Chain	Res	Type
1	S	129	ARG
1	T	129	ARG

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 molecules 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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	152/157 (96%)	2.31	84 (55%)	0	3	270, 310, 365, 448	0
1	B	152/157 (96%)	2.06	60 (39%)	0	3	255, 299, 357, 413	0
1	C	152/157 (96%)	1.90	51 (33%)	0	3	261, 303, 346, 387	0
1	D	152/157 (96%)	2.27	80 (52%)	0	3	268, 317, 350, 408	0
1	E	152/157 (96%)	1.90	65 (42%)	0	3	271, 308, 369, 416	0
1	F	152/157 (96%)	2.37	87 (57%)	0	3	273, 318, 363, 405	0
1	G	152/157 (96%)	2.08	69 (45%)	0	3	236, 294, 343, 395	0
1	H	152/157 (96%)	1.27	29 (19%)	2	6	232, 277, 335, 401	0
1	I	152/157 (96%)	1.83	63 (41%)	0	3	238, 283, 333, 382	0
1	J	152/157 (96%)	1.96	54 (35%)	0	3	241, 283, 348, 416	0
1	K	152/157 (96%)	2.17	73 (48%)	0	3	267, 305, 357, 442	0
1	L	152/157 (96%)	1.91	54 (35%)	0	3	249, 295, 350, 403	0
1	M	152/157 (96%)	1.85	53 (34%)	0	3	273, 303, 357, 406	0
1	N	152/157 (96%)	2.39	81 (53%)	0	3	275, 313, 348, 413	0
1	O	152/157 (96%)	2.02	72 (47%)	0	3	261, 307, 361, 413	0
1	P	152/157 (96%)	2.28	75 (49%)	0	3	271, 314, 364, 404	0
1	Q	152/157 (96%)	2.09	74 (48%)	0	3	238, 293, 343, 392	0
1	R	152/157 (96%)	1.27	26 (17%)	2	6	234, 280, 339, 403	0
1	S	152/157 (96%)	1.75	59 (38%)	0	3	234, 286, 333, 404	0
1	T	152/157 (96%)	2.02	55 (36%)	0	3	239, 283, 341, 397	0
2	U	148/165 (89%)	2.23	60 (40%)	0	3	318, 375, 453, 476	0
2	V	148/165 (89%)	1.78	52 (35%)	0	3	293, 336, 392, 440	0
2	W	148/165 (89%)	2.26	72 (48%)	0	3	294, 360, 407, 437	0
2	X	148/165 (89%)	2.15	54 (36%)	0	3	313, 374, 446, 482	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
2	Y	148/165 (89%)	1.93	63 (42%)	0	3	302, 348, 391, 448	0
2	Z	148/165 (89%)	3.04	94 (63%)	0	2	332, 373, 427, 456	0
2	a	148/165 (89%)	2.04	62 (41%)	0	3	271, 337, 394, 444	0
2	b	148/165 (89%)	1.15	27 (18%)	2	6	270, 323, 394, 435	0
2	c	148/165 (89%)	1.75	55 (37%)	0	3	266, 322, 378, 431	0
2	d	148/165 (89%)	2.90	88 (59%)	0	2	285, 347, 409, 440	0
2	e	148/165 (89%)	2.08	54 (36%)	0	3	307, 370, 445, 476	0
2	f	148/165 (89%)	2.01	64 (43%)	0	3	287, 339, 391, 431	0
2	g	148/165 (89%)	2.24	73 (49%)	0	3	289, 359, 414, 441	0
2	h	148/165 (89%)	1.83	52 (35%)	0	3	318, 376, 441, 482	0
2	i	148/165 (89%)	1.84	60 (40%)	0	3	306, 349, 391, 443	0
2	j	148/165 (89%)	2.94	92 (62%)	0	2	323, 372, 421, 445	0
2	k	148/165 (89%)	1.68	53 (35%)	0	3	268, 334, 395, 446	0
2	l	148/165 (89%)	1.22	31 (20%)	1	5	271, 322, 379, 426	0
2	m	148/165 (89%)	1.87	65 (43%)	0	3	273, 320, 378, 432	0
2	n	148/165 (89%)	2.74	78 (52%)	0	3	283, 349, 411, 458	0
All	All	6000/6440 (93%)	2.03	2513 (41%)	0	3	232, 324, 409, 482	0

All (2513) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	U	156	PRO	17.4
2	X	156	PRO	16.3
2	a	157	ALA	14.5
2	X	155	PRO	12.2
2	X	15	HIS	11.8
2	U	157	ALA	11.7
2	d	70	VAL	11.7
2	X	157	ALA	11.6
2	a	156	PRO	11.4
2	j	70	VAL	11.2
2	e	156	PRO	11.2
2	e	12	ARG	11.1
2	d	100	GLU	10.8
2	W	71	ARG	10.7
2	U	15	HIS	10.7

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Mol	Chain	Res	Type	RSRZ
2	n	98	ALA	10.6
1	D	113	GLY	10.5
1	P	174	ASP	10.5
1	J	108	GLU	10.5
1	B	114	GLY	10.2
2	k	157	ALA	10.0
2	g	71	ARG	9.9
2	U	155	PRO	9.9
2	e	157	ALA	9.7
2	n	74	GLN	9.7
2	h	156	PRO	9.7
2	j	29	ALA	9.6
1	T	114	GLY	9.5
2	d	77	GLU	9.4
2	d	71	ARG	9.4
2	e	15	HIS	9.4
2	n	70	VAL	9.3
2	Z	29	ALA	9.2
1	C	174	ASP	9.2
1	T	108	GLU	9.2
2	f	157	ALA	9.1
2	n	100	GLU	9.0
2	d	157	ALA	9.0
2	e	154	LEU	9.0
1	P	114	GLY	8.9
2	Z	30	ALA	8.9
2	j	12	ARG	8.9
2	d	98	ALA	8.9
2	j	30	ALA	8.9
2	U	154	LEU	8.7
2	Z	154	LEU	8.7
1	N	174	ASP	8.6
2	n	71	ARG	8.5
1	F	114	GLY	8.3
2	e	155	PRO	8.3
2	g	70	VAL	8.3
1	K	110	ILE	8.3
1	T	113	GLY	8.2
2	W	70	VAL	8.1
1	C	108	GLU	8.1
2	W	29	ALA	8.0
2	l	157	ALA	7.9

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Mol	Chain	Res	Type	RSRZ
2	W	30	ALA	7.9
1	E	108	GLU	7.9
1	L	114	GLY	7.9
2	h	157	ALA	7.9
2	j	98	ALA	7.8
2	X	154	LEU	7.8
1	N	113	GLY	7.8
1	T	107	GLU	7.8
1	B	174	ASP	7.7
1	D	145	ASN	7.7
2	Z	12	ARG	7.7
2	h	15	HIS	7.6
2	j	71	ARG	7.6
2	d	76	ALA	7.6
2	j	154	LEU	7.6
1	D	174	ASP	7.6
1	J	174	ASP	7.6
2	e	14	PRO	7.5
2	Z	71	ARG	7.5
2	V	157	ALA	7.5
1	P	113	GLY	7.5
2	g	77	GLU	7.4
2	Z	101	GLY	7.4
2	a	30	ALA	7.4
2	Y	100	GLU	7.4
2	h	155	PRO	7.4
2	j	155	PRO	7.3
1	N	107	GLU	7.3
1	F	113	GLY	7.3
2	X	14	PRO	7.2
1	J	113	GLY	7.2
1	B	113	GLY	7.2
1	K	79	PRO	7.1
1	F	174	ASP	7.1
1	C	173	ALA	7.1
2	d	96	ALA	7.1
2	U	14	PRO	7.1
1	J	107	GLU	7.1
1	N	108	GLU	7.1
2	Z	155	PRO	7.1
2	n	76	ALA	7.1
1	G	80	GLY	7.0

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Mol	Chain	Res	Type	RSRZ
2	Z	98	ALA	7.0
2	b	157	ALA	7.0
2	n	77	GLU	7.0
1	C	114	GLY	7.0
2	j	103	GLU	7.0
2	X	98	ALA	6.9
2	g	74	GLN	6.9
2	e	13	HIS	6.9
1	L	174	ASP	6.9
1	N	114	GLY	6.9
1	O	108	GLU	6.9
1	L	108	GLU	6.9
1	P	173	ALA	6.8
2	f	70	VAL	6.8
2	W	100	GLU	6.8
2	n	97	THR	6.8
2	Z	157	ALA	6.8
1	A	110	ILE	6.8
1	A	111	LEU	6.8
1	D	114	GLY	6.8
2	c	157	ALA	6.7
1	P	110	ILE	6.7
2	n	157	ALA	6.7
1	G	79	PRO	6.7
1	M	108	GLU	6.7
1	P	111	LEU	6.6
2	h	154	LEU	6.6
2	l	29	ALA	6.6
2	Z	76	ALA	6.6
2	W	27	PRO	6.6
1	E	110	ILE	6.6
2	Z	70	VAL	6.5
1	G	110	ILE	6.5
2	W	28	ALA	6.5
2	a	155	PRO	6.5
1	M	110	ILE	6.5
2	d	17	GLN	6.5
2	n	30	ALA	6.4
2	d	14	PRO	6.4
1	A	83	ALA	6.4
2	d	74	GLN	6.4
2	W	101	GLY	6.4

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Mol	Chain	Res	Type	RSRZ
1	K	81	HIS	6.3
1	K	108	GLU	6.3
2	Y	77	GLU	6.3
1	C	177	TRP	6.3
1	J	109	PHE	6.3
1	J	176	LEU	6.3
1	T	109	PHE	6.3
1	H	108	GLU	6.3
2	f	100	GLU	6.3
1	E	109	PHE	6.2
2	f	156	PRO	6.2
2	Z	99	ALA	6.2
1	M	174	ASP	6.2
2	e	97	THR	6.2
2	g	29	ALA	6.2
2	U	12	ARG	6.2
2	e	11	LEU	6.2
2	d	99	ALA	6.2
1	Q	79	PRO	6.2
1	A	79	PRO	6.1
1	G	82	ALA	6.1
2	n	14	PRO	6.1
