Full wwPDB EM Validation Report ⓘ

Oct 1, 2024 – 02:28 pm BST

PDB ID	:	9FO3
EMDB ID	:	EMD-50615
Title	:	Structure of a gp140 SpyTag-SpyCatcher mi3 nanoparticle including mi3 density only.
Authors	:	Woodward, J.D.; Malebo, K.; Chapman, R.
Deposited on	:	2024-06-11
Resolution	:	5.30 Å(reported)
Based on initial model	:	.

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

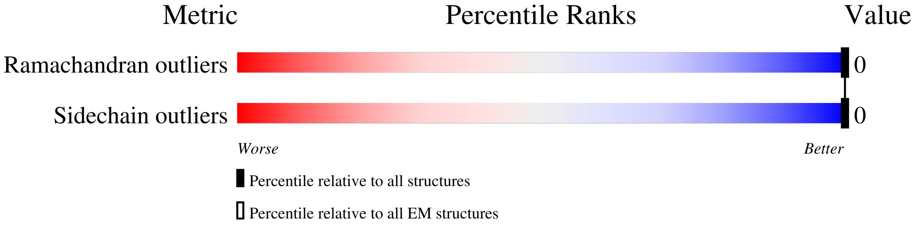
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

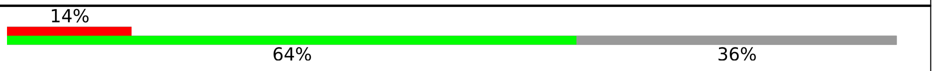
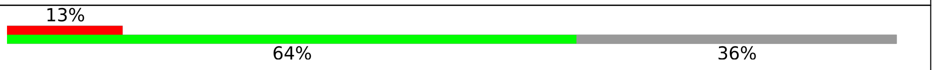
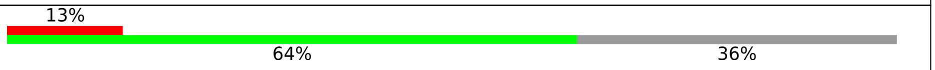
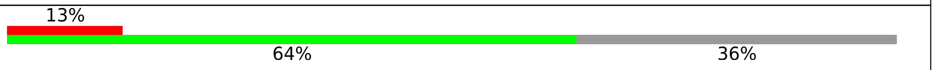
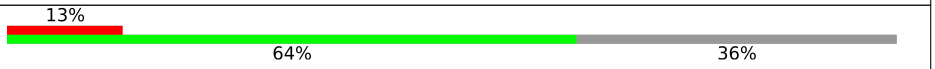
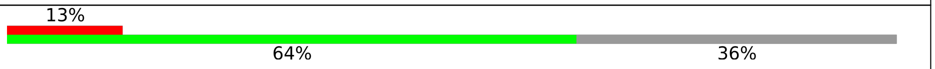
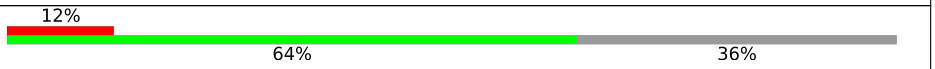
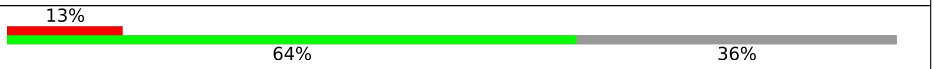
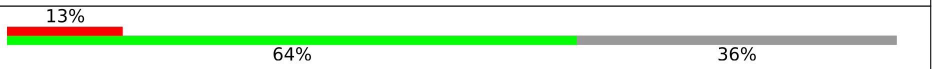
The reported resolution of this entry is 5.30 Å.

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)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	318	 14% 64% 36%
1	1	318	 13% 64% 36%
1	2	318	 13% 64% 36%
1	3	318	 13% 64% 36%
1	4	318	 13% 64% 36%
1	5	318	 13% 64% 36%
1	6	318	 12% 64% 36%
1	7	318	 13% 64% 36%
1	A	318	 13% 64% 36%

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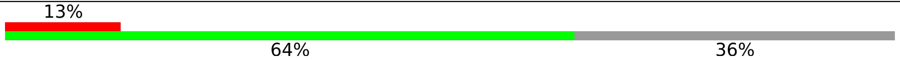
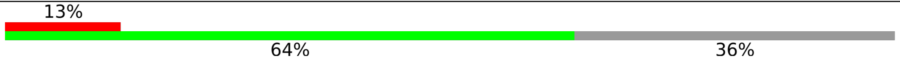
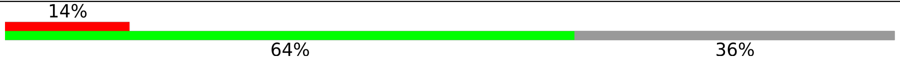
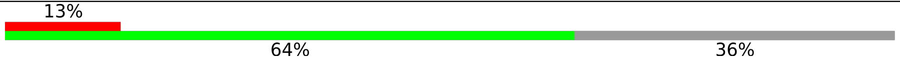
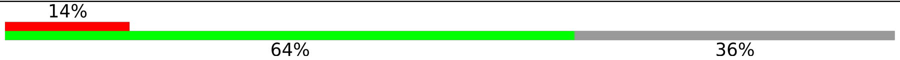
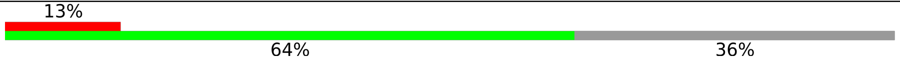
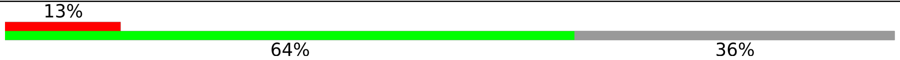
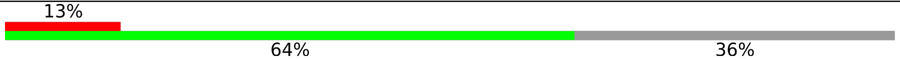
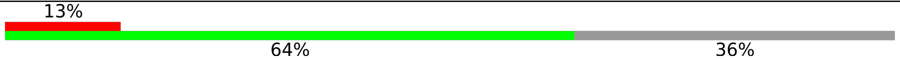
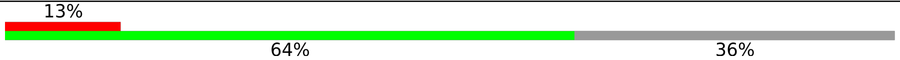
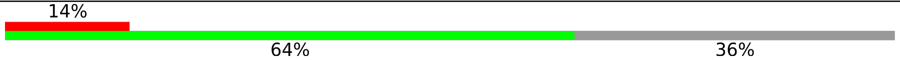
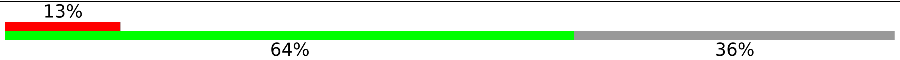
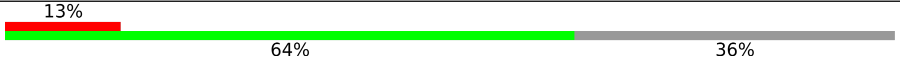
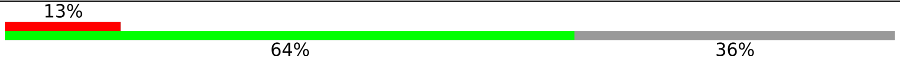
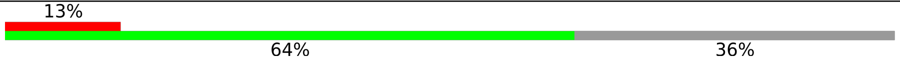
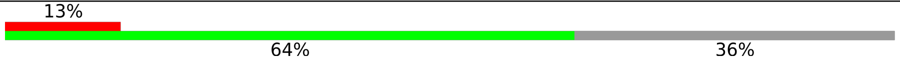
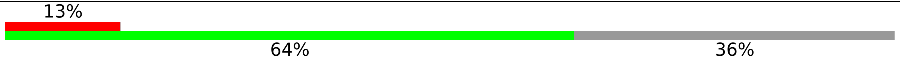
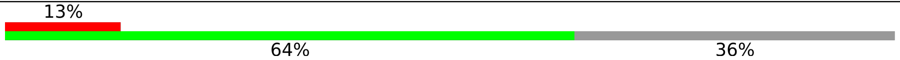
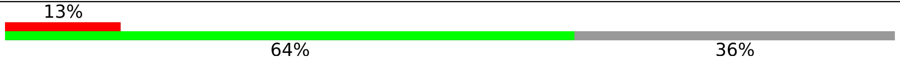
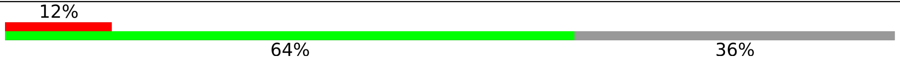
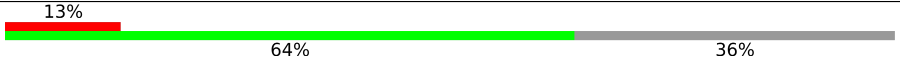
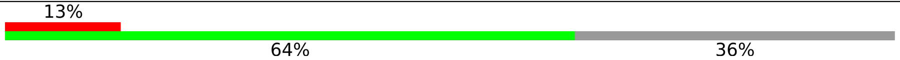
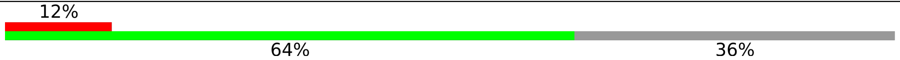
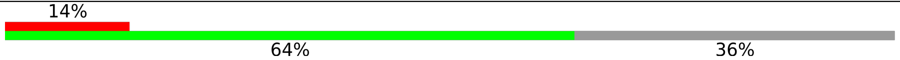
Mol	Chain	Length	Quality of chain
1	B	318	
1	C	318	
1	D	318	
1	E	318	
1	F	318	
1	G	318	
1	H	318	
1	I	318	
1	J	318	
1	K	318	
1	L	318	
1	M	318	
1	N	318	
1	O	318	
1	P	318	
1	Q	318	
1	R	318	
1	S	318	
1	T	318	
1	U	318	
1	V	318	
1	W	318	
1	X	318	
1	Y	318	
1	Z	318	

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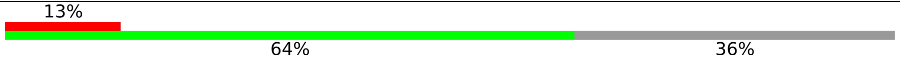
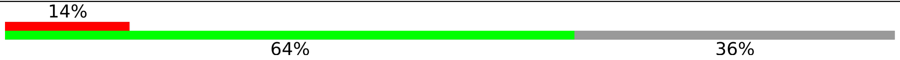
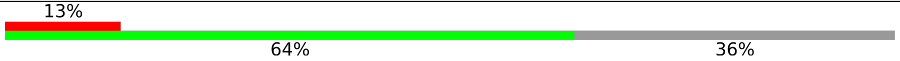
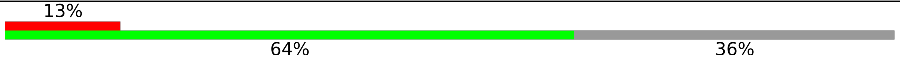
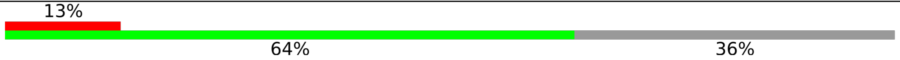
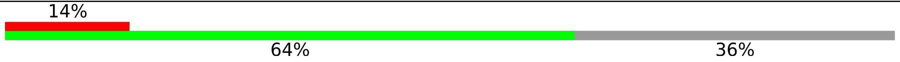
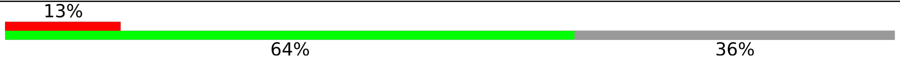
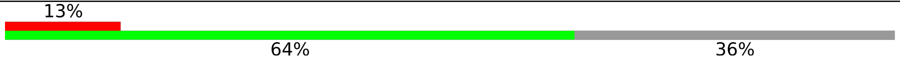
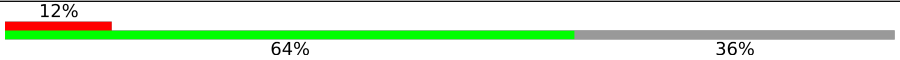
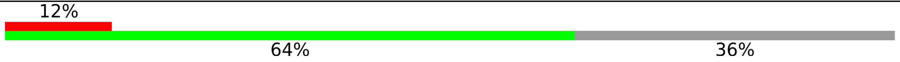
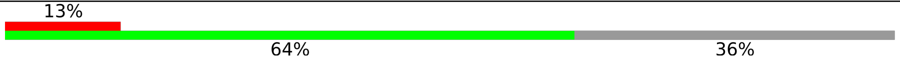
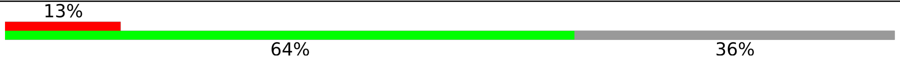
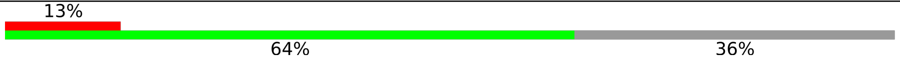
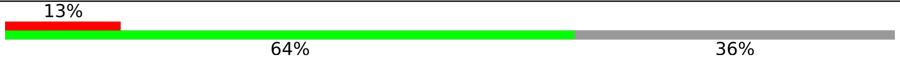
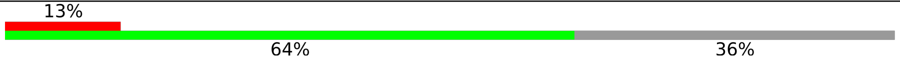
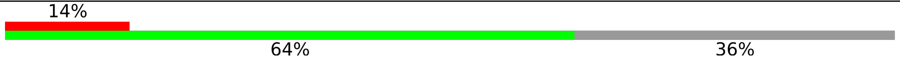
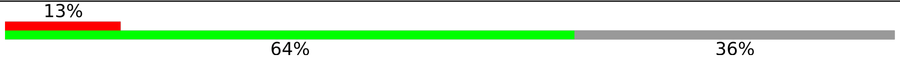
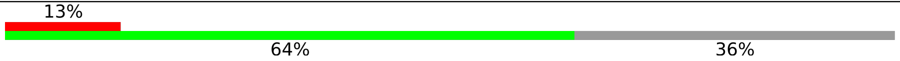
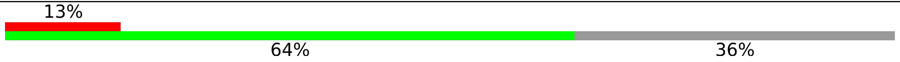
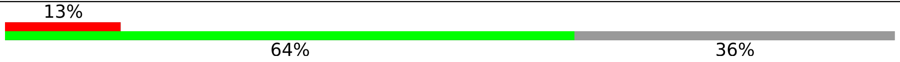
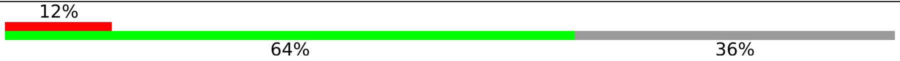
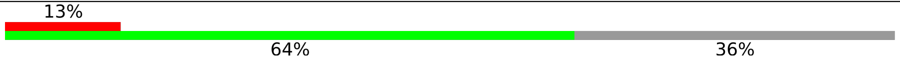
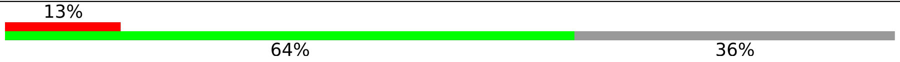
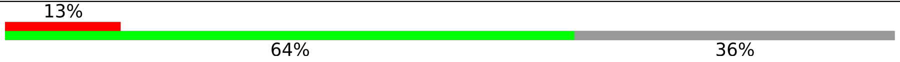
Mol	Chain	Length	Quality of chain
1	a	318	
1	b	318	
1	c	318	
1	d	318	
1	e	318	
1	f	318	
1	g	318	
1	h	318	
1	i	318	
1	j	318	
1	k	318	
1	l	318	
1	m	318	
1	n	318	
1	o	318	
1	p	318	
1	q	318	
1	r	318	
1	s	318	
1	t	318	
1	u	318	
1	v	318	
1	w	318	
1	x	318	
1	y	318	