2	a	14	PRO	6.1
2	g	76	ALA	6.1
2	j	97	THR	6.1
1	T	174	ASP	6.1
2	U	153	GLY	6.1
2	n	101	GLY	6.1
1	F	115	ALA	6.1
1	J	177	TRP	6.1
1	K	111	LEU	6.1
2	e	104	MET	6.1
2	g	101	GLY	6.1
2	g	100	GLU	6.1
2	Z	9	PHE	6.0
2	j	157	ALA	6.0
2	d	29	ALA	6.0
2	n	17	GLN	6.0
2	j	104	MET	6.0
2	m	29	ALA	5.9
1	J	114	GLY	5.9
2	Z	103	GLU	5.9

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Mol	Chain	Res	Type	RSRZ
1	G	109	PHE	5.9
2	Z	75	GLY	5.9
2	Z	25	ARG	5.9
1	J	112	PRO	5.9
1	N	145	ASN	5.9
2	W	77	GLU	5.9
2	U	100	GLU	5.9
2	g	30	ALA	5.9
2	X	103	GLU	5.9
1	P	176	LEU	5.8
1	P	108	GLU	5.8
2	n	99	ALA	5.8
1	D	103	LEU	5.8
2	d	97	THR	5.8
2	h	36	ARG	5.8
1	P	115	ALA	5.8
1	M	113	GLY	5.8
1	D	108	GLU	5.8
1	K	176	LEU	5.8
2	f	155	PRO	5.8
1	L	80	GLY	5.7
2	m	155	PRO	5.7
2	f	14	PRO	5.7
2	d	103	GLU	5.7
2	j	14	PRO	5.7
2	j	76	ALA	5.7
1	J	110	ILE	5.7
2	d	101	GLY	5.7
2	d	155	PRO	5.7
2	d	30	ALA	5.7
2	g	86	GLU	5.7
1	I	108	GLU	5.7
1	Q	110	ILE	5.7
1	E	174	ASP	5.7
2	m	32	ALA	5.7
2	Z	151	ALA	5.7
2	j	82	THR	5.7
2	X	29	ALA	5.6
1	K	109	PHE	5.6
1	M	114	GLY	5.6
1	R	79	PRO	5.6
1	K	83	ALA	5.6

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Mol	Chain	Res	Type	RSRZ
1	O	84	ILE	5.6
1	D	79	PRO	5.6
2	a	29	ALA	5.6
1	T	177	TRP	5.6
2	j	13	HIS	5.6
1	A	176	LEU	5.6
1	F	116	ARG	5.5
2	j	10	THR	5.5
1	H	114	GLY	5.5
2	j	11	LEU	5.5
2	i	70	VAL	5.5
1	K	80	GLY	5.5
1	F	111	LEU	5.5
1	J	145	ASN	5.5
2	n	13	HIS	5.5
2	U	97	THR	5.5
2	U	103	GLU	5.5
2	Y	70	VAL	5.5
2	k	71	ARG	5.5
1	M	109	PHE	5.5
2	a	71	ARG	5.5
2	i	71	ARG	5.5
2	U	101	GLY	5.5
1	D	81	HIS	5.4
1	N	116	ARG	5.4
1	F	112	PRO	5.4
1	P	177	TRP	5.4
1	O	110	ILE	5.4
2	j	27	PRO	5.4
2	c	30	ALA	5.4
2	d	154	LEU	5.4
1	J	111	LEU	5.4
1	A	108	GLU	5.4
1	Q	108	GLU	5.4
2	n	29	ALA	5.4
2	n	154	LEU	5.4
1	B	79	PRO	5.4
2	Z	100	GLU	5.4
1	M	80	GLY	5.4
2	j	101	GLY	5.4
2	Z	156	PRO	5.4
2	Z	11	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	I	145	ASN	5.4
1	L	84	ILE	5.3
2	Z	106	PHE	5.3
2	d	72	THR	5.3
2	f	71	ARG	5.3
1	L	81	HIS	5.3
2	b	30	ALA	5.3
1	B	108	GLU	5.3
1	Q	112	PRO	5.3
2	j	156	PRO	5.3
1	G	81	HIS	5.3
2	l	30	ALA	5.3
1	D	107	GLU	5.3
2	V	103	GLU	5.3
2	V	71	ARG	5.3
2	n	103	GLU	5.3
2	g	72	THR	5.3
2	m	154	LEU	5.3
1	Q	111	LEU	5.3
2	Y	157	ALA	5.3
1	A	174	ASP	5.3
2	n	75	GLY	5.3
2	V	154	LEU	5.3
2	a	154	LEU	5.3
1	D	112	PRO	5.3
2	W	76	ALA	5.3
2	n	73	PRO	5.2
2	W	98	ALA	5.2
2	U	29	ALA	5.2
2	n	12	ARG	5.2
2	Y	71	ARG	5.2
2	d	13	HIS	5.2
1	P	109	PHE	5.2
1	T	176	LEU	5.2
2	n	96	ALA	5.2
1	P	116	ARG	5.2
2	n	69	ILE	5.2
1	B	107	GLU	5.2
2	W	74	GLN	5.2
2	Z	13	HIS	5.2
2	k	81	LEU	5.1
2	W	99	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
2	e	103	GLU	5.1
2	n	72	THR	5.1
1	T	178	ASP	5.1
2	U	13	HIS	5.1
1	E	114	GLY	5.1
1	S	174	ASP	5.1
1	B	176	LEU	5.1
1	F	119	ALA	5.1
1	L	79	PRO	5.1
1	L	110	ILE	5.1
1	C	110	ILE	5.1
2	g	84	THR	5.1
1	K	82	ALA	5.1
1	K	177	TRP	5.1
1	N	176	LEU	5.1
2	k	30	ALA	5.1
2	c	155	PRO	5.1
1	J	178	ASP	5.0
2	U	99	ALA	5.0
1	B	84	ILE	5.0
1	F	110	ILE	5.0
1	B	110	ILE	5.0
2	h	14	PRO	5.0
1	O	174	ASP	5.0
1	P	175	VAL	5.0
1	L	145	ASN	5.0
2	e	29	ALA	5.0
2	Z	124	GLY	5.0
2	d	23	PHE	5.0
2	X	30	ALA	5.0
1	P	79	PRO	5.0
2	Z	69	ILE	5.0
1	G	83	ALA	5.0
1	G	108	GLU	5.0
1	O	112	PRO	5.0
1	M	112	PRO	5.0
2	U	11	LEU	5.0
2	m	157	ALA	5.0
1	N	104	PRO	5.0
2	Z	77	GLU	5.0
2	g	54	ARG	5.0
2	Z	27	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
2	m	156	PRO	4.9
1	N	81	HIS	4.9
2	j	75	GLY	4.9
2	j	105	ALA	4.9
2	Z	74	GLN	4.9
1	T	112	PRO	4.9
2	g	12	ARG	4.9
2	i	12	ARG	4.9
1	N	103	LEU	4.9
1	Q	31	ALA	4.9
1	L	71	ASP	4.9
2	k	156	PRO	4.9
2	g	87	ARG	4.9
2	m	150	LEU	4.9
1	H	79	PRO	4.9
1	T	79	PRO	4.9
2	Z	72	THR	4.9
2	d	156	PRO	4.9
2	W	72	THR	4.9
2	Z	82	THR	4.9
1	N	79	PRO	4.9
2	g	75	GLY	4.9
2	i	77	GLU	4.9
2	U	74	GLN	4.9
2	c	154	LEU	4.9
1	A	107	GLU	4.9
2	n	26	GLU	4.9
1	N	105	PRO	4.8
2	i	157	ALA	4.8
2	X	74	GLN	4.8
2	d	69	ILE	4.8
1	A	66	GLN	4.8
2	X	97	THR	4.8
1	L	111	LEU	4.8
2	W	12	ARG	4.8
2	d	79	ARG	4.8
1	O	113	GLY	4.8
2	Y	101	GLY	4.8
2	d	26	GLU	4.8
2	Y	54	ARG	4.8
2	j	23	PHE	4.8
1	R	114	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
2	X	102	GLY	4.8
2	j	106	PHE	4.8
2	n	10	THR	4.8
1	E	112	PRO	4.8
2	Z	150	LEU	4.8
2	c	70	VAL	4.8
1	D	164	ARG	4.7
2	i	54	ARG	4.7
2	Z	14	PRO	4.7
2	g	73	PRO	4.7
1	D	176	LEU	4.7
2	X	100	GLU	4.7
2	g	68	GLU	4.7
2	k	56	PRO	4.7
1	C	107	GLU	4.7
2	W	73	PRO	4.7
1	P	172	GLY	4.7
2	X	13	HIS	4.7
2	c	156	PRO	4.7
1	P	117	GLY	4.7
2	e	150	LEU	4.7
1	J	173	ALA	4.7
2	n	155	PRO	4.7
2	g	85	GLY	4.7
1	F	176	LEU	4.7
2	h	104	MET	4.7
1	L	113	GLY	4.7
2	d	12	ARG	4.7
2	a	70	VAL	4.7
2	h	150	LEU	4.7
2	m	71	ARG	4.6
2	d	116	THR	4.6
1	O	27	MET	4.6
2	j	150	LEU	4.6
1	I	79	PRO	4.6
2	n	20	ALA	4.6
1	E	113	GLY	4.6
1	Q	113	GLY	4.6
2	a	12	ARG	4.6
1	B	177	TRP	4.6
2	l	156	PRO	4.6
2	i	100	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
2	n	82	THR	4.6
2	f	12	ARG	4.6
2	d	73	PRO	4.6
2	X	12	ARG	4.6
1	B	83	ALA	4.6
1	M	81	HIS	4.6
2	j	24	VAL	4.6
1	E	84	ILE	4.6
2	b	29	ALA	4.6
2	W	154	LEU	4.6
2	Z	153	GLY	4.6
2	Y	103	GLU	4.6
1	T	111	LEU	4.6
2	d	25	ARG	4.6
2	V	70	VAL	4.6
2	V	29	ALA	4.6
2	e	98	ALA	4.6
2	j	72	THR	4.6
1	T	110	ILE	4.6
2	h	103	GLU	4.6
1	C	112	PRO	4.5
1	G	112	PRO	4.5
1	L	107	GLU	4.5
1	Q	81	HIS	4.5
1	L	83	ALA	4.5
1	T	145	ASN	4.5
2	X	36	ARG	4.5
2	d	104	MET	4.5
1	P	145	ASN	4.5
2	j	15	HIS	4.5
1	F	108	GLU	4.5
1	B	71	ASP	4.5
1	C	178	ASP	4.5
2	n	81	LEU	4.5
1	N	80	GLY	4.5
2	W	103	GLU	4.5
1	P	107	GLU	4.5
2	d	24	VAL	4.5
2	e	153	GLY	4.5
1	N	112	PRO	4.5
2	h	12	ARG	4.5
2	n	23	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	175	VAL	4.5
1	M	111	LEU	4.5
1	S	83	ALA	4.5
1	B	115	ALA	4.5
1	O	79	PRO	4.5
2	l	77	GLU	4.4
2	Z	97	THR	4.4
1	B	111	LEU	4.4
1	N	110	ILE	4.4
2	k	54	ARG	4.4
2	i	10	THR	4.4
2	f	29	ALA	4.4
1	S	108	GLU	4.4
2	i	11	LEU	4.4
2	n	16	GLY	4.4
1	K	174	ASP	4.4
2	j	28	ALA	4.4
1	T	116	ARG	4.4
2	n	104	MET	4.4
2	e	36	ARG	4.4
1	C	111	LEU	4.4
2	j	69	ILE	4.4
2	h	29	ALA	4.4
2	Z	28	ALA	4.4
1	F	148	PRO	4.4
1	H	81	HIS	4.4
2	V	12	ARG	4.4
2	g	114	LEU	4.4
1	L	176	LEU	4.4
2	j	77	GLU	4.4
2	j	74	GLN	4.4
1	L	82	ALA	4.4
2	Z	81	LEU	4.4
2	V	14	PRO	4.4
2	f	154	LEU	4.4
1	N	115	ALA	4.3
1	F	109	PHE	4.3
1	M	107	GLU	4.3
2	X	69	ILE	4.3
1	R	108	GLU	4.3
1	Q	51	ALA	4.3
2	j	9	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	164	ARG	4.3
2	n	150	LEU	4.3
1	C	113	GLY	4.3
1	O	83	ALA	4.3
2	X	11	LEU	4.3
1	F	107	GLU	4.3
2	k	12	ARG	4.3
1	A	84	ILE	4.3
2	Y	99	ALA	4.3
1	N	173	ALA	4.3
2	X	28	ALA	4.3
1	D	71	ASP	4.3
2	U	104	MET	4.3
2	h	30	ALA	4.3
1	R	113	GLY	4.3
2	n	66	ARG	4.3
1	N	111	LEU	4.3
1	O	107	GLU	4.3
2	e	70	VAL	4.3
2	f	150	LEU	4.3
2	c	29	ALA	4.3
1	N	84	ILE	4.3
2	a	5	ALA	4.3
2	j	20	ALA	4.3
1	A	81	HIS	4.3
1	K	112	PRO	4.3
1	M	38	ASP	4.3
2	V	156	PRO	4.2
2	b	154	LEU	4.2
2	W	69	ILE	4.2
2	e	69	ILE	4.2
2	U	102	GLY	4.2
2	d	75	GLY	4.2
1	I	144	LEU	4.2
2	j	25	ARG	4.2
1	G	113	GLY	4.2
2	W	17	GLN	4.2
2	Z	10	THR	4.2
2	k	57	LEU	4.2
2	X	101	GLY	4.2
2	Y	126	ALA	4.2
1	T	103	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
2	d	21	LEU	4.2
2	h	11	LEU	4.2
2	c	71	ARG	4.2
2	W	10	THR	4.2
2	Z	26	GLU	4.2
2	d	20	ALA	4.2
1	S	110	ILE	4.2
1	M	176	LEU	4.2
1	Q	174	ASP	4.2
1	G	114	GLY	4.2
1	J	116	ARG	4.2
1	Q	132	GLU	4.2
1	A	113	GLY	4.2
1	N	172	GLY	4.2
2	h	13	HIS	4.2
1	T	115	ALA	4.2
2	Y	76	ALA	4.2
1	N	106	LEU	4.2
1	H	109	PHE	4.2
1	M	145	ASN	4.2
1	A	112	PRO	4.2
1	F	172	GLY	4.2
2	b	71	ARG	4.2
1	A	31	ALA	4.2
2	X	153	GLY	4.2
2	h	74	GLN	4.2
2	V	56	PRO	4.2
2	V	30	ALA	4.2
2	Z	96	ALA	4.2
2	c	150	LEU	4.2
2	j	68	GLU	4.1
2	m	103	GLU	4.1
2	X	150	LEU	4.1
2	V	106	PHE	4.1
1	Q	145	ASN	4.1
2	Z	68	GLU	4.1
1	H	110	ILE	4.1
2	V	57	LEU	4.1
2	j	99	ALA	4.1
2	g	25	ARG	4.1
1	F	177	TRP	4.1
2	g	79	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	41	GLU	4.1
2	h	56	PRO	4.1
2	a	101	GLY	4.1
2	W	126	ALA	4.1
2	Z	73	PRO	4.1
2	c	12	ARG	4.1
2	i	56	PRO	4.1
1	S	177	TRP	4.1
2	c	14	PRO	4.1
2	j	151	ALA	4.1
2	k	58	LEU	4.1
1	H	116	ARG	4.1
1	E	116	ARG	4.1
1	P	58	VAL	4.1
1	N	177	TRP	4.1
1	P	80	GLY	4.1
2	Y	29	ALA	4.1
2	g	27	PRO	4.1
2	j	32	ALA	4.1
1	E	79	PRO	4.1
2	j	83	LEU	4.1
2	k	14	PRO	4.1
2	c	33	GLY	4.1
1	O	80	GLY	4.1
2	V	15	HIS	4.1
2	Z	17	GLN	4.1
1	N	83	ALA	4.1
1	Q	52	GLU	4.1
2	f	38	ARG	4.1
2	Y	55	VAL	4.0
1	B	175	VAL	4.0
2	d	105	ALA	4.0
1	A	103	LEU	4.0
2	g	69	ILE	4.0
2	f	68	GLU	4.0
2	g	78	LEU	4.0
1	D	80	GLY	4.0
1	J	172	GLY	4.0
2	U	150	LEU	4.0
2	j	102	GLY	4.0
1	K	105	PRO	4.0
1	N	164	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
2	Y	9	PHE	4.0
1	O	178	ASP	4.0
2	k	154	LEU	4.0
1	A	68	ASP	4.0
1	O	111	LEU	4.0
1	P	41	GLU	4.0
2	g	98	ALA	4.0
1	J	175	VAL	4.0
2	V	9	PHE	4.0
2	Y	56	PRO	4.0
2	a	54	ARG	4.0
1	T	144	LEU	4.0
2	d	150	LEU	4.0
1	E	35	ALA	4.0
1	Q	116	ARG	4.0
2	n	116	THR	4.0
2	m	30	ALA	4.0
1	N	117	GLY	4.0
2	V	104	MET	4.0
1	I	32	ARG	4.0
2	d	10	THR	4.0
2	e	101	GLY	4.0
1	G	51	ALA	4.0
1	N	100	ASN	4.0
2	X	54	ARG	4.0
2	i	57	LEU	3.9
1	A	177	TRP	3.9
1	G	116	ARG	3.9
2	g	157	ALA	3.9
1	K	175	VAL	3.9
2	U	23	PHE	3.9
2	U	26	GLU	3.9
2	g	126	ALA	3.9
1	O	109	PHE	3.9
2	V	150	LEU	3.9
1	C	164	ARG	3.9
1	I	174	ASP	3.9
2	m	70	VAL	3.9
1	C	109	PHE	3.9
2	f	101	GLY	3.9
2	n	86	GLU	3.9
2	U	96	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
2	d	83	LEU	3.9
2	k	10	THR	3.9
1	L	38	ASP	3.9
2	m	9	PHE	3.9
2	d	11	LEU	3.9
1	B	178	ASP	3.9
2	f	69	ILE	3.9
2	f	103	GLU	3.9
2	c	151	ALA	3.9
1	D	119	ALA	3.9
1	E	111	LEU	3.9
2	n	83	LEU	3.9
2	f	15	HIS	3.9
2	a	16	GLY	3.9
2	f	56	PRO	3.9
2	d	27	PRO	3.9
1	F	127	VAL	3.9
1	G	52	GLU	3.9
2	k	77	GLU	3.9
2	m	153	GLY	3.9
2	U	54	ARG	3.9
1	D	76	LEU	3.9
1	G	84	ILE	3.9
1	Q	176	LEU	3.9
2	m	33	GLY	3.8
1	C	102	GLN	3.8
2	Y	12	ARG	3.8
2	Y	124	GLY	3.8
2	j	54	ARG	3.8
1	R	112	PRO	3.8
1	A	114	GLY	3.8
2	V	97	THR	3.8
1	I	84	ILE	3.8
2	d	9	PHE	3.8
2	l	154	LEU	3.8
2	h	101	GLY	3.8
2	g	82	THR	3.8
1	A	80	GLY	3.8
2	n	24	VAL	3.8
2	n	25	ARG	3.8
2	b	156	PRO	3.8
2	l	14	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
2	h	54	ARG	3.8
2	j	114	LEU	3.8
1	D	52	GLU	3.8
1	Q	80	GLY	3.8
1	K	116	ARG	3.8
2	m	12	ARG	3.8
1	S	79	PRO	3.8
2	h	100	GLU	3.8
1	Q	130	ARG	3.8
1	S	32	ARG	3.8
1	M	102	GLN	3.8
2	W	155	PRO	3.8
2	Z	104	MET	3.8
1	A	102	GLN	3.8
1	M	164	ARG	3.8
2	U	36	ARG	3.8
2	g	14	PRO	3.8
1	H	113	GLY	3.8
1	O	81	HIS	3.8
2	Z	83	LEU	3.8
2	h	98	ALA	3.8
1	A	67	HIS	3.8
1	O	71	ASP	3.8
2	j	81	LEU	3.8
1	Q	114	GLY	3.8
2	g	11	LEU	3.8
2	n	15	HIS	3.8
1	G	111	LEU	3.8
1	N	89	LEU	3.8
1	A	116	ARG	3.8
1	D	75	GLU	3.8
2	Y	125	ALA	3.8
2	V	73	PRO	3.8
1	L	164	ARG	3.7
2	j	153	GLY	3.7
2	d	32	ALA	3.7
1	F	61	ALA	3.7
2	Z	24	VAL	3.7
2	U	56	PRO	3.7
1	A	82	ALA	3.7
2	a	15	HIS	3.7
1	O	116	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	N	144	LEU	3.7
1	F	173	ALA	3.7
2	g	16	GLY	3.7
2	V	98	ALA	3.7
2	g	150	LEU	3.7
1	N	119	ALA	3.7
2	k	28	ALA	3.7
2	h	10	THR	3.7
2	Z	126	ALA	3.7
2	V	105	ALA	3.7
2	f	99	ALA	3.7
2	i	126	ALA	3.7
2	h	70	VAL	3.7
1	F	164	ARG	3.7
2	a	17	GLN	3.7
1	I	38	ASP	3.7
2	i	29	ALA	3.7
1	L	75	GLU	3.7
1	S	116	ARG	3.7
2	a	28	ALA	3.7
2	b	77	GLU	3.7
1	A	109	PHE	3.7
2	l	23	PHE	3.7
2	m	36	ARG	3.7
2	n	112	ALA	3.7
1	N	175	VAL	3.7
2	d	15	HIS	3.7
2	l	124	GLY	3.7
1	D	45	GLN	3.7
2	h	148	GLN	3.7
1	A	99	TYR	3.6
2	Z	125	ALA	3.6
2	e	30	ALA	3.6
1	D	122	HIS	3.6
2	X	99	ALA	3.6
2	a	4	SER	3.6
1	N	71	ASP	3.6
1	R	174	ASP	3.6
2	n	54	ARG	3.6
1	L	175	VAL	3.6
1	S	112	PRO	3.6
1	T	118	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
2	b	155	PRO	3.6
1	R	110	ILE	3.6
1	K	107	GLU	3.6
1	Q	83	ALA	3.6
2	Z	38	ARG	3.6
1	C	84	ILE	3.6
2	U	10	THR	3.6
2	h	97	THR	3.6
2	n	102	GLY	3.6
2	Z	21	LEU	3.6
1	F	83	ALA	3.6
2	c	148	GLN	3.6
2	e	105	ALA	3.6
1	J	103	LEU	3.6
2	k	11	LEU	3.6
1	G	174	ASP	3.6