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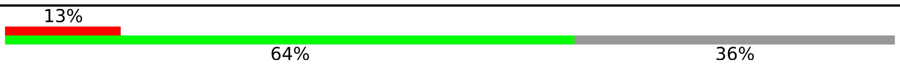
Mol	Chain	Length	Quality of chain
1	z	318	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 92520 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	204	Total C N O S 1542 1003 252 279 8	0	0
1	B	204	Total C N O S 1542 1003 252 279 8	0	0
1	C	204	Total C N O S 1542 1003 252 279 8	0	0
1	D	204	Total C N O S 1542 1003 252 279 8	0	0
1	E	204	Total C N O S 1542 1003 252 279 8	0	0
1	F	204	Total C N O S 1542 1003 252 279 8	0	0
1	G	204	Total C N O S 1542 1003 252 279 8	0	0
1	H	204	Total C N O S 1542 1003 252 279 8	0	0
1	I	204	Total C N O S 1542 1003 252 279 8	0	0
1	J	204	Total C N O S 1542 1003 252 279 8	0	0
1	K	204	Total C N O S 1542 1003 252 279 8	0	0
1	L	204	Total C N O S 1542 1003 252 279 8	0	0
1	M	204	Total C N O S 1542 1003 252 279 8	0	0
1	N	204	Total C N O S 1542 1003 252 279 8	0	0
1	O	204	Total C N O S 1542 1003 252 279 8	0	0
1	P	204	Total C N O S 1542 1003 252 279 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	R	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	S	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	T	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	U	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	V	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	W	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	X	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	Y	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	Z	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	a	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	b	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	c	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	d	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	e	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	f	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	g	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	h	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	i	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	j	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	k	204	Total 1542	C 1003	N 252	O 279	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	l	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	m	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	n	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	o	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	p	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	q	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	r	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	s	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	t	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	u	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	v	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	w	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	x	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	y	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	z	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	0	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	1	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	2	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	3	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	4	204	Total 1542	C 1003	N 252	O 279	S 8	0	0
1	5	204	Total 1542	C 1003	N 252	O 279	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	6	204	1542	1003	252	279	8	0	0
1	7	204	1542	1003	252	279	8	0	0

There are 420 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	LYS	GLU	conflict	UNP Q9WXS1
A	146	LEU	GLU	conflict	UNP Q9WXS1
A	174	MET	LYS	conflict	UNP Q9WXS1
A	189	ALA	CYS	conflict	UNP Q9WXS1
A	213	ALA	CYS	conflict	UNP Q9WXS1
A	300	VAL	ASP	conflict	UNP Q9WXS1
A	303	ALA	ARG	conflict	UNP Q9WXS1
B	139	LYS	GLU	conflict	UNP Q9WXS1
B	146	LEU	GLU	conflict	UNP Q9WXS1
B	174	MET	LYS	conflict	UNP Q9WXS1
B	189	ALA	CYS	conflict	UNP Q9WXS1
B	213	ALA	CYS	conflict	UNP Q9WXS1
B	300	VAL	ASP	conflict	UNP Q9WXS1
B	303	ALA	ARG	conflict	UNP Q9WXS1
C	139	LYS	GLU	conflict	UNP Q9WXS1
C	146	LEU	GLU	conflict	UNP Q9WXS1
C	174	MET	LYS	conflict	UNP Q9WXS1
C	189	ALA	CYS	conflict	UNP Q9WXS1
C	213	ALA	CYS	conflict	UNP Q9WXS1
C	300	VAL	ASP	conflict	UNP Q9WXS1
C	303	ALA	ARG	conflict	UNP Q9WXS1
D	139	LYS	GLU	conflict	UNP Q9WXS1
D	146	LEU	GLU	conflict	UNP Q9WXS1
D	174	MET	LYS	conflict	UNP Q9WXS1
D	189	ALA	CYS	conflict	UNP Q9WXS1
D	213	ALA	CYS	conflict	UNP Q9WXS1
D	300	VAL	ASP	conflict	UNP Q9WXS1
D	303	ALA	ARG	conflict	UNP Q9WXS1
E	139	LYS	GLU	conflict	UNP Q9WXS1
E	146	LEU	GLU	conflict	UNP Q9WXS1
E	174	MET	LYS	conflict	UNP Q9WXS1
E	189	ALA	CYS	conflict	UNP Q9WXS1
E	213	ALA	CYS	conflict	UNP Q9WXS1
E	300	VAL	ASP	conflict	UNP Q9WXS1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	303	ALA	ARG	conflict	UNP Q9WXS1
F	139	LYS	GLU	conflict	UNP Q9WXS1
F	146	LEU	GLU	conflict	UNP Q9WXS1
F	174	MET	LYS	conflict	UNP Q9WXS1
F	189	ALA	CYS	conflict	UNP Q9WXS1
F	213	ALA	CYS	conflict	UNP Q9WXS1
F	300	VAL	ASP	conflict	UNP Q9WXS1
F	303	ALA	ARG	conflict	UNP Q9WXS1
G	139	LYS	GLU	conflict	UNP Q9WXS1
G	146	LEU	GLU	conflict	UNP Q9WXS1
G	174	MET	LYS	conflict	UNP Q9WXS1
G	189	ALA	CYS	conflict	UNP Q9WXS1
G	213	ALA	CYS	conflict	UNP Q9WXS1
G	300	VAL	ASP	conflict	UNP Q9WXS1
G	303	ALA	ARG	conflict	UNP Q9WXS1
H	139	LYS	GLU	conflict	UNP Q9WXS1
H	146	LEU	GLU	conflict	UNP Q9WXS1
H	174	MET	LYS	conflict	UNP Q9WXS1
H	189	ALA	CYS	conflict	UNP Q9WXS1
H	213	ALA	CYS	conflict	UNP Q9WXS1
H	300	VAL	ASP	conflict	UNP Q9WXS1
H	303	ALA	ARG	conflict	UNP Q9WXS1
I	139	LYS	GLU	conflict	UNP Q9WXS1
I	146	LEU	GLU	conflict	UNP Q9WXS1
I	174	MET	LYS	conflict	UNP Q9WXS1
I	189	ALA	CYS	conflict	UNP Q9WXS1
I	213	ALA	CYS	conflict	UNP Q9WXS1
I	300	VAL	ASP	conflict	UNP Q9WXS1
I	303	ALA	ARG	conflict	UNP Q9WXS1
J	139	LYS	GLU	conflict	UNP Q9WXS1
J	146	LEU	GLU	conflict	UNP Q9WXS1
J	174	MET	LYS	conflict	UNP Q9WXS1
J	189	ALA	CYS	conflict	UNP Q9WXS1
J	213	ALA	CYS	conflict	UNP Q9WXS1
J	300	VAL	ASP	conflict	UNP Q9WXS1
J	303	ALA	ARG	conflict	UNP Q9WXS1
K	139	LYS	GLU	conflict	UNP Q9WXS1
K	146	LEU	GLU	conflict	UNP Q9WXS1
K	174	MET	LYS	conflict	UNP Q9WXS1
K	189	ALA	CYS	conflict	UNP Q9WXS1
K	213	ALA	CYS	conflict	UNP Q9WXS1
K	300	VAL	ASP	conflict	UNP Q9WXS1

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Chain	Residue	Modelled	Actual	Comment	Reference
K	303	ALA	ARG	conflict	UNP Q9WXS1
L	139	LYS	GLU	conflict	UNP Q9WXS1
L	146	LEU	GLU	conflict	UNP Q9WXS1
L	174	MET	LYS	conflict	UNP Q9WXS1
L	189	ALA	CYS	conflict	UNP Q9WXS1
L	213	ALA	CYS	conflict	UNP Q9WXS1
L	300	VAL	ASP	conflict	UNP Q9WXS1
L	303	ALA	ARG	conflict	UNP Q9WXS1
M	139	LYS	GLU	conflict	UNP Q9WXS1
M	146	LEU	GLU	conflict	UNP Q9WXS1
M	174	MET	LYS	conflict	UNP Q9WXS1
M	189	ALA	CYS	conflict	UNP Q9WXS1
M	213	ALA	CYS	conflict	UNP Q9WXS1
M	300	VAL	ASP	conflict	UNP Q9WXS1
M	303	ALA	ARG	conflict	UNP Q9WXS1
N	139	LYS	GLU	conflict	UNP Q9WXS1
N	146	LEU	GLU	conflict	UNP Q9WXS1
N	174	MET	LYS	conflict	UNP Q9WXS1
N	189	ALA	CYS	conflict	UNP Q9WXS1
N	213	ALA	CYS	conflict	UNP Q9WXS1
N	300	VAL	ASP	conflict	UNP Q9WXS1
N	303	ALA	ARG	conflict	UNP Q9WXS1
O	139	LYS	GLU	conflict	UNP Q9WXS1
O	146	LEU	GLU	conflict	UNP Q9WXS1
O	174	MET	LYS	conflict	UNP Q9WXS1
O	189	ALA	CYS	conflict	UNP Q9WXS1
O	213	ALA	CYS	conflict	UNP Q9WXS1
O	300	VAL	ASP	conflict	UNP Q9WXS1
O	303	ALA	ARG	conflict	UNP Q9WXS1
P	139	LYS	GLU	conflict	UNP Q9WXS1
P	146	LEU	GLU	conflict	UNP Q9WXS1
P	174	MET	LYS	conflict	UNP Q9WXS1
P	189	ALA	CYS	conflict	UNP Q9WXS1
P	213	ALA	CYS	conflict	UNP Q9WXS1
P	300	VAL	ASP	conflict	UNP Q9WXS1
P	303	ALA	ARG	conflict	UNP Q9WXS1
Q	139	LYS	GLU	conflict	UNP Q9WXS1
Q	146	LEU	GLU	conflict	UNP Q9WXS1
Q	174	MET	LYS	conflict	UNP Q9WXS1
Q	189	ALA	CYS	conflict	UNP Q9WXS1
Q	213	ALA	CYS	conflict	UNP Q9WXS1
Q	300	VAL	ASP	conflict	UNP Q9WXS1

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	303	ALA	ARG	conflict	UNP Q9WXS1
R	139	LYS	GLU	conflict	UNP Q9WXS1
R	146	LEU	GLU	conflict	UNP Q9WXS1
R	174	MET	LYS	conflict	UNP Q9WXS1
R	189	ALA	CYS	conflict	UNP Q9WXS1
R	213	ALA	CYS	conflict	UNP Q9WXS1
R	300	VAL	ASP	conflict	UNP Q9WXS1
R	303	ALA	ARG	conflict	UNP Q9WXS1
S	139	LYS	GLU	conflict	UNP Q9WXS1
S	146	LEU	GLU	conflict	UNP Q9WXS1
S	174	MET	LYS	conflict	UNP Q9WXS1
S	189	ALA	CYS	conflict	UNP Q9WXS1
S	213	ALA	CYS	conflict	UNP Q9WXS1
S	300	VAL	ASP	conflict	UNP Q9WXS1
S	303	ALA	ARG	conflict	UNP Q9WXS1
T	139	LYS	GLU	conflict	UNP Q9WXS1
T	146	LEU	GLU	conflict	UNP Q9WXS1
T	174	MET	LYS	conflict	UNP Q9WXS1
T	189	ALA	CYS	conflict	UNP Q9WXS1
T	213	ALA	CYS	conflict	UNP Q9WXS1
T	300	VAL	ASP	conflict	UNP Q9WXS1
T	303	ALA	ARG	conflict	UNP Q9WXS1
U	139	LYS	GLU	conflict	UNP Q9WXS1
U	146	LEU	GLU	conflict	UNP Q9WXS1
U	174	MET	LYS	conflict	UNP Q9WXS1
U	189	ALA	CYS	conflict	UNP Q9WXS1
U	213	ALA	CYS	conflict	UNP Q9WXS1
U	300	VAL	ASP	conflict	UNP Q9WXS1
U	303	ALA	ARG	conflict	UNP Q9WXS1
V	139	LYS	GLU	conflict	UNP Q9WXS1
V	146	LEU	GLU	conflict	UNP Q9WXS1
V	174	MET	LYS	conflict	UNP Q9WXS1
V	189	ALA	CYS	conflict	UNP Q9WXS1
V	213	ALA	CYS	conflict	UNP Q9WXS1
V	300	VAL	ASP	conflict	UNP Q9WXS1
V	303	ALA	ARG	conflict	UNP Q9WXS1
W	139	LYS	GLU	conflict	UNP Q9WXS1
W	146	LEU	GLU	conflict	UNP Q9WXS1
W	174	MET	LYS	conflict	UNP Q9WXS1
W	189	ALA	CYS	conflict	UNP Q9WXS1
W	213	ALA	CYS	conflict	UNP Q9WXS1
W	300	VAL	ASP	conflict	UNP Q9WXS1