2	a	10	THR	3.6
2	a	103	GLU	3.6
2	g	83	LEU	3.6
1	F	103	LEU	3.6
1	I	111	LEU	3.6
1	C	176	LEU	3.6
1	D	104	PRO	3.6
1	C	103	LEU	3.6
1	D	110	ILE	3.6
2	f	77	GLU	3.6
2	W	157	ALA	3.6
2	W	75	GLY	3.6
2	X	104	MET	3.6
1	G	145	ASN	3.6
2	d	87	ARG	3.6
2	e	76	ALA	3.6
1	C	116	ARG	3.6
1	I	116	ARG	3.6
1	T	175	VAL	3.6
2	n	18	ALA	3.6
1	K	75	GLU	3.6
1	Q	175	VAL	3.6
1	S	178	ASP	3.6
2	Y	98	ALA	3.6
1	C	175	VAL	3.6
1	D	49	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	e	74	GLN	3.6
2	j	16	GLY	3.6
1	D	100	ASN	3.5
1	T	104	PRO	3.5
2	j	21	LEU	3.5
2	k	70	VAL	3.5
1	B	116	ARG	3.5
2	W	26	GLU	3.5
2	V	74	GLN	3.5
2	Z	66	ARG	3.5
2	k	17	GLN	3.5
1	P	144	LEU	3.5
1	E	164	ARG	3.5
1	F	32	ARG	3.5
1	Q	109	PHE	3.5
2	Z	36	ARG	3.5
1	T	173	ALA	3.5
2	m	76	ALA	3.5
2	W	86	GLU	3.5
2	i	5	ALA	3.5
2	f	9	PHE	3.5
2	W	84	THR	3.5
2	W	16	GLY	3.5
1	F	175	VAL	3.5
2	U	98	ALA	3.5
2	n	67	SER	3.5
2	Y	58	LEU	3.5
2	k	101	GLY	3.5
1	F	145	ASN	3.5
1	D	116	ARG	3.5
1	F	132	GLU	3.5
1	E	44	SER	3.5
1	T	172	GLY	3.5
2	e	151	ALA	3.5
1	F	57	ASP	3.5
2	f	130	MET	3.5
2	h	102	GLY	3.5
2	d	28	ALA	3.5
2	l	155	PRO	3.5
1	D	82	ALA	3.5
1	G	130	ARG	3.5
1	T	119	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	d	54	ARG	3.5
1	M	175	VAL	3.5
1	O	117	GLY	3.5
2	l	71	ARG	3.5
1	K	38	ASP	3.5
1	Q	144	LEU	3.5
2	k	150	LEU	3.5
2	m	73	PRO	3.5
2	e	71	ARG	3.5
2	k	104	MET	3.5
2	W	3	LEU	3.5
2	f	76	ALA	3.5
2	n	27	PRO	3.5
1	D	175	VAL	3.5
1	A	28	GLY	3.5
1	P	45	GLN	3.5
2	V	11	LEU	3.5
2	U	151	ALA	3.5
2	Z	102	GLY	3.5
2	g	17	GLN	3.5
1	F	125	ARG	3.4
2	h	47	VAL	3.5
2	e	96	ALA	3.4
2	m	151	ALA	3.4
2	m	104	MET	3.4
2	X	10	THR	3.4
1	O	145	ASN	3.4
2	Y	11	LEU	3.4
2	m	14	PRO	3.4
2	U	46	GLN	3.4
2	d	3	LEU	3.4
1	A	43	ASN	3.4
1	M	79	PRO	3.4
2	Y	10	THR	3.4
1	Q	54	LEU	3.4
1	S	176	LEU	3.4
2	Y	83	LEU	3.4
2	a	38	ARG	3.4
2	g	88	ALA	3.4
2	h	153	GLY	3.4
1	M	148	PRO	3.4
1	A	51	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	N	167	ASN	3.4
2	a	56	PRO	3.4
1	C	172	GLY	3.4
2	U	71	ARG	3.4
2	m	106	PHE	3.4
1	N	38	ASP	3.4
2	g	125	ALA	3.4
1	O	114	GLY	3.4
1	N	146	ILE	3.4
1	F	118	ALA	3.4
1	C	76	LEU	3.4
1	A	95	TRP	3.4
2	j	26	GLU	3.4
2	j	125	ALA	3.4
1	I	110	ILE	3.4
2	d	92	VAL	3.4
1	H	115	ALA	3.4
1	I	41	GLU	3.4
2	V	100	GLU	3.4
2	Y	74	GLN	3.4
2	g	155	PRO	3.4
2	n	11	LEU	3.4
1	S	38	ASP	3.4
1	Q	82	ALA	3.4
2	k	103	GLU	3.4
1	C	75	GLU	3.4
1	F	45	GLN	3.4
1	N	125	ARG	3.4
2	d	102	GLY	3.4
2	i	144	MET	3.4
1	A	32	ARG	3.4
1	A	125	ARG	3.4
2	b	81	LEU	3.4
2	c	81	LEU	3.4
1	D	102	GLN	3.4
1	E	41	GLU	3.4
1	A	171	GLY	3.4
1	S	114	GLY	3.4
2	d	78	LEU	3.4
1	B	81	HIS	3.4
1	Q	71	ASP	3.4
1	G	48	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
2	W	25	ARG	3.4
2	c	57	LEU	3.4
1	N	109	PHE	3.3
2	j	79	ARG	3.3
1	P	103	LEU	3.3
1	N	122	HIS	3.3
2	U	81	LEU	3.3
1	C	79	PRO	3.3
2	Y	17	GLN	3.3
1	D	144	LEU	3.3
2	j	112	ALA	3.3
1	D	177	TRP	3.3
2	a	9	PHE	3.3
2	g	124	GLY	3.3
1	N	32	ARG	3.3
1	E	48	VAL	3.3
2	k	9	PHE	3.3
2	n	124	GLY	3.3
1	K	104	PRO	3.3
1	P	112	PRO	3.3
1	Q	68	ASP	3.3
1	Q	173	ALA	3.3
2	Z	92	VAL	3.3
1	J	144	LEU	3.3
2	W	83	LEU	3.3
2	g	115	ALA	3.3
1	A	172	GLY	3.3
1	O	144	LEU	3.3
1	G	49	LEU	3.3
2	a	13	HIS	3.3
1	F	84	ILE	3.3
1	T	48	VAL	3.3
1	S	113	GLY	3.3
2	f	30	ALA	3.3
1	K	84	ILE	3.3
2	U	148	GLN	3.3
1	F	122	HIS	3.3
2	g	96	ALA	3.3
1	G	50	LEU	3.3
1	L	72	LEU	3.3
1	R	107	GLU	3.3
1	B	167	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
2	f	98	ALA	3.3
2	m	92	VAL	3.3
1	I	112	PRO	3.3
1	C	99	TYR	3.3
2	m	74	GLN	3.3
1	D	72	LEU	3.3
1	M	99	TYR	3.3
1	P	148	PRO	3.3
1	S	109	PHE	3.3
1	B	145	ASN	3.3
1	L	70	PHE	3.3
2	b	130	MET	3.3
1	L	146	ILE	3.3
1	H	111	LEU	3.3
1	D	83	ALA	3.3
2	Y	94	GLY	3.3
1	J	32	ARG	3.3
1	K	125	ARG	3.3
1	O	41	GLU	3.3
1	P	164	ARG	3.3
2	d	82	THR	3.3
2	f	57	LEU	3.3
1	I	31	ALA	3.3
1	K	99	TYR	3.2
2	Z	15	HIS	3.2
1	G	35	ALA	3.2
1	E	45	GLN	3.2
1	O	164	ARG	3.2
2	W	54	ARG	3.2
1	N	76	LEU	3.2
2	i	58	LEU	3.2
2	W	78	LEU	3.2
2	j	126	ALA	3.2
1	S	111	LEU	3.2
1	E	80	GLY	3.2
1	H	112	PRO	3.2
2	Y	82	THR	3.2
1	R	111	LEU	3.2
2	d	115	ALA	3.2
1	A	104	PRO	3.2
2	h	23	PHE	3.2
2	l	37	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	m	130	MET	3.2
1	G	70	PHE	3.2
1	P	167	ASN	3.2
1	B	41	GLU	3.2
2	Z	114	LEU	3.2
2	W	125	ALA	3.2
2	Y	110	PHE	3.2
2	f	110	PHE	3.2
1	P	55	PRO	3.2
2	d	124	GLY	3.2
2	f	73	PRO	3.2
2	Z	23	PHE	3.2
1	O	175	VAL	3.2
2	c	69	ILE	3.2
2	V	79	ARG	3.2
2	h	71	ARG	3.2
1	O	165	VAL	3.2
2	k	79	ARG	3.2
1	J	41	GLU	3.2
2	Z	105	ALA	3.2
2	n	105	ALA	3.2
1	G	32	ARG	3.2
1	T	122	HIS	3.2
2	m	15	HIS	3.2
1	F	42	LEU	3.2
1	O	52	GLU	3.2
2	Y	69	ILE	3.2
1	K	113	GLY	3.2
1	B	76	LEU	3.2
2	i	92	VAL	3.2
2	c	36	ARG	3.2
2	g	10	THR	3.2
1	L	45	GLN	3.2
1	Q	48	VAL	3.2
2	k	155	PRO	3.2
1	B	75	GLU	3.2
1	O	146	ILE	3.2
1	S	115	ALA	3.2
2	j	18	ALA	3.2
1	G	176	LEU	3.2
1	T	41	GLU	3.2
1	A	70	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
2	k	13	HIS	3.2
2	Z	3	LEU	3.2
1	I	68	ASP	3.2
2	a	110	PHE	3.2
2	i	150	LEU	3.1
1	K	68	ASP	3.1
1	O	35	ALA	3.1
2	j	17	GLN	3.1
1	S	126	THR	3.1
2	X	77	GLU	3.1
2	W	23	PHE	3.1
1	K	71	ASP	3.1
2	a	81	LEU	3.1
2	V	82	THR	3.1
2	e	99	ALA	3.1
2	Z	47	VAL	3.1
2	W	82	THR	3.1
2	j	100	GLU	3.1
2	X	27	PRO	3.1
2	m	147	PRO	3.1
2	j	130	MET	3.1
1	E	178	ASP	3.1
2	i	124	GLY	3.1
2	m	11	LEU	3.1
1	G	146	ILE	3.1
1	S	84	ILE	3.1
1	B	112	PRO	3.1
2	W	87	ARG	3.1
1	D	111	LEU	3.1
1	I	83	ALA	3.1
2	n	79	ARG	3.1
1	G	71	ASP	3.1
2	U	152	ALA	3.1
1	P	104	PRO	3.1
1	L	40	ASP	3.1
1	C	104	PRO	3.1
2	i	154	LEU	3.1
1	E	73	GLY	3.1
1	O	177	TRP	3.1
2	j	36	ARG	3.1
1	A	145	ASN	3.1
1	F	144	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	70	PHE	3.1
2	i	14	PRO	3.1
2	n	126	ALA	3.1
1	I	176	LEU	3.1
1	C	81	HIS	3.1
2	V	23	PHE	3.1
2	a	23	PHE	3.1
2	j	110	PHE	3.1
1	M	177	TRP	3.1
1	S	75	GLU	3.1
2	d	16	GLY	3.1
1	G	173	ALA	3.1
1	K	103	LEU	3.1
2	i	9	PHE	3.1
1	B	29	ASP	3.1
2	e	102	GLY	3.1