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Chain	Residue	Modelled	Actual	Comment	Reference
W	303	ALA	ARG	conflict	UNP Q9WXS1
X	139	LYS	GLU	conflict	UNP Q9WXS1
X	146	LEU	GLU	conflict	UNP Q9WXS1
X	174	MET	LYS	conflict	UNP Q9WXS1
X	189	ALA	CYS	conflict	UNP Q9WXS1
X	213	ALA	CYS	conflict	UNP Q9WXS1
X	300	VAL	ASP	conflict	UNP Q9WXS1
X	303	ALA	ARG	conflict	UNP Q9WXS1
Y	139	LYS	GLU	conflict	UNP Q9WXS1
Y	146	LEU	GLU	conflict	UNP Q9WXS1
Y	174	MET	LYS	conflict	UNP Q9WXS1
Y	189	ALA	CYS	conflict	UNP Q9WXS1
Y	213	ALA	CYS	conflict	UNP Q9WXS1
Y	300	VAL	ASP	conflict	UNP Q9WXS1
Y	303	ALA	ARG	conflict	UNP Q9WXS1
Z	139	LYS	GLU	conflict	UNP Q9WXS1
Z	146	LEU	GLU	conflict	UNP Q9WXS1
Z	174	MET	LYS	conflict	UNP Q9WXS1
Z	189	ALA	CYS	conflict	UNP Q9WXS1
Z	213	ALA	CYS	conflict	UNP Q9WXS1
Z	300	VAL	ASP	conflict	UNP Q9WXS1
Z	303	ALA	ARG	conflict	UNP Q9WXS1
a	139	LYS	GLU	conflict	UNP Q9WXS1
a	146	LEU	GLU	conflict	UNP Q9WXS1
a	174	MET	LYS	conflict	UNP Q9WXS1
a	189	ALA	CYS	conflict	UNP Q9WXS1
a	213	ALA	CYS	conflict	UNP Q9WXS1
a	300	VAL	ASP	conflict	UNP Q9WXS1
a	303	ALA	ARG	conflict	UNP Q9WXS1
b	139	LYS	GLU	conflict	UNP Q9WXS1
b	146	LEU	GLU	conflict	UNP Q9WXS1
b	174	MET	LYS	conflict	UNP Q9WXS1
b	189	ALA	CYS	conflict	UNP Q9WXS1
b	213	ALA	CYS	conflict	UNP Q9WXS1
b	300	VAL	ASP	conflict	UNP Q9WXS1
b	303	ALA	ARG	conflict	UNP Q9WXS1
c	139	LYS	GLU	conflict	UNP Q9WXS1
c	146	LEU	GLU	conflict	UNP Q9WXS1
c	174	MET	LYS	conflict	UNP Q9WXS1
c	189	ALA	CYS	conflict	UNP Q9WXS1
c	213	ALA	CYS	conflict	UNP Q9WXS1
c	300	VAL	ASP	conflict	UNP Q9WXS1

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Chain	Residue	Modelled	Actual	Comment	Reference
c	303	ALA	ARG	conflict	UNP Q9WXS1
d	139	LYS	GLU	conflict	UNP Q9WXS1
d	146	LEU	GLU	conflict	UNP Q9WXS1
d	174	MET	LYS	conflict	UNP Q9WXS1
d	189	ALA	CYS	conflict	UNP Q9WXS1
d	213	ALA	CYS	conflict	UNP Q9WXS1
d	300	VAL	ASP	conflict	UNP Q9WXS1
d	303	ALA	ARG	conflict	UNP Q9WXS1
e	139	LYS	GLU	conflict	UNP Q9WXS1
e	146	LEU	GLU	conflict	UNP Q9WXS1
e	174	MET	LYS	conflict	UNP Q9WXS1
e	189	ALA	CYS	conflict	UNP Q9WXS1
e	213	ALA	CYS	conflict	UNP Q9WXS1
e	300	VAL	ASP	conflict	UNP Q9WXS1
e	303	ALA	ARG	conflict	UNP Q9WXS1
f	139	LYS	GLU	conflict	UNP Q9WXS1
f	146	LEU	GLU	conflict	UNP Q9WXS1
f	174	MET	LYS	conflict	UNP Q9WXS1
f	189	ALA	CYS	conflict	UNP Q9WXS1
f	213	ALA	CYS	conflict	UNP Q9WXS1
f	300	VAL	ASP	conflict	UNP Q9WXS1
f	303	ALA	ARG	conflict	UNP Q9WXS1
g	139	LYS	GLU	conflict	UNP Q9WXS1
g	146	LEU	GLU	conflict	UNP Q9WXS1
g	174	MET	LYS	conflict	UNP Q9WXS1
g	189	ALA	CYS	conflict	UNP Q9WXS1
g	213	ALA	CYS	conflict	UNP Q9WXS1
g	300	VAL	ASP	conflict	UNP Q9WXS1
g	303	ALA	ARG	conflict	UNP Q9WXS1
h	139	LYS	GLU	conflict	UNP Q9WXS1
h	146	LEU	GLU	conflict	UNP Q9WXS1
h	174	MET	LYS	conflict	UNP Q9WXS1
h	189	ALA	CYS	conflict	UNP Q9WXS1
h	213	ALA	CYS	conflict	UNP Q9WXS1
h	300	VAL	ASP	conflict	UNP Q9WXS1
h	303	ALA	ARG	conflict	UNP Q9WXS1
i	139	LYS	GLU	conflict	UNP Q9WXS1
i	146	LEU	GLU	conflict	UNP Q9WXS1
i	174	MET	LYS	conflict	UNP Q9WXS1
i	189	ALA	CYS	conflict	UNP Q9WXS1
i	213	ALA	CYS	conflict	UNP Q9WXS1
i	300	VAL	ASP	conflict	UNP Q9WXS1

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Chain	Residue	Modelled	Actual	Comment	Reference
i	303	ALA	ARG	conflict	UNP Q9WXS1
j	139	LYS	GLU	conflict	UNP Q9WXS1
j	146	LEU	GLU	conflict	UNP Q9WXS1
j	174	MET	LYS	conflict	UNP Q9WXS1
j	189	ALA	CYS	conflict	UNP Q9WXS1
j	213	ALA	CYS	conflict	UNP Q9WXS1
j	300	VAL	ASP	conflict	UNP Q9WXS1
j	303	ALA	ARG	conflict	UNP Q9WXS1
k	139	LYS	GLU	conflict	UNP Q9WXS1
k	146	LEU	GLU	conflict	UNP Q9WXS1
k	174	MET	LYS	conflict	UNP Q9WXS1
k	189	ALA	CYS	conflict	UNP Q9WXS1
k	213	ALA	CYS	conflict	UNP Q9WXS1
k	300	VAL	ASP	conflict	UNP Q9WXS1
k	303	ALA	ARG	conflict	UNP Q9WXS1
l	139	LYS	GLU	conflict	UNP Q9WXS1
l	146	LEU	GLU	conflict	UNP Q9WXS1
l	174	MET	LYS	conflict	UNP Q9WXS1
l	189	ALA	CYS	conflict	UNP Q9WXS1
l	213	ALA	CYS	conflict	UNP Q9WXS1
l	300	VAL	ASP	conflict	UNP Q9WXS1
l	303	ALA	ARG	conflict	UNP Q9WXS1
m	139	LYS	GLU	conflict	UNP Q9WXS1
m	146	LEU	GLU	conflict	UNP Q9WXS1
m	174	MET	LYS	conflict	UNP Q9WXS1
m	189	ALA	CYS	conflict	UNP Q9WXS1
m	213	ALA	CYS	conflict	UNP Q9WXS1
m	300	VAL	ASP	conflict	UNP Q9WXS1
m	303	ALA	ARG	conflict	UNP Q9WXS1
n	139	LYS	GLU	conflict	UNP Q9WXS1
n	146	LEU	GLU	conflict	UNP Q9WXS1
n	174	MET	LYS	conflict	UNP Q9WXS1
n	189	ALA	CYS	conflict	UNP Q9WXS1
n	213	ALA	CYS	conflict	UNP Q9WXS1
n	300	VAL	ASP	conflict	UNP Q9WXS1
n	303	ALA	ARG	conflict	UNP Q9WXS1
o	139	LYS	GLU	conflict	UNP Q9WXS1
o	146	LEU	GLU	conflict	UNP Q9WXS1
o	174	MET	LYS	conflict	UNP Q9WXS1
o	189	ALA	CYS	conflict	UNP Q9WXS1
o	213	ALA	CYS	conflict	UNP Q9WXS1
o	300	VAL	ASP	conflict	UNP Q9WXS1

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Chain	Residue	Modelled	Actual	Comment	Reference
o	303	ALA	ARG	conflict	UNP Q9WXS1
p	139	LYS	GLU	conflict	UNP Q9WXS1
p	146	LEU	GLU	conflict	UNP Q9WXS1
p	174	MET	LYS	conflict	UNP Q9WXS1
p	189	ALA	CYS	conflict	UNP Q9WXS1
p	213	ALA	CYS	conflict	UNP Q9WXS1
p	300	VAL	ASP	conflict	UNP Q9WXS1
p	303	ALA	ARG	conflict	UNP Q9WXS1
q	139	LYS	GLU	conflict	UNP Q9WXS1
q	146	LEU	GLU	conflict	UNP Q9WXS1
q	174	MET	LYS	conflict	UNP Q9WXS1
q	189	ALA	CYS	conflict	UNP Q9WXS1
q	213	ALA	CYS	conflict	UNP Q9WXS1
q	300	VAL	ASP	conflict	UNP Q9WXS1
q	303	ALA	ARG	conflict	UNP Q9WXS1
r	139	LYS	GLU	conflict	UNP Q9WXS1
r	146	LEU	GLU	conflict	UNP Q9WXS1
r	174	MET	LYS	conflict	UNP Q9WXS1
r	189	ALA	CYS	conflict	UNP Q9WXS1
r	213	ALA	CYS	conflict	UNP Q9WXS1
r	300	VAL	ASP	conflict	UNP Q9WXS1
r	303	ALA	ARG	conflict	UNP Q9WXS1
s	139	LYS	GLU	conflict	UNP Q9WXS1
s	146	LEU	GLU	conflict	UNP Q9WXS1
s	174	MET	LYS	conflict	UNP Q9WXS1
s	189	ALA	CYS	conflict	UNP Q9WXS1
s	213	ALA	CYS	conflict	UNP Q9WXS1
s	300	VAL	ASP	conflict	UNP Q9WXS1
s	303	ALA	ARG	conflict	UNP Q9WXS1
t	139	LYS	GLU	conflict	UNP Q9WXS1
t	146	LEU	GLU	conflict	UNP Q9WXS1
t	174	MET	LYS	conflict	UNP Q9WXS1
t	189	ALA	CYS	conflict	UNP Q9WXS1
t	213	ALA	CYS	conflict	UNP Q9WXS1
t	300	VAL	ASP	conflict	UNP Q9WXS1
t	303	ALA	ARG	conflict	UNP Q9WXS1
u	139	LYS	GLU	conflict	UNP Q9WXS1
u	146	LEU	GLU	conflict	UNP Q9WXS1
u	174	MET	LYS	conflict	UNP Q9WXS1
u	189	ALA	CYS	conflict	UNP Q9WXS1
u	213	ALA	CYS	conflict	UNP Q9WXS1
u	300	VAL	ASP	conflict	UNP Q9WXS1

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Chain	Residue	Modelled	Actual	Comment	Reference
u	303	ALA	ARG	conflict	UNP Q9WXS1
v	139	LYS	GLU	conflict	UNP Q9WXS1
v	146	LEU	GLU	conflict	UNP Q9WXS1
v	174	MET	LYS	conflict	UNP Q9WXS1
v	189	ALA	CYS	conflict	UNP Q9WXS1
v	213	ALA	CYS	conflict	UNP Q9WXS1
v	300	VAL	ASP	conflict	UNP Q9WXS1
v	303	ALA	ARG	conflict	UNP Q9WXS1
w	139	LYS	GLU	conflict	UNP Q9WXS1
w	146	LEU	GLU	conflict	UNP Q9WXS1
w	174	MET	LYS	conflict	UNP Q9WXS1
w	189	ALA	CYS	conflict	UNP Q9WXS1
w	213	ALA	CYS	conflict	UNP Q9WXS1
w	300	VAL	ASP	conflict	UNP Q9WXS1
w	303	ALA	ARG	conflict	UNP Q9WXS1
x	139	LYS	GLU	conflict	UNP Q9WXS1
x	146	LEU	GLU	conflict	UNP Q9WXS1
x	174	MET	LYS	conflict	UNP Q9WXS1
x	189	ALA	CYS	conflict	UNP Q9WXS1
x	213	ALA	CYS	conflict	UNP Q9WXS1
x	300	VAL	ASP	conflict	UNP Q9WXS1
x	303	ALA	ARG	conflict	UNP Q9WXS1
y	139	LYS	GLU	conflict	UNP Q9WXS1
y	146	LEU	GLU	conflict	UNP Q9WXS1
y	174	MET	LYS	conflict	UNP Q9WXS1
y	189	ALA	CYS	conflict	UNP Q9WXS1
y	213	ALA	CYS	conflict	UNP Q9WXS1
y	300	VAL	ASP	conflict	UNP Q9WXS1
y	303	ALA	ARG	conflict	UNP Q9WXS1
z	139	LYS	GLU	conflict	UNP Q9WXS1
z	146	LEU	GLU	conflict	UNP Q9WXS1
z	174	MET	LYS	conflict	UNP Q9WXS1
z	189	ALA	CYS	conflict	UNP Q9WXS1
z	213	ALA	CYS	conflict	UNP Q9WXS1
z	300	VAL	ASP	conflict	UNP Q9WXS1
z	303	ALA	ARG	conflict	UNP Q9WXS1
0	139	LYS	GLU	conflict	UNP Q9WXS1
0	146	LEU	GLU	conflict	UNP Q9WXS1
0	174	MET	LYS	conflict	UNP Q9WXS1
0	189	ALA	CYS	conflict	UNP Q9WXS1
0	213	ALA	CYS	conflict	UNP Q9WXS1
0	300	VAL	ASP	conflict	UNP Q9WXS1