2	j	66	ARG	3.1
1	T	83	ALA	3.1
1	E	146	ILE	3.1
1	D	50	LEU	3.1
1	K	102	GLN	3.1
2	V	10	THR	3.1
2	h	99	ALA	3.1
2	i	156	PRO	3.1
1	B	109	PHE	3.1
1	D	89	LEU	3.1
1	M	95	TRP	3.1
2	Y	7	GLN	3.1
2	n	21	LEU	3.1
1	M	41	GLU	3.1
2	k	100	GLU	3.1
2	X	70	VAL	3.1
2	j	92	VAL	3.1
2	d	94	GLY	3.1
1	B	104	PRO	3.1
2	U	73	PRO	3.1
1	N	118	ALA	3.1
1	Q	35	ALA	3.1
2	U	30	ALA	3.1
1	F	104	PRO	3.1
2	d	86	GLU	3.1
1	P	57	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
2	b	23	PHE	3.1
2	X	16	GLY	3.1
2	m	68	GLU	3.0
2	n	92	VAL	3.1
1	F	166	LEU	3.0
1	L	109	PHE	3.0
2	U	72	THR	3.0
1	A	71	ASP	3.0
1	E	115	ALA	3.0
2	Y	96	ALA	3.0
2	m	101	GLY	3.0
2	Z	80	PRO	3.0
2	Z	147	PRO	3.0
2	a	69	ILE	3.0
2	a	150	LEU	3.0
2	a	151	ALA	3.0
2	h	37	LEU	3.0
1	O	70	PHE	3.0
2	n	45	GLU	3.0
1	C	41	GLU	3.0
1	Q	70	PHE	3.0
2	d	68	GLU	3.0
1	T	146	ILE	3.0
1	J	38	ASP	3.0
1	F	105	PRO	3.0
2	c	17	GLN	3.0
2	b	70	VAL	3.0
2	c	77	GLU	3.0
2	c	133	ALA	3.0
2	h	76	ALA	3.0
2	m	105	ALA	3.0
1	E	103	LEU	3.0
1	T	75	GLU	3.0
2	n	68	GLU	3.0
1	B	70	PHE	3.0
1	C	126	THR	3.0
1	A	130	ARG	3.0
1	M	130	ARG	3.0
2	U	130	MET	3.0
2	g	15	HIS	3.0
2	Y	57	LEU	3.0
1	B	45	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
2	g	23	PHE	3.0
2	Y	78	LEU	3.0
1	F	130	ARG	3.0
2	b	54	ARG	3.0
2	g	24	VAL	3.0
1	G	41	GLU	3.0
2	g	103	GLU	3.0
2	i	125	ALA	3.0
1	Q	84	ILE	3.0
2	c	58	LEU	3.0
2	f	74	GLN	3.0
2	U	82	THR	3.0
1	J	164	ARG	3.0
1	K	115	ALA	3.0
1	D	115	ALA	3.0
1	N	99	TYR	3.0
2	e	10	THR	3.0
2	a	3	LEU	3.0
2	f	67	SER	3.0
2	i	78	LEU	3.0
2	V	77	GLU	3.0
1	D	178	ASP	3.0
1	K	31	ALA	3.0
1	R	81	HIS	3.0
1	Q	146	ILE	3.0
2	n	47	VAL	3.0
2	k	29	ALA	3.0
1	A	44	SER	3.0
2	X	73	PRO	3.0
2	f	11	LEU	3.0
2	Z	32	ALA	3.0
1	J	104	PRO	3.0
1	M	48	VAL	3.0
2	c	82	THR	3.0
1	J	106	LEU	3.0
1	Q	142	GLU	3.0
2	m	100	GLU	3.0
2	V	38	ARG	3.0
1	E	176	LEU	2.9
1	K	32	ARG	2.9
1	L	144	LEU	2.9
2	W	85	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	f	40	LEU	2.9
2	f	54	ARG	2.9
2	m	148	GLN	2.9
1	G	38	ASP	2.9
1	D	84	ILE	2.9
2	a	57	LEU	2.9
1	D	38	ASP	2.9
1	E	175	VAL	2.9
1	O	48	VAL	2.9
1	R	115	ALA	2.9
2	U	76	ALA	2.9
2	m	75	GLY	2.9
1	N	160	PHE	2.9
2	g	81	LEU	2.9
2	c	130	MET	2.9
1	A	49	LEU	2.9
2	X	55	VAL	2.9
2	d	110	PHE	2.9
2	n	9	PHE	2.9
2	X	60	GLU	2.9
1	K	124	CYS	2.9
2	Z	46	GLN	2.9
2	g	36	ARG	2.9
1	C	95	TRP	2.9
2	d	18	ALA	2.9
2	a	100	GLU	2.9
2	e	100	GLU	2.9
1	D	146	ILE	2.9
1	I	129	ARG	2.9
1	Q	167	ASN	2.9
1	S	175	VAL	2.9
2	W	11	LEU	2.9
2	d	114	LEU	2.9
2	i	82	THR	2.9
2	n	144	MET	2.9
1	D	117	GLY	2.9
1	I	76	LEU	2.9
2	W	14	PRO	2.9
2	Z	56	PRO	2.9
2	i	133	ALA	2.9
1	H	80	GLY	2.9
1	K	122	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	116	ARG	2.9
1	Q	78	ILE	2.9
1	N	82	ALA	2.9
2	l	125	ALA	2.9
1	A	50	LEU	2.9
2	Z	146	LEU	2.9
2	f	106	PHE	2.9
1	A	52	GLU	2.9
2	d	66	ARG	2.9
1	H	176	LEU	2.9
2	c	56	PRO	2.9
2	V	55	VAL	2.9
1	D	67	HIS	2.9
1	N	130	ARG	2.9
1	C	80	GLY	2.9
2	Z	88	ALA	2.9
2	e	81	LEU	2.9
2	Y	14	PRO	2.9
2	V	153	GLY	2.9
1	T	130	ARG	2.9
2	c	126	ALA	2.9
2	U	144	MET	2.9
1	F	58	VAL	2.9
1	A	41	GLU	2.9
1	G	36	ILE	2.9
2	d	106	PHE	2.9
2	i	103	GLU	2.9
1	I	77	CYS	2.9
1	K	43	ASN	2.9
1	L	43	ASN	2.9
2	Z	64	PRO	2.9
2	b	14	PRO	2.9
2	i	83	LEU	2.9
2	j	3	LEU	2.9
1	D	118	ALA	2.9
1	E	148	PRO	2.9
1	K	42	LEU	2.9
2	j	31	LEU	2.9
1	A	40	ASP	2.9
1	P	61	ALA	2.9
2	b	99	ALA	2.9
2	g	110	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	Q	75	GLU	2.9
1	E	117	GLY	2.9
1	F	43	ASN	2.9
1	F	44	SER	2.9
1	D	70	PHE	2.9
1	D	51	ALA	2.8
1	E	99	TYR	2.8
1	E	166	LEU	2.8
1	G	132	GLU	2.8
1	J	29	ASP	2.8
1	M	58	VAL	2.8
2	g	92	VAL	2.8
2	n	46	GLN	2.8
1	S	76	LEU	2.8
1	I	109	PHE	2.8
2	V	155	PRO	2.8
1	Q	99	TYR	2.8
2	Z	112	ALA	2.8
2	g	94	GLY	2.8
1	D	54	LEU	2.8
2	Y	144	MET	2.8
2	Z	44	GLY	2.8
1	R	176	LEU	2.8
2	f	37	LEU	2.8
2	i	55	VAL	2.8
1	E	130	ARG	2.8
2	W	68	GLU	2.8
2	d	81	LEU	2.8
2	f	104	MET	2.8
2	V	33	GLY	2.8
1	H	107	GLU	2.8
1	O	95	TRP	2.8
1	T	81	HIS	2.8
2	i	76	ALA	2.8
1	S	130	ARG	2.8
2	V	54	ARG	2.8
1	A	173	ALA	2.8
1	P	160	PHE	2.8
2	Y	108	PHE	2.8
1	A	138	LEU	2.8
2	n	78	LEU	2.8
2	f	105	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	i	104	MET	2.8
2	m	96	ALA	2.8
2	V	130	MET	2.8
2	d	95	GLN	2.8
1	F	79	PRO	2.8
1	T	106	LEU	2.8
1	B	160	PHE	2.8
1	B	165	VAL	2.8
1	C	58	VAL	2.8
1	E	83	ALA	2.8
1	P	130	ARG	2.8
1	B	67	HIS	2.8
2	U	16	GLY	2.8
2	Z	42	SER	2.8
2	j	96	ALA	2.8
2	l	69	ILE	2.8
1	C	57	ASP	2.8
1	R	116	ARG	2.8
2	W	96	ALA	2.8
2	j	131	VAL	2.8
1	D	148	PRO	2.8
2	W	13	HIS	2.8
2	i	69	ILE	2.8
1	L	177	TRP	2.8
2	i	129	VAL	2.8
2	Z	78	LEU	2.8
2	f	97	THR	2.8
2	n	3	LEU	2.8
2	Z	142	VAL	2.8
1	K	65	ILE	2.8
1	L	36	ILE	2.8
1	L	116	ARG	2.8
2	b	150	LEU	2.8
1	K	95	TRP	2.8
2	d	93	SER	2.8
2	m	7	GLN	2.8
1	H	174	ASP	2.8
1	I	125	ARG	2.8
1	I	126	THR	2.8
2	g	93	SER	2.8
2	f	92	VAL	2.8
1	G	103	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	48	VAL	2.8
1	Q	45	GLN	2.8
1	I	36	ILE	2.8
1	P	38	ASP	2.8
1	T	164	ARG	2.8
2	k	66	ARG	2.8
1	N	102	GLN	2.8
2	e	56	PRO	2.8
2	l	150	LEU	2.8
2	Z	54	ARG	2.8
1	I	48	VAL	2.8
1	J	27	MET	2.8
1	L	76	LEU	2.8
2	Z	79	ARG	2.8
2	f	36	ARG	2.8
1	A	45	GLN	2.8
1	J	52	GLU	2.8
1	Q	36	ILE	2.8
2	X	37	LEU	2.8
2	V	151	ALA	2.8
2	d	85	GLY	2.8
1	K	136	LYS	2.8
1	F	151	TYR	2.8
1	L	95	TRP	2.8
1	G	75	GLU	2.7
1	Q	53	PRO	2.7
2	a	148	GLN	2.7
2	f	10	THR	2.7
1	S	77	CYS	2.7
1	L	48	VAL	2.7
1	O	32	ARG	2.7
2	W	24	VAL	2.7
1	A	35	ALA	2.7
1	D	66	GLN	2.7
2	d	40	LEU	2.7
1	P	32	ARG	2.7
1	M	51	ALA	2.7
1	E	77	CYS	2.7
1	H	177	TRP	2.7
1	R	50	LEU	2.7
2	X	82	THR	2.7
2	e	68	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	i	60	GLU	2.7
1	M	84	ILE	2.7
2	j	19	ALA	2.7
1	T	102	GLN	2.7
2	i	4	SER	2.7
2	i	17	GLN	2.7
2	j	33	GLY	2.7
1	T	49	LEU	2.7
2	k	106	PHE	2.7
1	S	41	GLU	2.7
2	h	55	VAL	2.7
2	W	110	PHE	2.7
1	I	45	GLN	2.7
2	i	101	GLY	2.7
2	f	126	ALA	2.7
2	l	32	ALA	2.7
1	P	95	TRP	2.7
1	P	132	GLU	2.7