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Chain	Residue	Modelled	Actual	Comment	Reference
0	303	ALA	ARG	conflict	UNP Q9WXS1
1	139	LYS	GLU	conflict	UNP Q9WXS1
1	146	LEU	GLU	conflict	UNP Q9WXS1
1	174	MET	LYS	conflict	UNP Q9WXS1
1	189	ALA	CYS	conflict	UNP Q9WXS1
1	213	ALA	CYS	conflict	UNP Q9WXS1
1	300	VAL	ASP	conflict	UNP Q9WXS1
1	303	ALA	ARG	conflict	UNP Q9WXS1
2	139	LYS	GLU	conflict	UNP Q9WXS1
2	146	LEU	GLU	conflict	UNP Q9WXS1
2	174	MET	LYS	conflict	UNP Q9WXS1
2	189	ALA	CYS	conflict	UNP Q9WXS1
2	213	ALA	CYS	conflict	UNP Q9WXS1
2	300	VAL	ASP	conflict	UNP Q9WXS1
2	303	ALA	ARG	conflict	UNP Q9WXS1
3	139	LYS	GLU	conflict	UNP Q9WXS1
3	146	LEU	GLU	conflict	UNP Q9WXS1
3	174	MET	LYS	conflict	UNP Q9WXS1
3	189	ALA	CYS	conflict	UNP Q9WXS1
3	213	ALA	CYS	conflict	UNP Q9WXS1
3	300	VAL	ASP	conflict	UNP Q9WXS1
3	303	ALA	ARG	conflict	UNP Q9WXS1
4	139	LYS	GLU	conflict	UNP Q9WXS1
4	146	LEU	GLU	conflict	UNP Q9WXS1
4	174	MET	LYS	conflict	UNP Q9WXS1
4	189	ALA	CYS	conflict	UNP Q9WXS1
4	213	ALA	CYS	conflict	UNP Q9WXS1
4	300	VAL	ASP	conflict	UNP Q9WXS1
4	303	ALA	ARG	conflict	UNP Q9WXS1
5	139	LYS	GLU	conflict	UNP Q9WXS1
5	146	LEU	GLU	conflict	UNP Q9WXS1
5	174	MET	LYS	conflict	UNP Q9WXS1
5	189	ALA	CYS	conflict	UNP Q9WXS1
5	213	ALA	CYS	conflict	UNP Q9WXS1
5	300	VAL	ASP	conflict	UNP Q9WXS1
5	303	ALA	ARG	conflict	UNP Q9WXS1
6	139	LYS	GLU	conflict	UNP Q9WXS1
6	146	LEU	GLU	conflict	UNP Q9WXS1
6	174	MET	LYS	conflict	UNP Q9WXS1
6	189	ALA	CYS	conflict	UNP Q9WXS1
6	213	ALA	CYS	conflict	UNP Q9WXS1
6	300	VAL	ASP	conflict	UNP Q9WXS1

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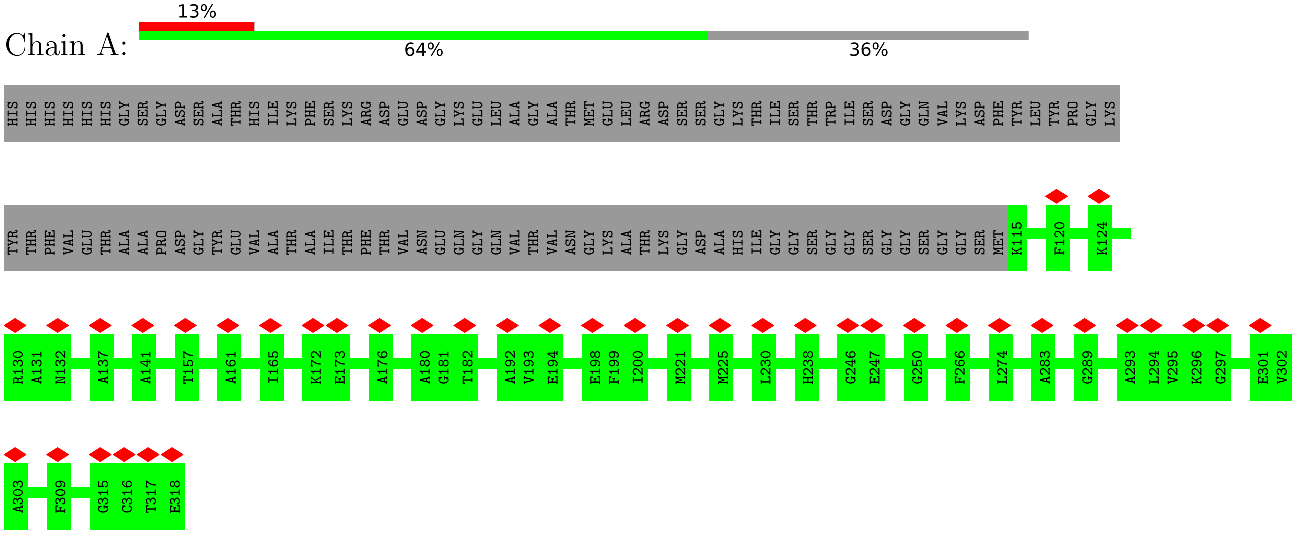
Chain	Residue	Modelled	Actual	Comment	Reference
6	303	ALA	ARG	conflict	UNP Q9WXS1
7	139	LYS	GLU	conflict	UNP Q9WXS1
7	146	LEU	GLU	conflict	UNP Q9WXS1
7	174	MET	LYS	conflict	UNP Q9WXS1
7	189	ALA	CYS	conflict	UNP Q9WXS1
7	213	ALA	CYS	conflict	UNP Q9WXS1
7	300	VAL	ASP	conflict	UNP Q9WXS1
7	303	ALA	ARG	conflict	UNP Q9WXS1

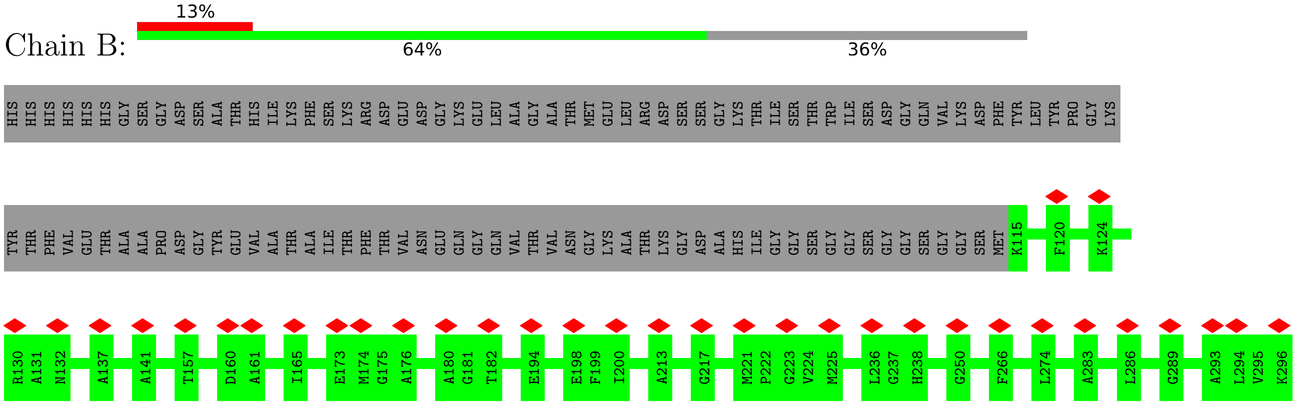
3 Residue-property plots ⓘ

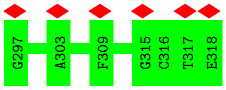
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase



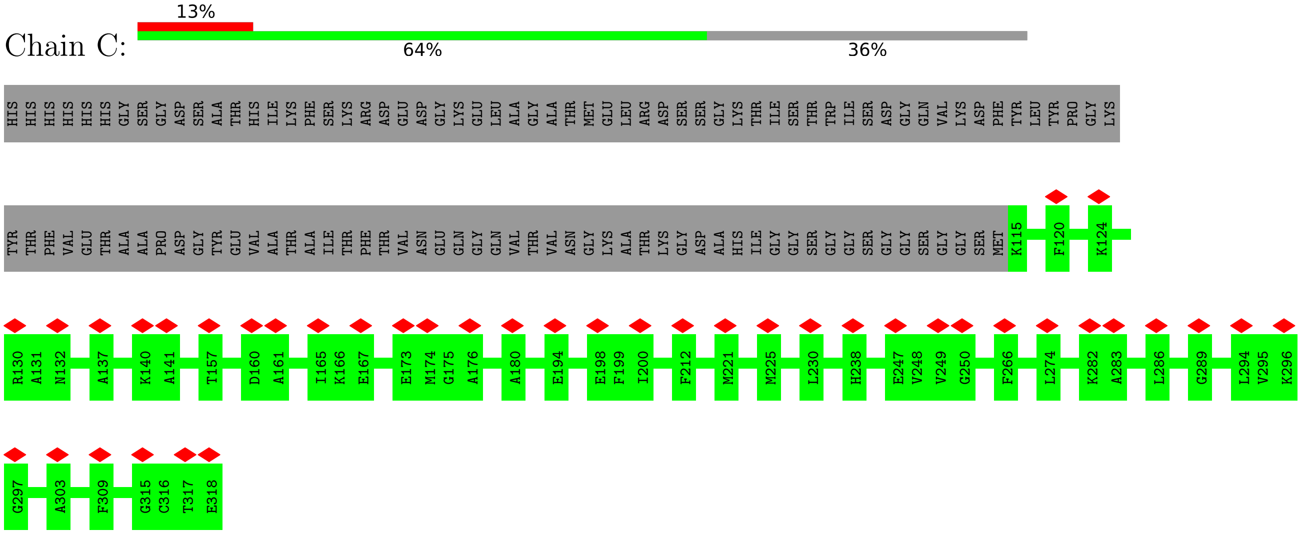
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase





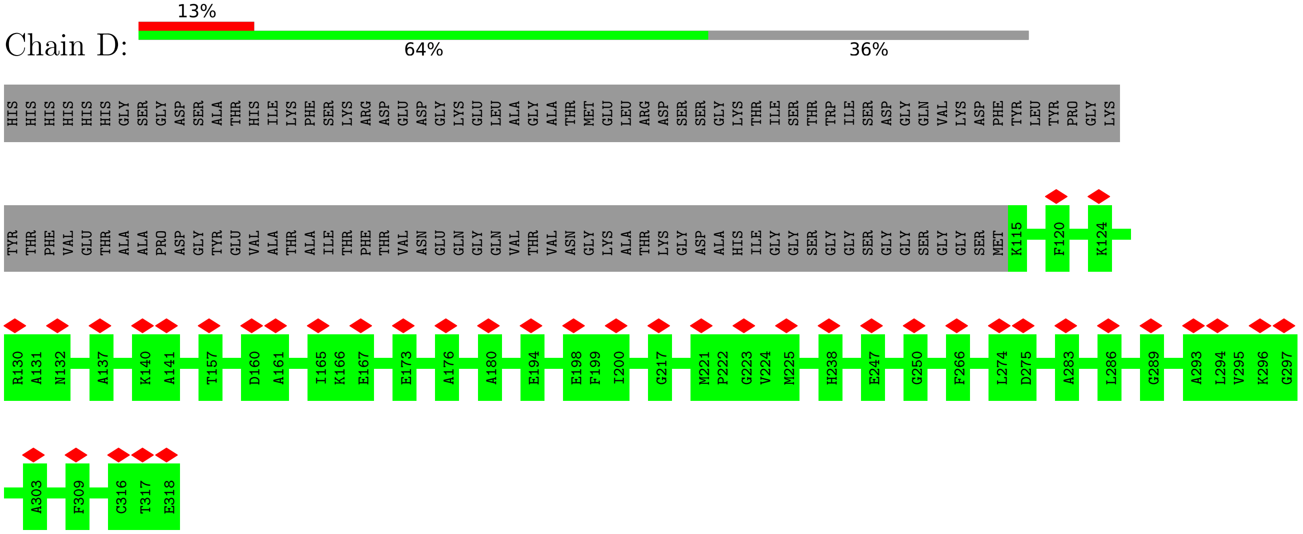
• Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain C:



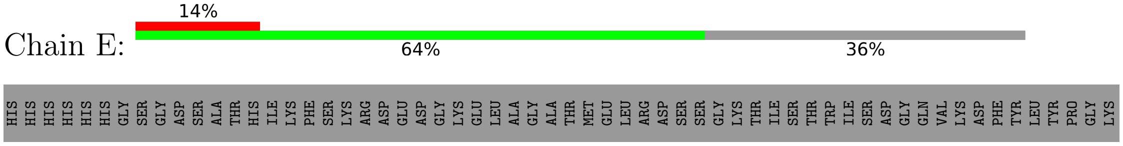
• Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