2	l	26	GLU	2.7
1	F	62	LEU	2.7
1	K	66	GLN	2.7
2	Z	18	ALA	2.7
1	B	146	ILE	2.7
1	N	95	TRP	2.7
1	O	75	GLU	2.7
2	j	132	GLN	2.7
1	Q	103	LEU	2.7
1	A	61	ALA	2.7
1	K	67	HIS	2.7
2	m	67	SER	2.7
1	K	49	LEU	2.7
1	Q	49	LEU	2.7
1	R	41	GLU	2.7
1	S	27	MET	2.7
1	T	143	PRO	2.7
2	U	27	PRO	2.7
2	b	83	LEU	2.7
2	i	110	PHE	2.7
2	e	82	THR	2.7
2	n	87	ARG	2.7
1	I	172	GLY	2.7
1	T	38	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	d	64	PRO	2.7
1	P	119	ALA	2.7
2	j	84	THR	2.7
2	j	86	GLU	2.7
1	P	106	LEU	2.7
2	Z	87	ARG	2.7
2	m	25	ARG	2.7
1	A	135	ILE	2.7
1	Q	148	PRO	2.7
1	K	58	VAL	2.7
1	O	86	GLU	2.7
1	E	144	LEU	2.7
1	P	54	LEU	2.7
2	Z	67	SER	2.7
2	a	60	GLU	2.7
1	J	45	GLN	2.7
1	A	127	VAL	2.7
2	m	69	ILE	2.7
1	J	115	ALA	2.7
1	C	130	ARG	2.7
1	R	109	PHE	2.7
2	a	11	LEU	2.7
2	i	146	LEU	2.7
1	H	84	ILE	2.7
1	F	120	LEU	2.7
2	Y	92	VAL	2.7
2	m	28	ALA	2.7
1	K	135	ILE	2.7
1	I	177	TRP	2.7
2	V	32	ALA	2.7
2	Z	91	ALA	2.7
1	B	38	ASP	2.7
1	K	41	GLU	2.7
1	K	78	ILE	2.7
1	B	28	GLY	2.7
2	j	78	LEU	2.7
2	Z	152	ALA	2.7
1	D	41	GLU	2.7
1	N	27	MET	2.7
2	c	54	ARG	2.7
1	F	99	TYR	2.7
1	F	117	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	Q	117	GLY	2.7
1	A	122	HIS	2.7
2	c	104	MET	2.7
2	l	81	LEU	2.7
2	m	77	GLU	2.7
1	H	145	ASN	2.7
1	M	35	ALA	2.7
1	Q	66	GLN	2.7
2	k	148	GLN	2.7
1	O	29	ASP	2.6
1	S	122	HIS	2.7
2	Z	37	LEU	2.7
2	Z	45	GLU	2.7
2	a	40	LEU	2.7
2	h	38	ARG	2.7
1	A	106	LEU	2.6
2	Y	104	MET	2.6
1	I	124	CYS	2.6
2	h	77	GLU	2.6
1	B	82	ALA	2.6
2	X	124	GLY	2.6
2	k	16	GLY	2.6
1	G	167	ASN	2.6
1	M	144	LEU	2.6
1	O	45	GLN	2.6
2	X	148	GLN	2.6
2	f	83	LEU	2.6
2	W	97	THR	2.6
2	b	100	GLU	2.6
1	Q	177	TRP	2.6
2	l	99	ALA	2.6
1	A	144	LEU	2.6
1	F	165	VAL	2.6
1	J	79	PRO	2.6
2	W	150	LEU	2.6
2	l	83	LEU	2.6
2	m	34	VAL	2.6
1	E	52	GLU	2.6
2	W	15	HIS	2.6
2	e	46	GLN	2.6
1	I	37	GLY	2.6
1	I	75	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	126	THR	2.6
1	O	74	GLY	2.6
2	Y	15	HIS	2.6
2	Y	30	ALA	2.6
2	e	75	GLY	2.6
1	G	175	VAL	2.6
1	J	143	PRO	2.6
2	a	74	GLN	2.6
2	c	9	PHE	2.6
1	A	75	GLU	2.6
2	d	112	ALA	2.6
2	k	98	ALA	2.6
1	G	44	SER	2.6
2	a	67	SER	2.6
2	g	97	THR	2.6
1	I	71	ASP	2.6
1	R	177	TRP	2.6
2	n	114	LEU	2.6
1	Q	107	GLU	2.6
1	S	172	GLY	2.6
2	m	102	GLY	2.6
2	X	9	PHE	2.6
1	D	68	ASP	2.6
1	M	45	GLN	2.6
2	i	81	LEU	2.6
2	k	3	LEU	2.6
1	O	173	ALA	2.6
1	P	46	ILE	2.6
2	V	36	ARG	2.6
2	X	126	ALA	2.6
1	Q	166	LEU	2.6
2	V	81	LEU	2.6
2	W	81	LEU	2.6
1	F	95	TRP	2.6
2	Y	95	GLN	2.6
2	b	69	ILE	2.6
2	f	148	GLN	2.6
1	E	165	VAL	2.6
2	V	13	HIS	2.6
2	a	58	LEU	2.6
1	D	109	PHE	2.6
1	K	45	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	68	ASP	2.6
1	J	168	ARG	2.6
2	Y	154	LEU	2.6
2	e	77	GLU	2.6
1	F	46	ILE	2.6
1	B	80	GLY	2.6
1	Q	69	LEU	2.6
2	a	92	VAL	2.6
2	h	151	ALA	2.6
1	A	63	SER	2.6
1	L	132	GLU	2.6
2	Z	20	ALA	2.6
2	b	126	ALA	2.6
2	g	154	LEU	2.6
2	c	23	PHE	2.6
2	k	60	GLU	2.6
1	C	50	LEU	2.6
1	C	100	ASN	2.6
1	I	89	LEU	2.6
1	O	166	LEU	2.6
1	T	168	ARG	2.6
2	c	15	HIS	2.6
2	e	106	PHE	2.6
1	C	48	VAL	2.6
1	E	93	ALA	2.6
1	O	176	LEU	2.6
2	X	53	VAL	2.6
1	K	171	GLY	2.6
1	I	130	ARG	2.6
1	B	132	GLU	2.6
2	e	110	PHE	2.6
2	m	23	PHE	2.6
2	W	114	LEU	2.6
2	a	76	ALA	2.6
1	O	135	ILE	2.6
2	V	101	GLY	2.6
2	n	156	PRO	2.6
1	B	32	ARG	2.6
2	i	74	GLN	2.6
1	I	99	TYR	2.6
1	S	144	LEU	2.6
1	J	170	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	c	76	ALA	2.6
2	j	111	GLN	2.6
1	Q	41	GLU	2.6
2	U	75	GLY	2.6
1	G	166	LEU	2.6
1	I	49	LEU	2.6
2	V	110	PHE	2.6
2	d	80	PRO	2.6
1	N	75	GLU	2.6
1	N	142	GLU	2.6
1	Q	131	ALA	2.6
2	a	32	ALA	2.6
1	B	135	ILE	2.6
1	E	50	LEU	2.6
2	Z	40	LEU	2.6
2	c	11	LEU	2.6
1	M	125	ARG	2.5
2	U	66	ARG	2.5
1	M	142	GLU	2.5
2	Z	110	PHE	2.5
2	l	57	LEU	2.5
2	W	79	ARG	2.5
2	n	34	VAL	2.5
1	A	76	LEU	2.5
1	G	73	GLY	2.5
1	K	76	LEU	2.5
1	O	171	GLY	2.5
2	W	9	PHE	2.5
1	A	170	ALA	2.5
1	C	83	ALA	2.5
1	K	35	ALA	2.5
2	Y	28	ALA	2.5
2	m	54	ARG	2.5
2	m	35	GLN	2.5
2	Z	16	GLY	2.5
1	B	72	LEU	2.5
1	C	77	CYS	2.5
1	B	173	ALA	2.5
1	J	130	ARG	2.5
1	S	49	LEU	2.5
2	U	105	ALA	2.5
1	G	45	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	73	GLY	2.5
1	M	165	VAL	2.5
1	S	45	GLN	2.5
1	C	43	ASN	2.5
1	O	82	ALA	2.5
1	P	149	ALA	2.5
1	S	82	ALA	2.5
2	e	32	ALA	2.5
2	j	88	ALA	2.5
1	I	102	GLN	2.5
1	N	68	ASP	2.5
1	F	72	LEU	2.5
1	N	72	LEU	2.5
1	S	145	ASN	2.5
2	Y	147	PRO	2.5
2	c	25	ARG	2.5
1	Q	127	VAL	2.5
1	B	52	GLU	2.5
1	E	145	ASN	2.5
1	E	76	LEU	2.5
1	F	80	GLY	2.5
2	l	70	VAL	2.5
1	N	166	LEU	2.5
1	P	89	LEU	2.5
1	O	31	ALA	2.5
2	W	20	ALA	2.5
2	X	23	PHE	2.5
2	g	156	PRO	2.5
2	m	144	MET	2.5
1	K	145	ASN	2.5
2	W	36	ARG	2.5
1	P	166	LEU	2.5
1	F	124	CYS	2.5
1	G	115	ALA	2.5
1	G	131	ALA	2.5
1	L	41	GLU	2.5
2	d	108	PHE	2.5
2	h	140	LEU	2.5
2	a	144	MET	2.5
1	D	143	PRO	2.5
2	U	3	LEU	2.5
2	a	153	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	f	23	PHE	2.5
1	N	45	GLN	2.5
2	V	68	GLU	2.5
2	a	77	GLU	2.5
2	X	47	VAL	2.5
2	c	35	GLN	2.5
2	n	28	ALA	2.5
2	f	153	GLY	2.5
1	N	149	ALA	2.5
2	f	81	LEU	2.5
1	Q	32	ARG	2.5
1	N	169	ALA	2.5
1	H	52	GLU	2.5
2	m	81	LEU	2.5
1	G	168	ARG	2.5
1	P	62	LEU	2.5
1	P	118	ALA	2.5
2	g	116	THR	2.5
1	O	36	ILE	2.5
1	Q	27	MET	2.5
1	Q	44	SER	2.5
2	W	4	SER	2.5
1	O	58	VAL	2.5
1	F	102	GLN	2.5
1	G	177	TRP	2.5
1	N	41	GLU	2.5
1	C	61	ALA	2.5
1	D	173	ALA	2.5
1	F	106	LEU	2.5
1	F	149	ALA	2.5
1	S	117	GLY	2.5
1	T	27	MET	2.5
2	W	102	GLY	2.5
2	f	151	ALA	2.5
2	U	110	PHE	2.5
2	k	55	VAL	2.5
1	N	120	LEU	2.5
1	Q	164	ARG	2.5
1	F	36	ILE	2.5
1	Q	38	ASP	2.5
2	W	112	ALA	2.5
2	f	55	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	102	GLN	2.5
1	J	49	LEU	2.5
1	F	171	GLY	2.5
2	W	56	PRO	2.5
1	Q	39	VAL	2.5
1	A	38	ASP	2.5
1	M	57	ASP	2.5
1	O	99	TYR	2.4
2	X	56	PRO	2.4
2	j	129	VAL	2.4
1	D	106	LEU	2.4
1	G	39	VAL	2.4
1	J	146	ILE	2.4
1	Q	55	PRO	2.4
2	e	23	PHE	2.4
2	i	64	PRO	2.4
1	A	93	ALA	2.4
1	A	105	PRO	2.4
1	H	75	GLU	2.4
1	T	171	GLY	2.4
2	i	30	ALA	2.4
1	G	54	LEU	2.4
1	O	50	LEU	2.4
2	Y	93	SER	2.4
1	T	126	THR	2.4
1	L	69	LEU	2.4
1	N	86	GLU	2.4
1	T	142	GLU	2.4
2	f	28	ALA	2.4
2	f	39	GLY	2.4
2	i	128	GLU	2.4
2	k	153	GLY	2.4
1	F	66	GLN	2.4
1	B	36	ILE	2.4
1	F	38	ASP	2.4
2	U	28	ALA	2.4
2	V	37	LEU	2.4
2	f	91	ALA	2.4
2	m	146	LEU	2.4
2	X	35	GLN	2.4
2	Z	130	MET	2.4
2	h	69	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	138	LEU	2.4
2	V	66	ARG	2.4
2	X	71	ARG	2.4
2	n	110	PHE	2.4
2	m	16	GLY	2.4
1	C	125	ARG	2.4
2	l	54	ARG	2.4
2	W	31	LEU	2.4
2	Y	129	VAL	2.4
2	e	24	VAL	2.4
2	c	98	ALA	2.4
2	g	58	LEU	2.4
2	m	78	LEU	2.4
1	C	91	ARG	2.4
1	P	168	ARG	2.4
2	l	73	PRO	2.4
1	D	27	MET	2.4
1	Q	135	ILE	2.4
1	S	127	VAL	2.4
2	h	35	GLN	2.4
1	J	122	HIS	2.4
1	N	148	PRO	2.4
2	k	15	HIS	2.4
1	E	27	MET	2.4
1	A	115	ALA	2.4
1	N	93	ALA	2.4
1	P	35	ALA	2.4
2	l	28	ALA	2.4
1	H	54	LEU	2.4
2	c	73	PRO	2.4
2	g	26	GLU	2.4
2	Y	33	GLY	2.4
2	b	17	GLN	2.4
1	G	133	ARG	2.4
1	K	106	LEU	2.4
2	i	72	THR	2.4
1	N	52	GLU	2.4
2	a	68	GLU	2.4
1	H	144	LEU	2.4
2	c	147	PRO	2.4
2	d	84	THR	2.4
1	E	54	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	P	49	LEU	2.4
1	Q	151	TYR	2.4
2	W	94	GLY	2.4
2	c	153	GLY	2.4
1	J	148	PRO	2.4
1	L	112	PRO	2.4
2	d	47	VAL	2.4
2	l	82	THR	2.4
1	T	52	GLU	2.4
1	B	144	LEU	2.4
1	P	178	ASP	2.4
2	Y	153	GLY	2.4
2	j	146	LEU	2.4
2	W	104	MET	2.4
2	k	53	VAL	2.4
1	C	122	HIS	2.4
2	Y	156	PRO	2.4
2	i	36	ARG	2.4
2	j	87	ARG	2.4
2	m	79	ARG	2.4
1	P	84	ILE	2.4
1	T	138	LEU	2.4
2	V	69	ILE	2.4
2	i	151	ALA	2.4
2	i	148	GLN	2.4
1	K	148	PRO	2.4
1	M	173	ALA	2.4
1	P	125	ARG	2.4
2	c	13	HIS	2.4
2	j	73	PRO	2.4
1	D	95	TRP	2.4
1	N	78	ILE	2.4
2	Y	81	LEU	2.4
2	a	78	LEU	2.4
1	B	66	GLN	2.4
1	E	38	ASP	2.4
1	D	147	ALA	2.4
1	M	146	ILE	2.4
2	b	82	THR	2.4
2	n	84	THR	2.4
1	T	80	GLY	2.4
2	a	39	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	c	92	VAL	2.4
1	F	167	ASN	2.4
1	N	70	PHE	2.4
2	Y	106	PHE	2.4
1	D	165	VAL	2.4
1	E	151	TYR	2.4
1	J	127	VAL	2.4
1	N	73	GLY	2.4
1	B	54	LEU	2.4
1	M	135	ILE	2.4
2	c	37	LEU	2.4
1	O	115	ALA	2.4
1	T	32	ARG	2.4
2	d	151	ALA	2.4
2	c	144	MET	2.4
1	G	46	ILE	2.4
1	I	72	LEU	2.4
2	X	31	LEU	2.4
2	m	108	PHE	2.4
1	K	178	ASP	2.4
1	L	151	TYR	2.4
1	O	68	ASP	2.4
1	K	52	GLU	2.4
1	O	44	SER	2.3
1	L	168	ARG	2.3
2	Y	148	GLN	2.3
2	m	152	ALA	2.3
1	I	27	MET	2.3
1	K	172	GLY	2.3
2	Y	72	THR	2.3
2	n	106	PHE	2.3
1	G	66	GLN	2.3
2	a	99	ALA	2.3
2	n	151	ALA	2.3
1	M	43	ASN	2.3
1	Q	76	LEU	2.3
1	B	27	MET	2.3
1	A	33	ILE	2.3
1	H	172	GLY	2.3
2	U	37	LEU	2.3
2	b	114	LEU	2.3
2	U	45	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	d	44	GLY	2.3
2	j	128	GLU	2.3
1	A	48	VAL	2.3
1	A	123	VAL	2.3
1	F	170	ALA	2.3
1	S	31	ALA	2.3
2	l	98	ALA	2.3
1	P	59	ARG	2.3
2	c	101	GLY	2.3
1	A	42	LEU	2.3
1	K	72	LEU	2.3
1	T	99	TYR	2.3
2	Z	57	LEU	2.3
2	d	48	TRP	2.3
1	P	63	SER	2.3
1	F	47	GLY	2.3
1	T	125	ARG	2.3
2	k	110	PHE	2.3
1	N	170	ALA	2.3
1	O	51	ALA	2.3
1	P	138	LEU	2.3
2	j	34	VAL	2.3
2	V	144	MET	2.3
2	g	104	MET	2.3
1	I	113	GLY	2.3
1	K	40	ASP	2.3
1	Q	90	LEU	2.3
2	Y	150	LEU	2.3
2	c	34	VAL	2.3
1	T	29	ASP	2.3
2	h	28	ALA	2.3
2	n	65	PHE	2.3
1	D	161	VAL	2.3
2	c	74	GLN	2.3
1	G	90	LEU	2.3
1	I	151	TYR	2.3
2	d	126	ALA	2.3
2	i	99	ALA	2.3
1	D	130	ARG	2.3
1	P	44	SER	2.3
1	J	147	ALA	2.3
1	K	126	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	Q	115	ALA	2.3
1	F	27	MET	2.3
1	Q	43	ASN	2.3
1	K	48	VAL	2.3
1	O	130	ARG	2.3
1	B	77	CYS	2.3
1	Q	123	VAL	2.3
2	W	153	GLY	2.3
1	R	119	ALA	2.3
1	S	167	ASN	2.3
1	E	107	GLU	2.3
1	L	165	VAL	2.3
1	T	76	LEU	2.3
2	X	140	LEU	2.3
2	b	78	LEU	2.3
1	G	148	PRO	2.3
2	e	27	PRO	2.3
1	E	122	HIS	2.3
1	T	45	GLN	2.3
1	J	142	GLU	2.3
2	h	83	LEU	2.3
1	D	99	TYR	2.3
2	b	92	VAL	2.3
1	F	76	LEU	2.3
2	W	57	LEU	2.3
2	g	9	PHE	2.3
2	h	86	GLU	2.3
1	Q	95	TRP	2.3
1	A	169	ALA	2.3
1	P	67	HIS	2.3
1	Q	147	ALA	2.3
2	a	98	ALA	2.3
2	a	34	VAL	2.3
1	B	149	ALA	2.3
1	A	178	ASP	2.3
1	E	72	LEU	2.3
1	K	44	SER	2.3
2	m	13	HIS	2.3
1	F	75	GLU	2.3
1	G	107	GLU	2.3
2	k	68	GLU	2.3
1	A	164	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	89	LEU	2.3
2	i	145	ALA	2.3
1	C	165	VAL	2.3
1	F	153	ASN	2.3
1	S	124	CYS	2.3
1	B	103	LEU	2.3
1	D	172	GLY	2.3
1	K	144	LEU	2.3
1	O	28	GLY	2.3
2	m	26	GLU	2.3
1	H	125	ARG	2.3
2	Y	5	ALA	2.3
1	G	58	VAL	2.3
1	S	71	ASP	2.3
1	K	62	LEU	2.3
1	S	78	ILE	2.3
1	F	29	ASP	2.3
1	I	66	GLN	2.3
1	Q	50	LEU	2.3
2	c	103	GLU	2.3
2	n	95	GLN	2.3
1	G	164	ARG	2.3
1	M	82	ALA	2.3
1	N	165	VAL	2.3
1	P	165	VAL	2.3
1	Q	129	ARG	2.3
1	S	173	ALA	2.3
2	e	152	ALA	2.3
2	d	67	SER	2.3
2	i	127	PHE	2.3
1	J	99	TYR	2.3
1	P	146	ILE	2.3
2	c	114	LEU	2.3
2	h	132	GLN	2.3
2	i	37	LEU	2.3
2	i	108	PHE	2.3
2	k	99	ALA	2.3
2	Z	55	VAL	2.3
2	g	28	ALA	2.2
2	X	142	VAL	2.2
1	A	72	LEU	2.2
1	J	54	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	44	SER	2.2
2	f	13	HIS	2.2
1	F	40	ASP	2.2
1	H	102	GLN	2.2
1	J	75	GLU	2.2
2	k	76	ALA	2.2
2	m	82	THR	2.2
1	A	148	PRO	2.2
1	I	168	ARG	2.2
2	Y	38	ARG	2.2
2	U	42	SER	2.2
2	V	67	SER	2.2
1	E	51	ALA	2.2
1	J	31	ALA	2.2
1	N	28	GLY	2.2
2	j	124	GLY	2.2
1	Q	168	ARG	2.2
2	U	69	ILE	2.2
2	W	21	LEU	2.2
1	G	47	GLY	2.2
2	g	99	ALA	2.2
2	k	112	ALA	2.2
1	G	72	LEU	2.2
1	T	84	ILE	2.2
2	d	139	LEU	2.2
2	i	3	LEU	2.2
2	j	38	ARG	2.2
1	K	70	PHE	2.2
1	B	69	LEU	2.2
2	i	130	MET	2.2
2	i	131	VAL	2.2
2	j	22	ALA	2.2
1	F	146	ILE	2.2
1	E	55	PRO	2.2
1	K	164	ARG	2.2
2	e	7	GLN	2.2
2	e	66	ARG	2.2
1	J	48	VAL	2.2
1	K	173	ALA	2.2
1	P	42	LEU	2.2
1	P	81	HIS	2.2
2	k	67	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	Z	111	GLN	2.2
1	C	167	ASN	2.2
1	G	144	LEU	2.2
1	I	30	ASP	2.2
1	F	81	HIS	2.2
1	P	135	ILE	2.2
2	U	17	GLN	2.2
1	F	49	LEU	2.2
1	F	63	SER	2.2
1	G	127	VAL	2.2
1	G	138	LEU	2.2
1	O	106	LEU	2.2
2	a	147	PRO	2.2
1	N	151	TYR	2.2
1	S	81	HIS	2.2
1	O	132	GLU	2.2
2	h	60	GLU	2.2
1	I	114	GLY	2.2
1	J	124	CYS	2.2
1	E	125	ARG	2.2
2	V	58	LEU	2.2
2	f	78	LEU	2.2
1	D	35	ALA	2.2
1	I	115	ALA	2.2
1	L	78	ILE	2.2
1	P	36	ILE	2.2
1	S	74	GLY	2.2
1	T	135	ILE	2.2
2	f	142	VAL	2.2
2	h	144	MET	2.2
1	R	123	VAL	2.2
2	j	55	VAL	2.2
2	k	130	MET	2.2
1	K	114	GLY	2.2
2	d	33	GLY	2.2
1	A	57	ASP	2.2
1	B	89	LEU	2.2
1	E	177	TRP	2.2
1	F	159	LEU	2.2
1	N	88	HIS	2.2
2	a	31	LEU	2.2
1	N	147	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	P	147	ALA	2.2
2	Y	25	ARG	2.2
2	c	96	ALA	2.2
1	C	70	PHE	2.2
1	E	49	LEU	2.2
1	K	138	LEU	2.2
1	A	59	ARG	2.2
1	I	175	VAL	2.2
1	J	169	ALA	2.2
2	X	151	ALA	2.2
1	S	103	LEU	2.2
2	m	114	LEU	2.2
1	G	125	ARG	2.2
1	M	75	GLU	2.2
2	Y	112	ALA	2.2
2	c	149	GLY	2.2
2	h	72	THR	2.2
2	k	102	GLY	2.2
2	k	92	VAL	2.2
1	O	148	PRO	2.2
1	P	105	PRO	2.2
2	U	77	GLU	2.2
2	g	56	PRO	2.2
2	j	89	TRP	2.2
2	k	82	THR	2.2
1	A	65	ILE	2.2
1	F	33	ILE	2.2
1	J	135	ILE	2.2
1	K	61	ALA	2.2
1	M	103	LEU	2.2
2	a	79	ARG	2.2
2	n	57	LEU	2.2
1	B	102	GLN	2.2
1	E	167	ASN	2.2
1	I	135	ILE	2.2
1	M	66	GLN	2.2
2	j	47	VAL	2.2
1	K	134	SER	2.2
1	S	70	PHE	2.2
2	j	67	SER	2.2
1	D	46	ILE	2.2
2	X	46	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	105	PRO	2.2
1	E	36	ILE	2.2
1	F	28	GLY	2.2
2	g	53	VAL	2.2
2	j	147	PRO	2.2
1	C	54	LEU	2.2
1	S	66	GLN	2.2
1	D	32	ARG	2.2
2	Y	97	THR	2.2
2	d	45	GLU	2.2
1	S	102	GLN	2.2
2	m	132	GLN	2.2
1	A	146	ILE	2.2
1	I	122	HIS	2.2
1	I	142	GLU	2.1
1	A	126	THR	2.1
1	E	70	PHE	2.1
1	R	54	LEU	2.1
2	U	106	PHE	2.1
1	I	127	VAL	2.1
1	P	86	GLU	2.1
2	e	60	GLU	2.1
1	F	157	ASP	2.1
2	h	46	GLN	2.1
2	a	66	ARG	2.1
2	e	47	VAL	2.1
1	B	40	ASP	2.1
1	E	170	ALA	2.1
1	P	99	TYR	2.1
1	G	40	ASP	2.1
1	A	124	CYS	2.1
1	F	50	LEU	2.1
1	H	78	ILE	2.1
2	e	28	ALA	2.1
1	K	123	VAL	2.1
2	i	132	GLN	2.1
1	J	125	ARG	2.1
1	L	74	GLY	2.1
1	P	47	GLY	2.1
2	l	56	PRO	2.1
1	D	78	ILE	2.1
1	Q	118	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	V	152	ALA	2.1
2	c	28	ALA	2.1
2	d	22	ALA	2.1
2	d	43	ASP	2.1
1	E	132	GLU	2.1
1	O	170	ALA	2.1
1	S	72	LEU	2.1
2	a	106	PHE	2.1
2	b	57	LEU	2.1
2	g	20	ALA	2.1
1	D	47	GLY	2.1
2	Y	102	GLY	2.1
1	F	35	ALA	2.1
1	O	43	ASN	2.1
1	D	160	PHE	2.1
2	V	83	LEU	2.1
2	f	58	LEU	2.1
2	i	114	LEU	2.1
1	N	139	GLY	2.1
2	f	7	GLN	2.1
2	g	102	GLY	2.1
1	S	125	ARG	2.1
1	K	69	LEU	2.1
2	c	32	ALA	2.1
2	g	5	ALA	2.1
1	L	99	TYR	2.1
1	L	35	ALA	2.1
1	L	130	ARG	2.1
1	M	76	LEU	2.1
1	O	103	LEU	2.1
2	W	156	PRO	2.1
2	c	79	ARG	2.1
2	n	62	ASP	2.1
2	i	106	PHE	2.1
1	O	167	ASN	2.1
1	I	92	LEU	2.1
1	O	61	ALA	2.1
1	R	146	ILE	2.1
1	S	36	ILE	2.1
2	m	17	GLN	2.1
1	T	148	PRO	2.1
2	m	93	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	142	GLU	2.1
1	H	49	LEU	2.1
1	L	66	GLN	2.1
1	N	62	LEU	2.1
1	O	49	LEU	2.1
2	b	37	LEU	2.1
2	h	130	MET	2.1
1	N	91	ARG	2.1
2	W	18	ALA	2.1
2	g	13	HIS	2.1
1	M	104	PRO	2.1
2	h	24	VAL	2.1
2	m	98	ALA	2.1
1	R	52	GLU	2.1
1	S	52	GLU	2.1
1	S	132	GLU	2.1
1	N	126	THR	2.1
1	D	133	ARG	2.1
1	N	168	ARG	2.1
2	f	79	ARG	2.1
1	E	135	ILE	2.1
1	P	151	TYR	2.1
2	a	83	LEU	2.1
2	h	58	LEU	2.1
1	D	167	ASN	2.1
2	e	9	PHE	2.1
1	Q	133	ARG	2.1
2	e	148	GLN	2.1
1	A	69	LEU	2.1
2	k	27	PRO	2.1
2	Z	86	GLU	2.1
2	k	78	LEU	2.1
2	f	33	GLY	2.1
1	A	100	ASN	2.1
1	D	125	ARG	2.1
1	L	149	ALA	2.1
2	W	53	VAL	2.1
1	G	120	LEU	2.1
2	g	57	LEU	2.1
1	R	80	GLY	2.1
2	j	108	PHE	2.1
1	K	91	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	122	HIS	2.1
2	W	151	ALA	2.1
1	A	36	ILE	2.1
1	P	120	LEU	2.1
2	f	66	ARG	2.1
2	g	3	LEU	2.1
2	m	37	LEU	2.1
1	F	31	ALA	2.1
1	F	123	VAL	2.1
1	I	95	TRP	2.1
1	N	49	LEU	2.1
1	S	147	ALA	2.1
2	Z	89	TRP	2.1
2	h	82	THR	2.1
1	O	102	GLN	2.1
1	B	68	ASP	2.1
1	M	161	VAL	2.1
2	l	3	LEU	2.1
1	I	81	HIS	2.1
1	K	46	ILE	2.1
1	P	102	GLN	2.1
2	Y	73	PRO	2.1
1	D	127	VAL	2.1
1	E	86	GLU	2.1
2	f	90	VAL	2.1
1	I	93	ALA	2.1
1	O	149	ALA	2.1
2	j	5	ALA	2.1
1	N	66	GLN	2.1
1	R	122	HIS	2.1
1	S	164	ARG	2.1
2	a	61	VAL	2.1
2	d	53	VAL	2.1
2	e	92	VAL	2.1
2	Y	91	ALA	2.1
1	E	71	ASP	2.1
1	M	178	ASP	2.1
2	U	38	ARG	2.1
2	Z	84	THR	2.1
1	G	123	VAL	2.1
1	I	73	GLY	2.1
1	J	53	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	148	PRO	2.1
2	e	61	VAL	2.1
2	j	141	LEU	2.1
1	B	78	ILE	2.1
2	d	36	ARG	2.1
2	m	110	PHE	2.1
1	C	161	VAL	2.1
2	U	57	LEU	2.1
2	U	95	GLN	2.1
2	g	55	VAL	2.1
1	A	78	ILE	2.1
1	G	147	ALA	2.1
1	G	172	GLY	2.1
1	L	93	ALA	2.1
2	U	60	GLU	2.1
1	I	29	ASP	2.0
1	I	69	LEU	2.0
2	j	61	VAL	2.0
1	E	173	ALA	2.0
1	F	39	VAL	2.0
1	I	164	ARG	2.0
1	L	39	VAL	2.0
2	a	53	VAL	2.0
2	f	21	LEU	2.0
2	n	40	LEU	2.0
1	C	35	ALA	2.0
1	D	135	ILE	2.0
1	G	95	TRP	2.0
1	I	148	PRO	2.0
2	Y	8	SER	2.0
2	m	8	SER	2.0
1	B	106	LEU	2.0
1	R	76	LEU	2.0
2	k	114	LEU	2.0
1	F	126	THR	2.0
1	R	78	ILE	2.0
2	d	4	SER	2.0
2	d	7	GLN	2.0
1	P	143	PRO	2.0
1	S	135	ILE	2.0
2	X	20	ALA	2.0
2	f	96	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	f	145	ALA	2.0
2	n	56	PRO	2.0
1	D	120	LEU	2.0
2	W	52	LEU	2.0
2	a	37	LEU	2.0
1	I	146	ILE	2.0
1	J	28	GLY	2.0
1	N	67	HIS	2.0
1	P	70	PHE	2.0
1	N	138	LEU	2.0
1	S	89	LEU	2.0
2	X	67	SER	2.0
2	Z	148	GLN	2.0
1	I	78	ILE	2.0
1	A	54	LEU	2.0
1	M	167	ASN	2.0
1	O	67	HIS	2.0
2	g	21	LEU	2.0
1	C	66	GLN	2.0
1	H	38	ASP	2.0
1	O	38	ASP	2.0
2	n	148	GLN	2.0
1	M	70	PHE	2.0
2	c	106	PHE	2.0
1	N	35	ALA	2.0
1	O	72	LEU	2.0
1	O	73	GLY	2.0
1	Q	138	LEU	2.0
2	W	92	VAL	2.0
1	C	38	ASP	2.0
1	D	166	LEU	2.0
1	F	69	LEU	2.0
1	M	52	GLU	2.0
2	Z	108	PHE	2.0
1	J	171	GLY	2.0
1	O	147	ALA	2.0
1	S	120	LEU	2.0
2	W	38	ARG	2.0
2	X	114	LEU	2.0
2	l	58	LEU	2.0
2	l	100	GLU	2.0
1	F	128	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	62	LEU	2.0
1	M	166	LEU	2.0
1	P	40	ASP	2.0
1	E	119	ALA	2.0
1	H	35	ALA	2.0
1	O	119	ALA	2.0
1	S	142	GLU	2.0
2	c	18	ALA	2.0
2	k	33	GLY	2.0
1	E	43	ASN	2.0
1	E	78	ILE	2.0
2	a	108	PHE	2.0
1	A	165	VAL	2.0
1	B	151	TYR	2.0
1	D	31	ALA	2.0
1	D	93	ALA	2.0
1	L	68	ASP	2.0
2	j	42	SER	2.0
2	g	112	ALA	2.0
2	Z	131	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.