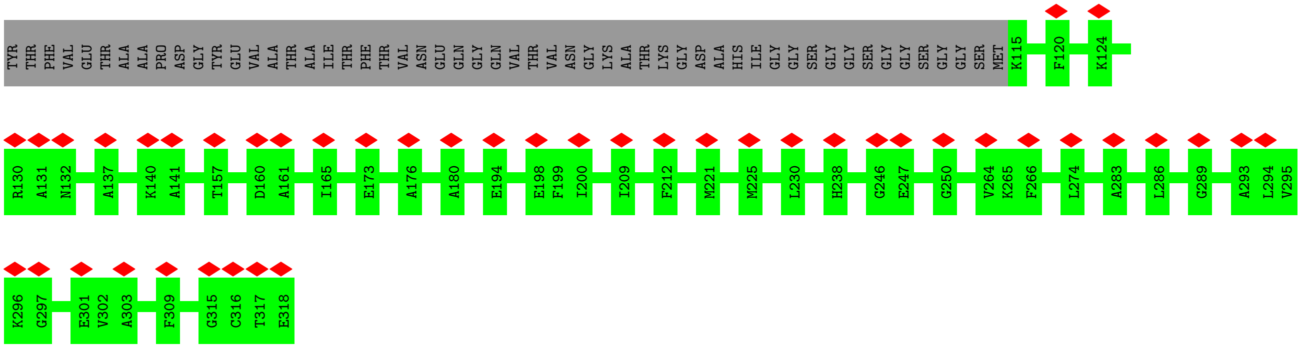
Chain D:



• Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

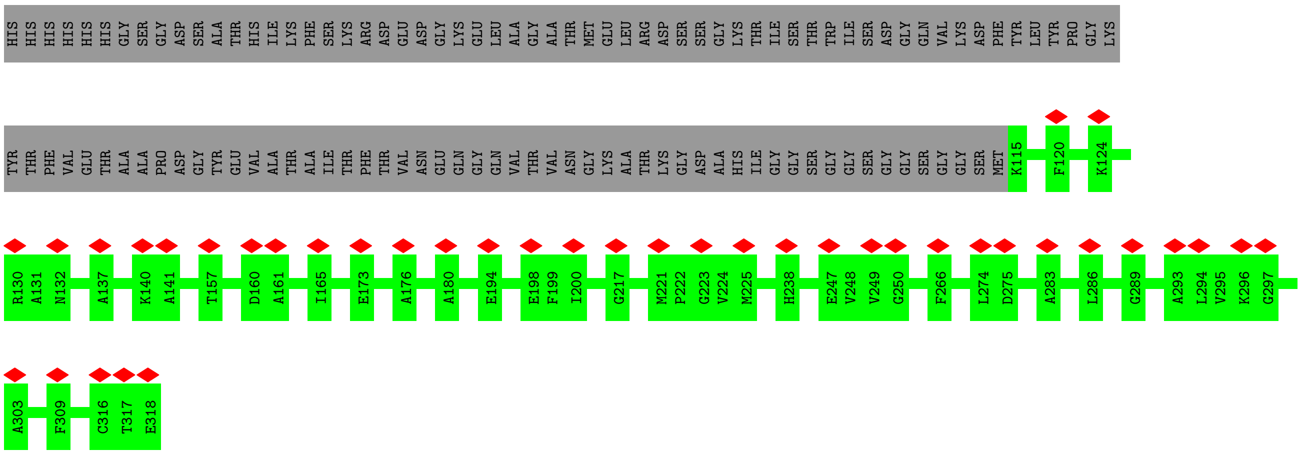
Chain E:





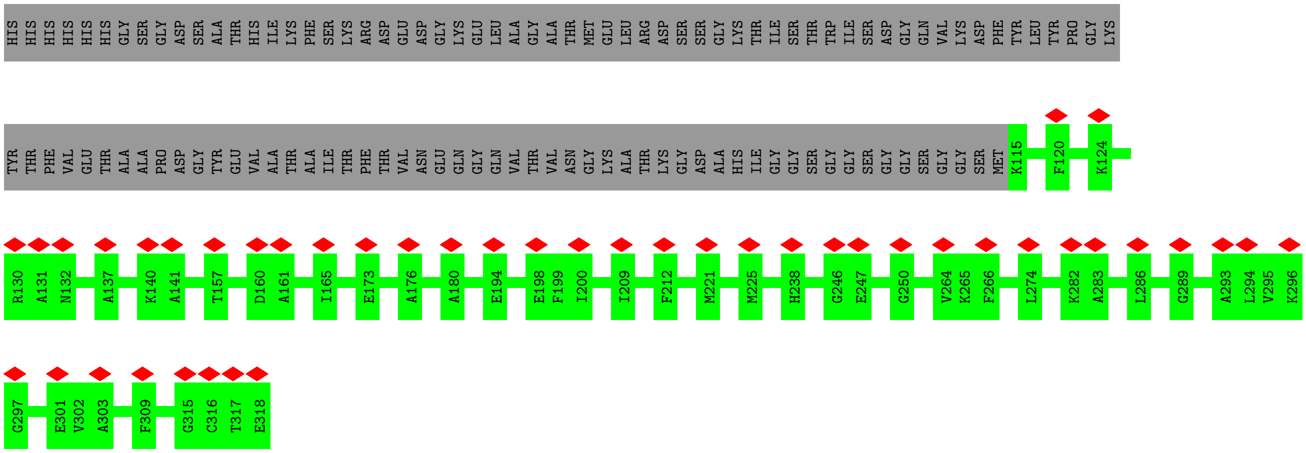
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain F:

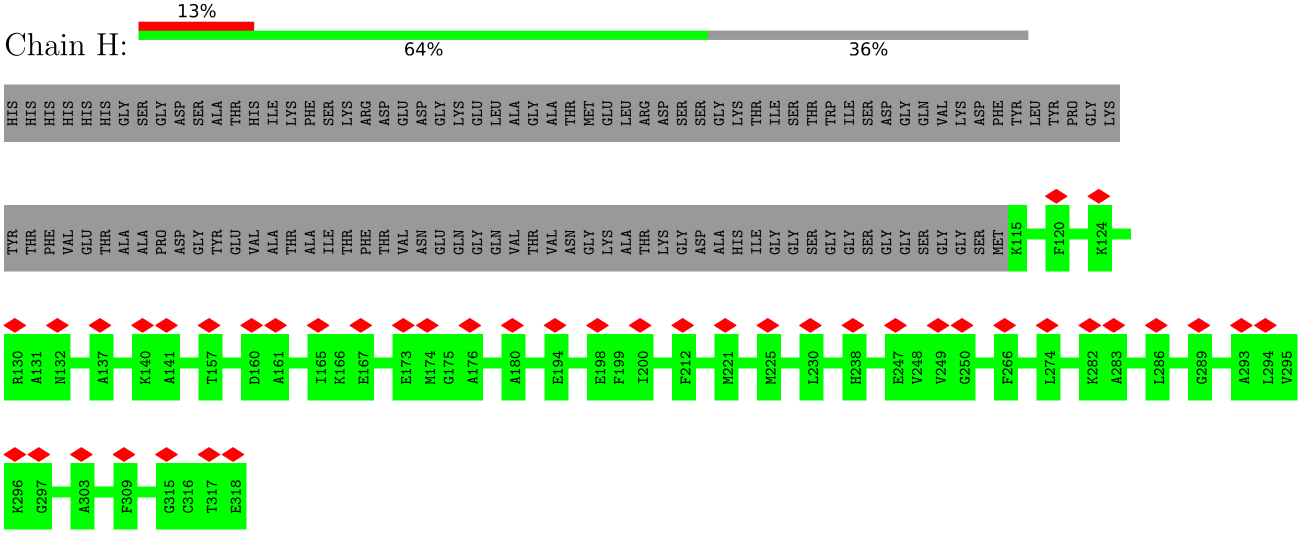


- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

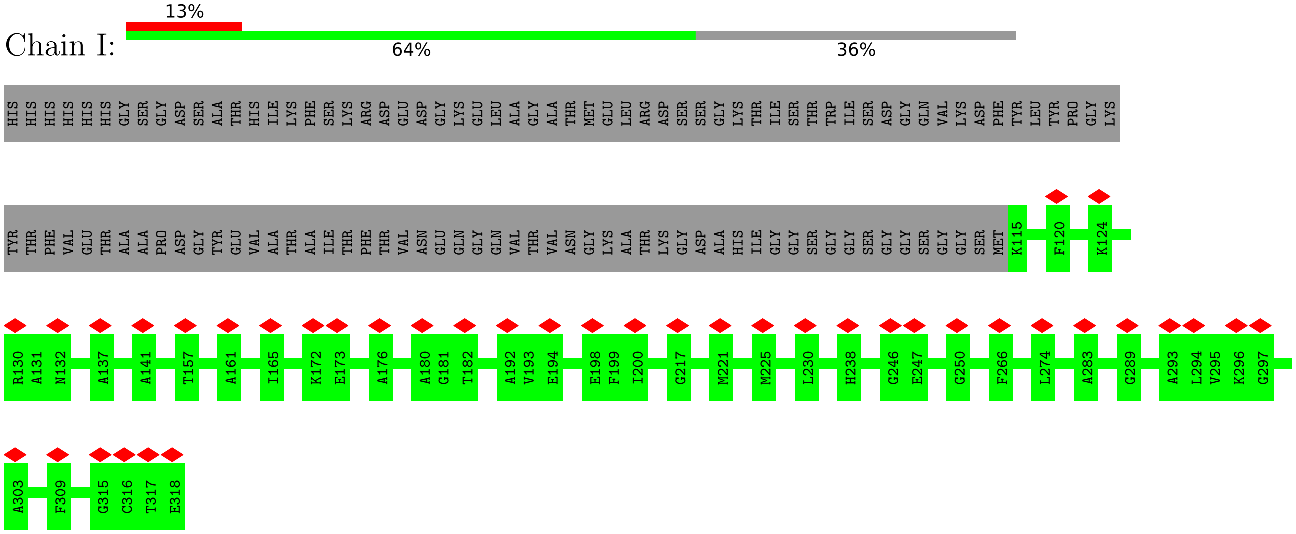
Chain G:



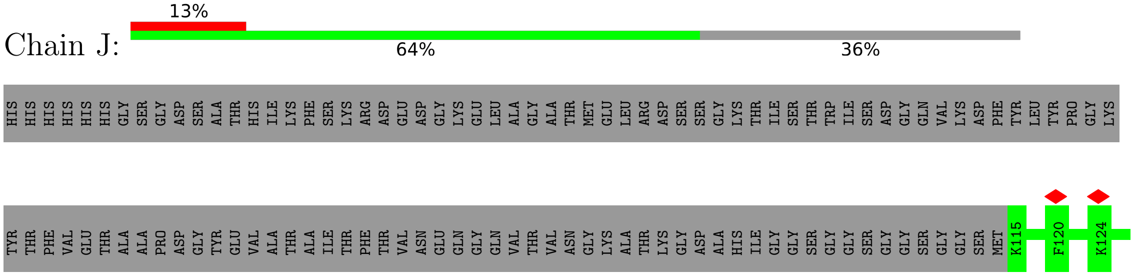
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

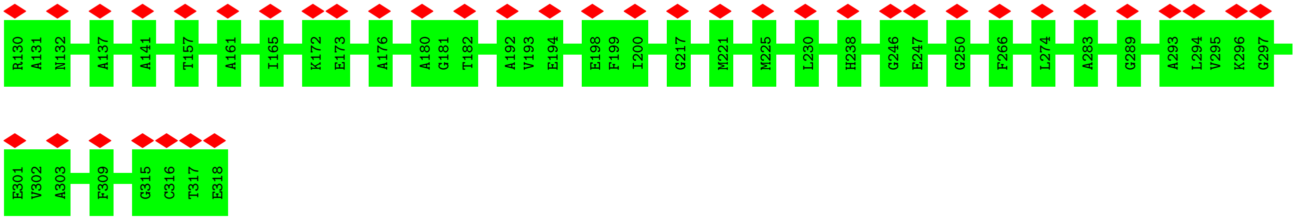


- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase



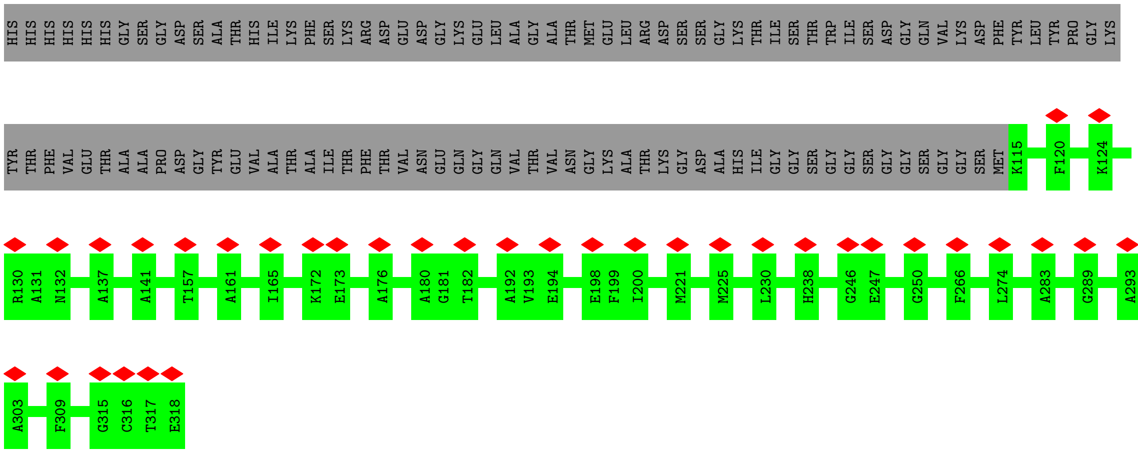
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase





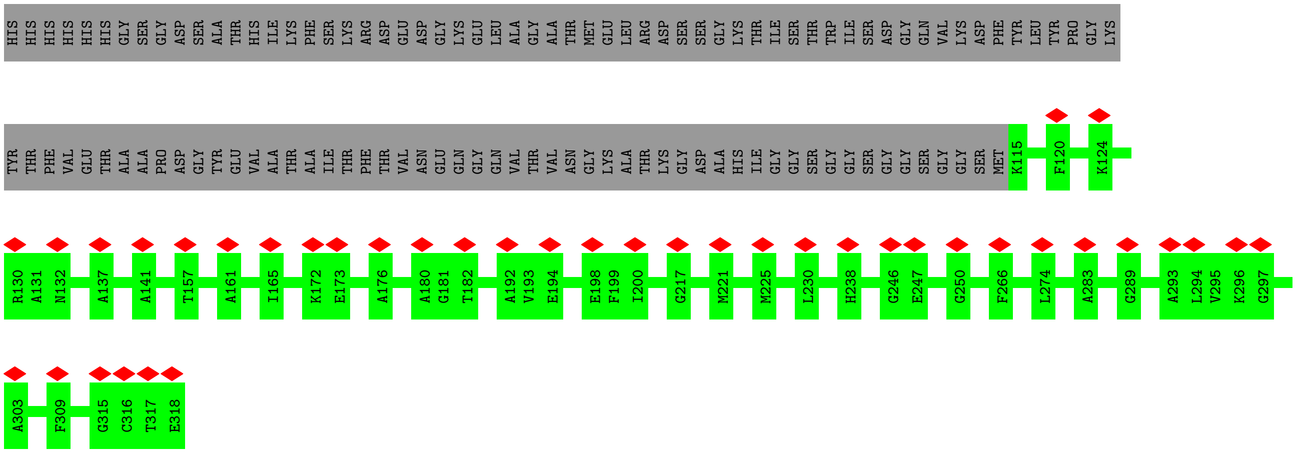
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain K:



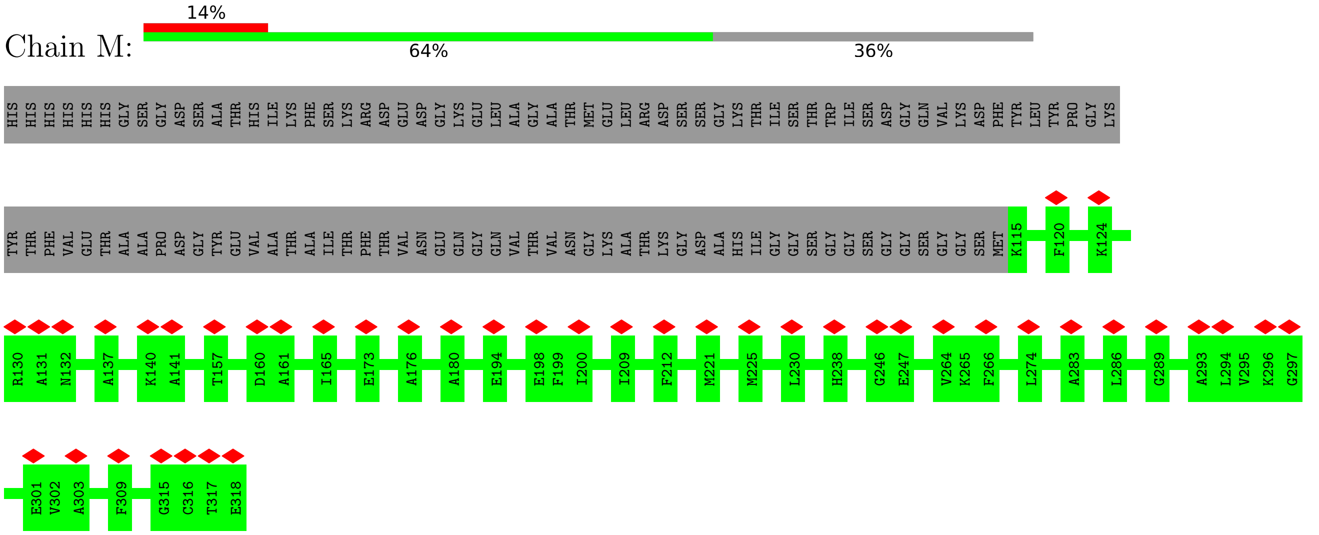
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain L:



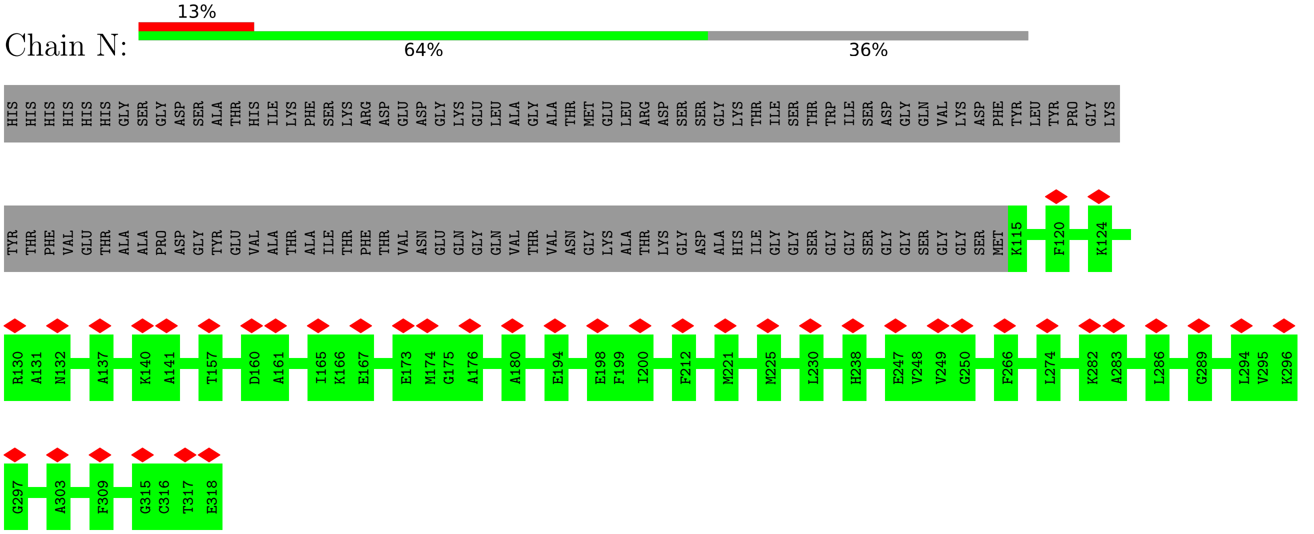
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain M:



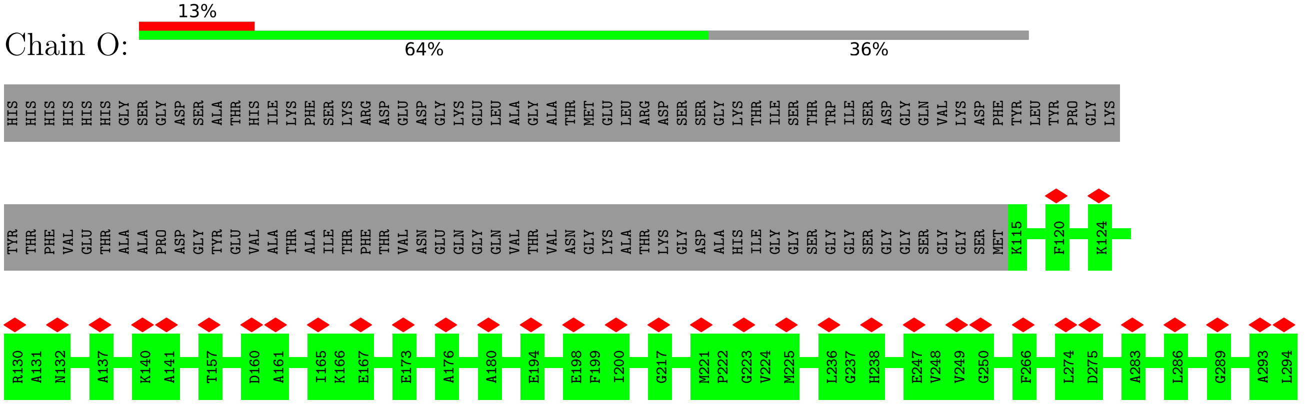
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

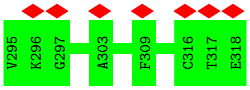
Chain N:



- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

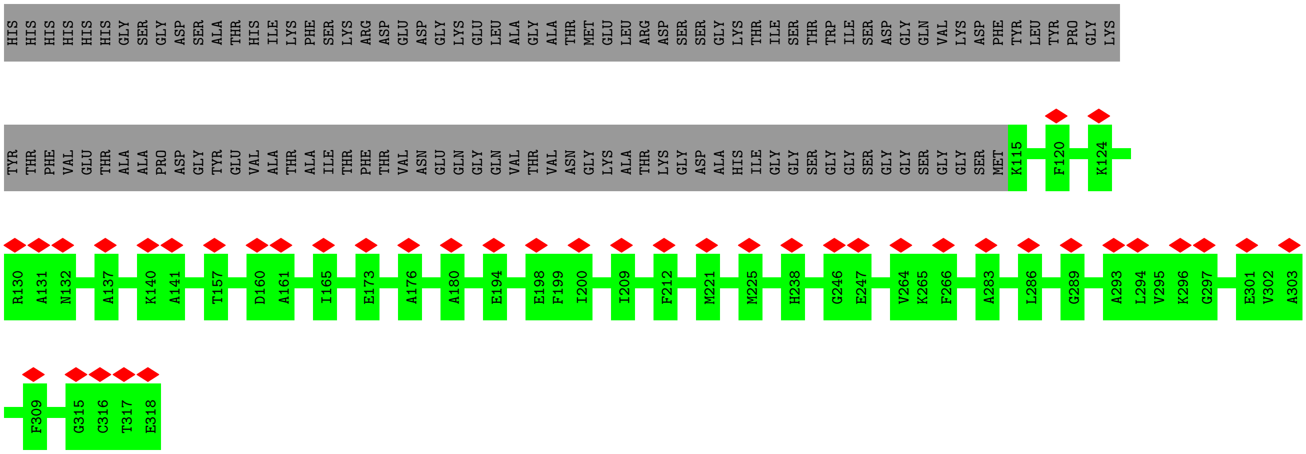
Chain O:





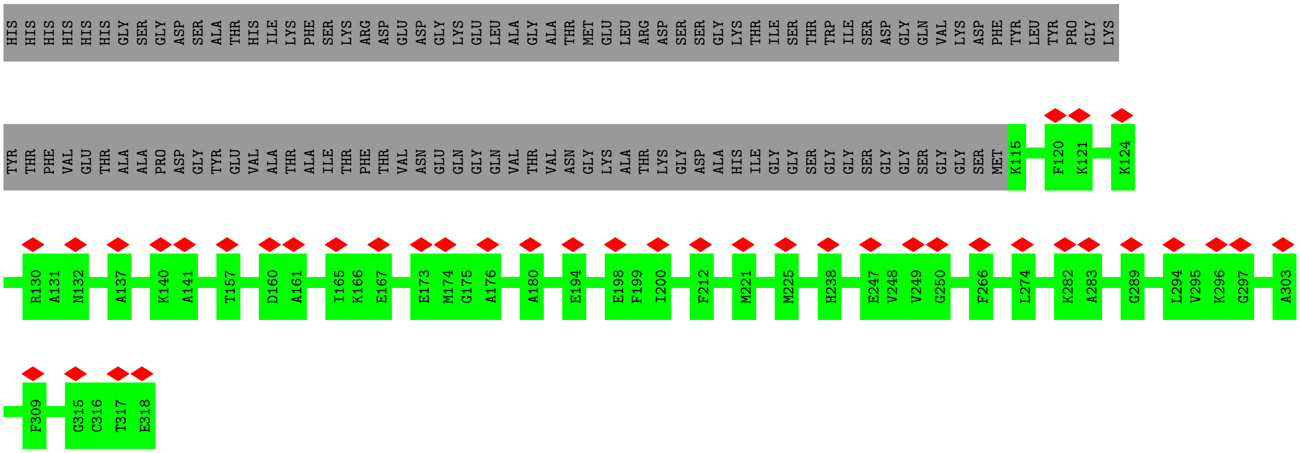
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain P:



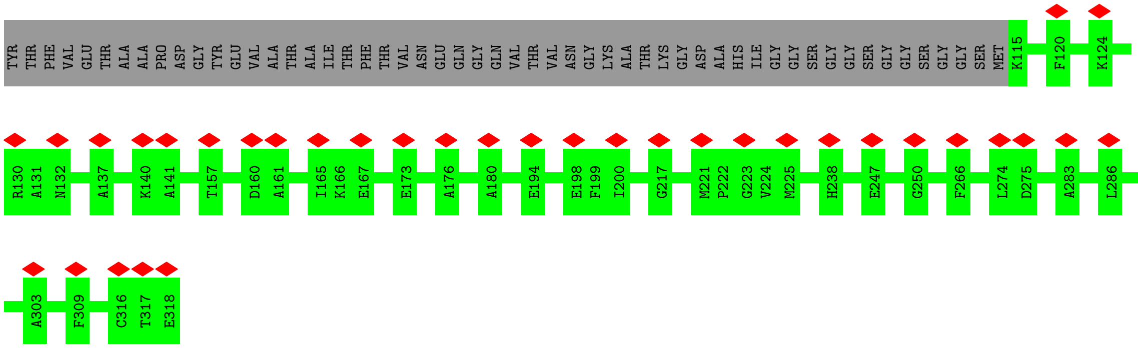
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain Q:



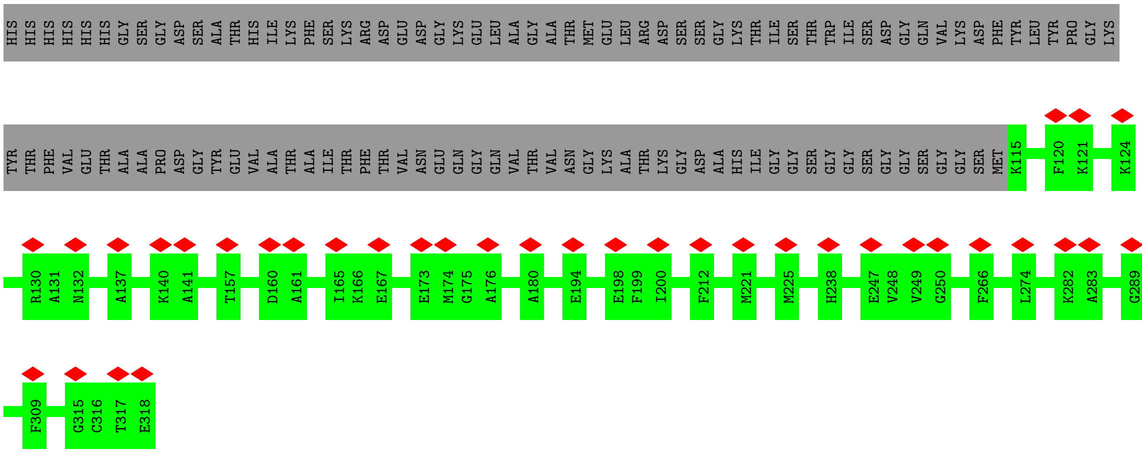
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain R:



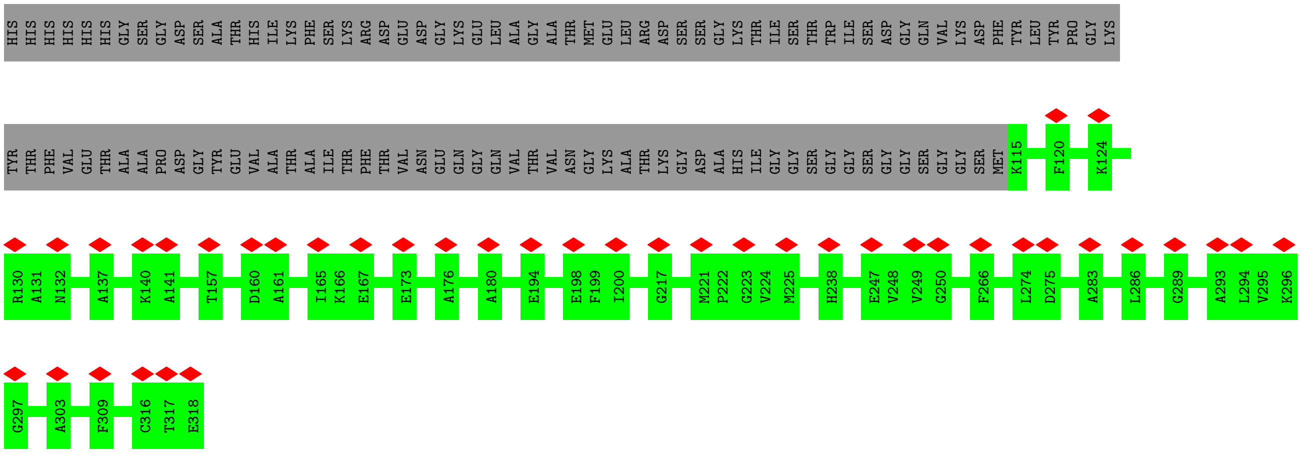
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain S:

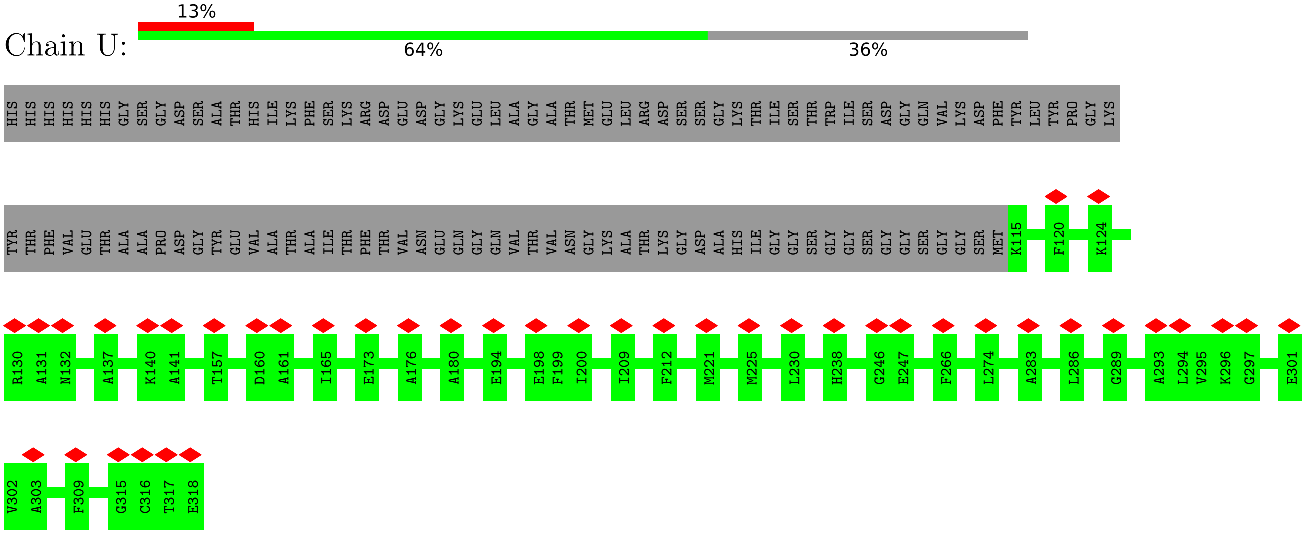


- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

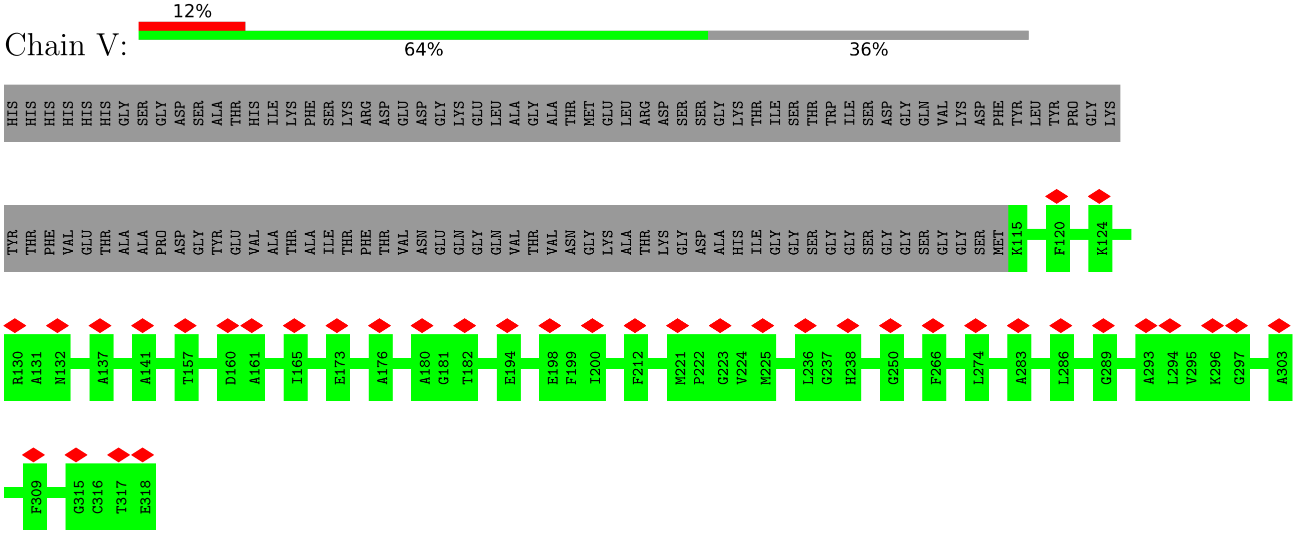
Chain T:



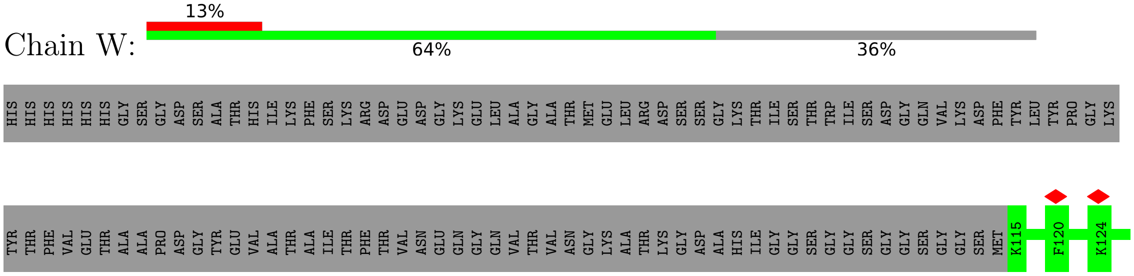
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

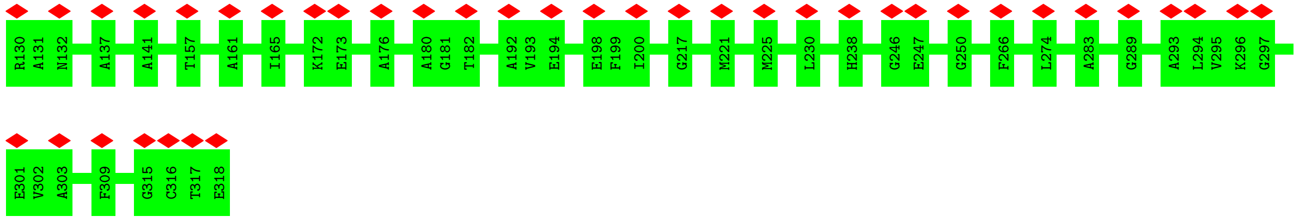


- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase



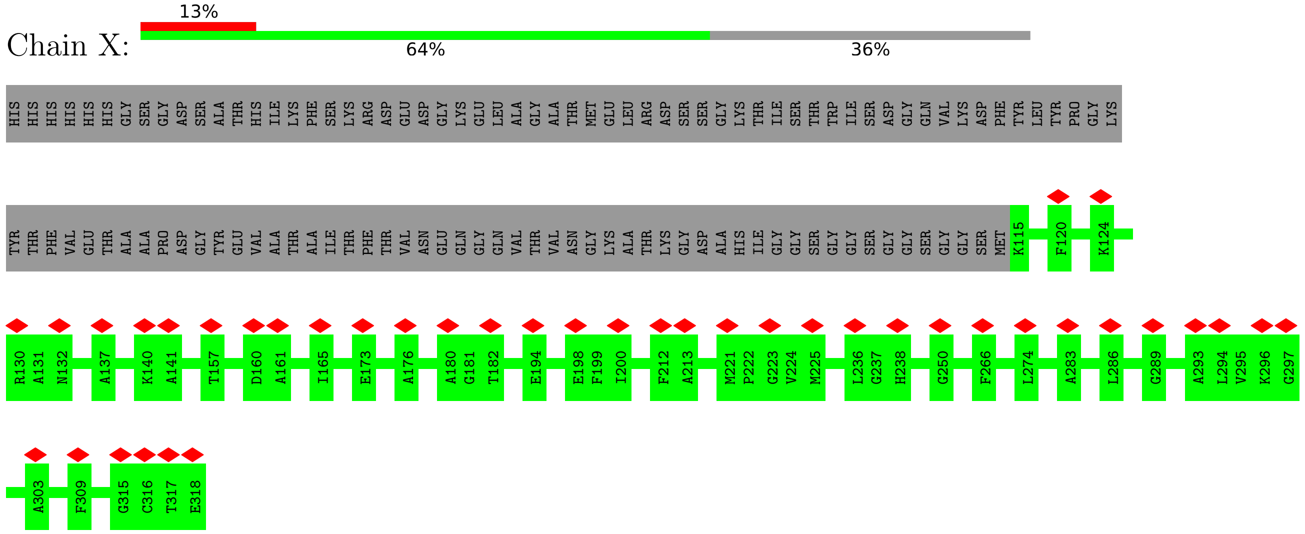
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase





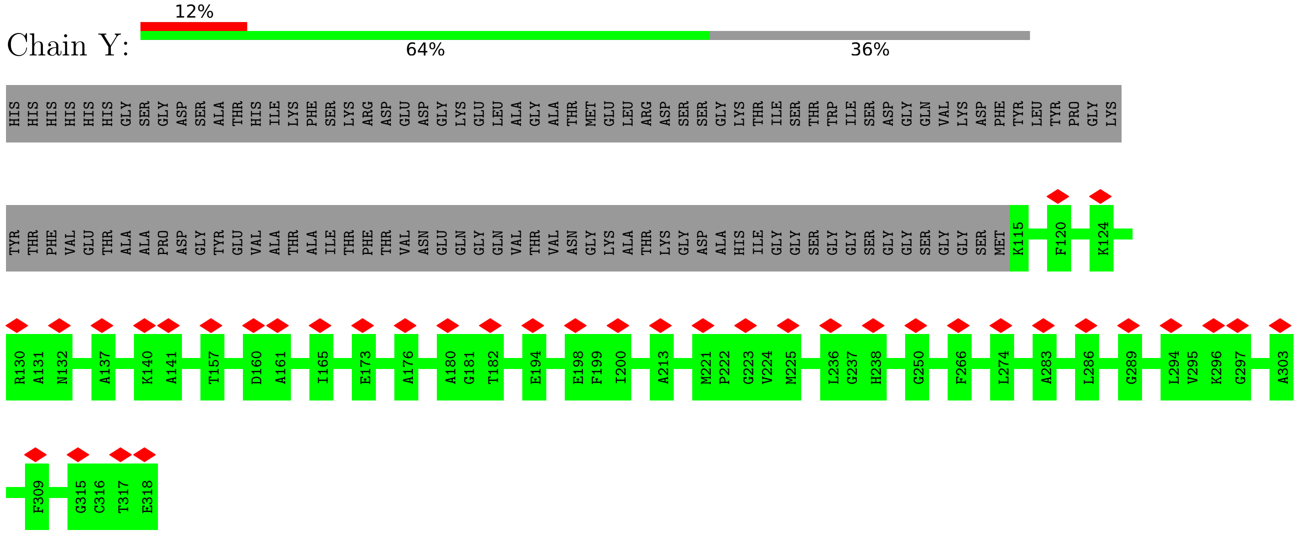
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain X:



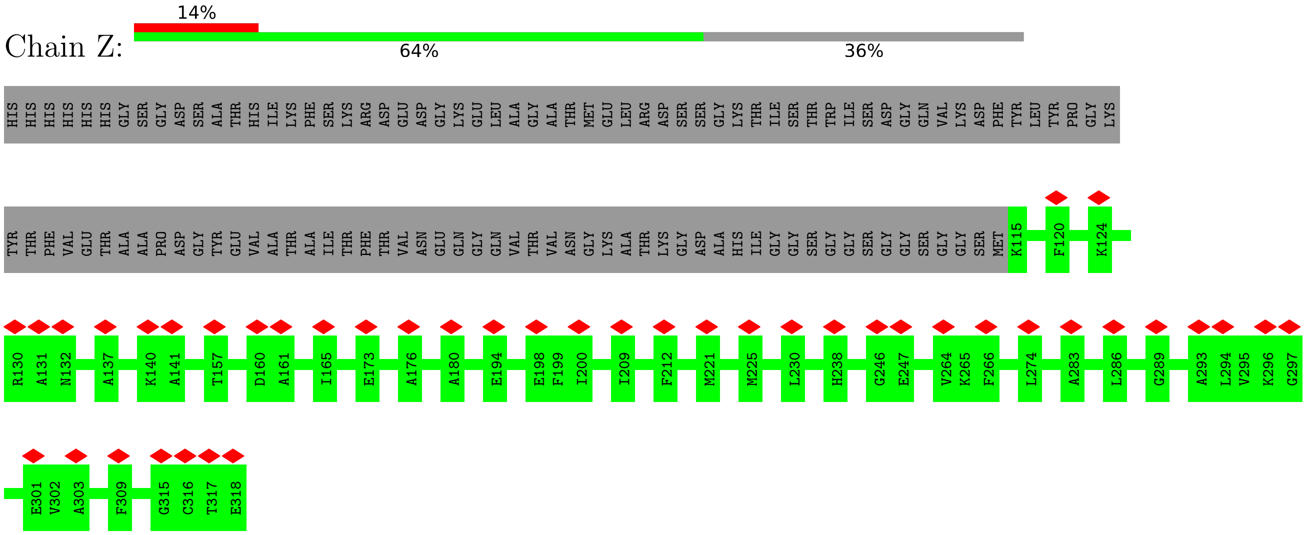
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain Y:



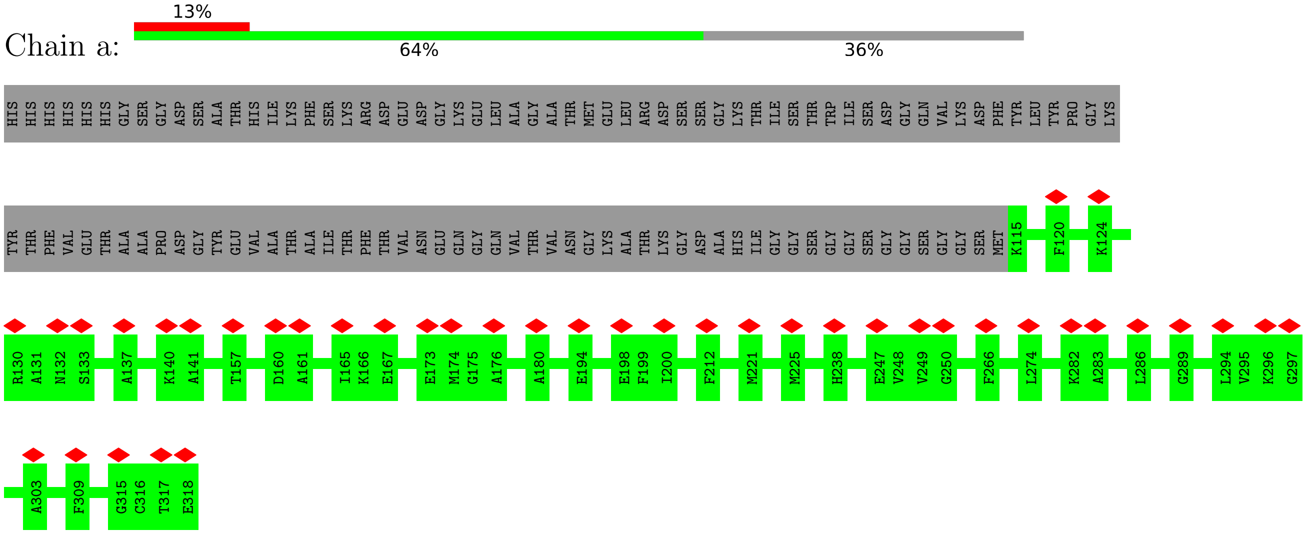
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain Z:



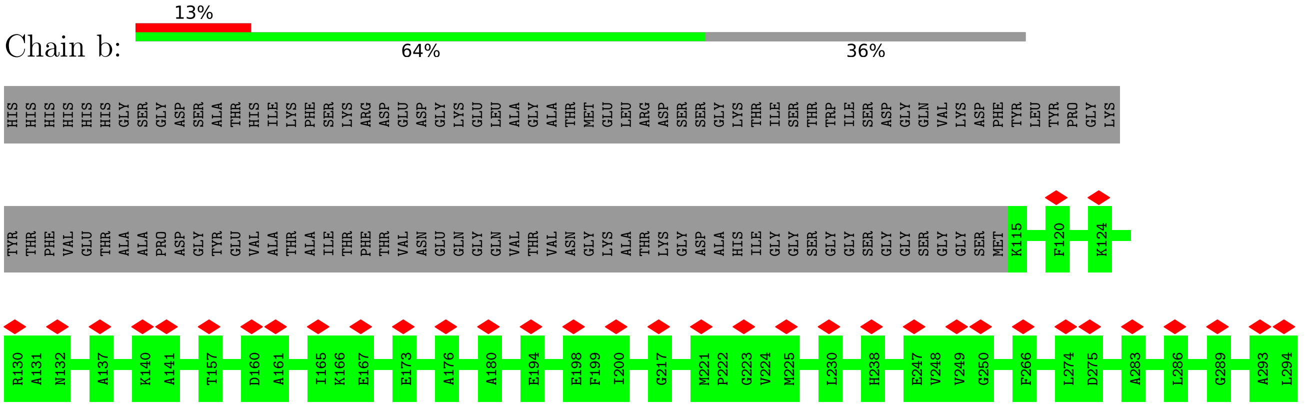
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

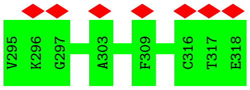
Chain a:



- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

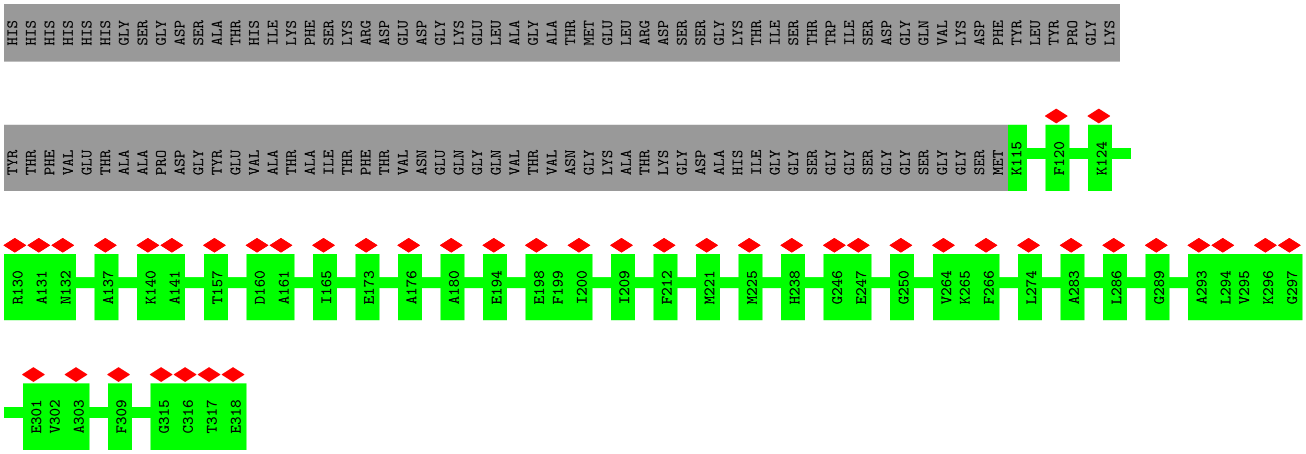
Chain b:





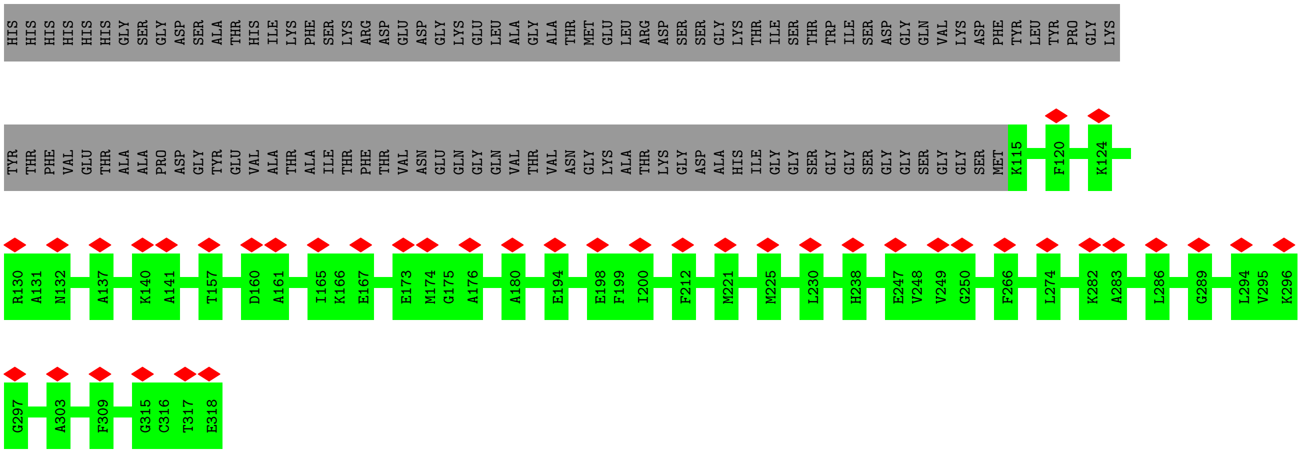
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain c:



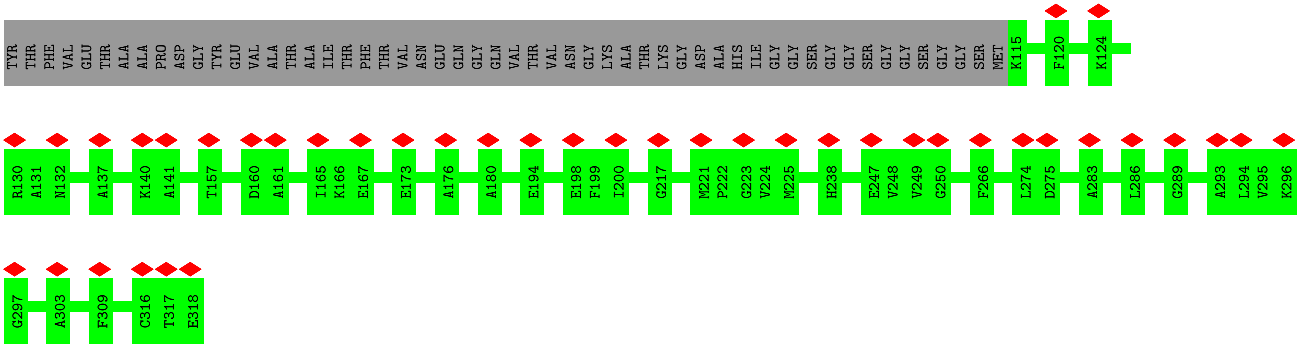
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain d:



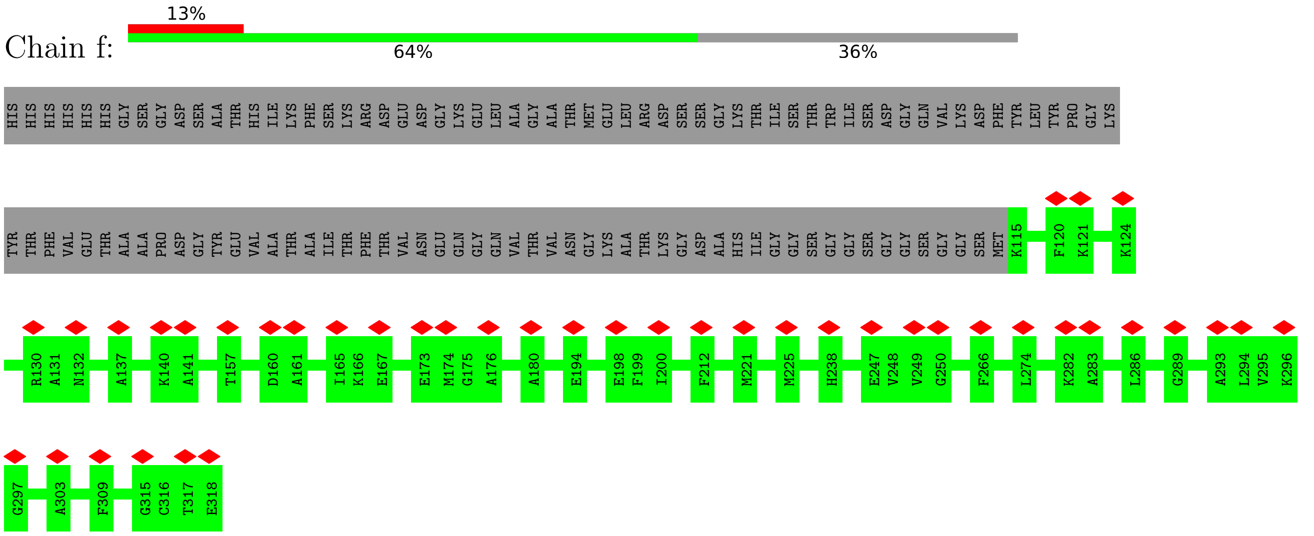
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain e:



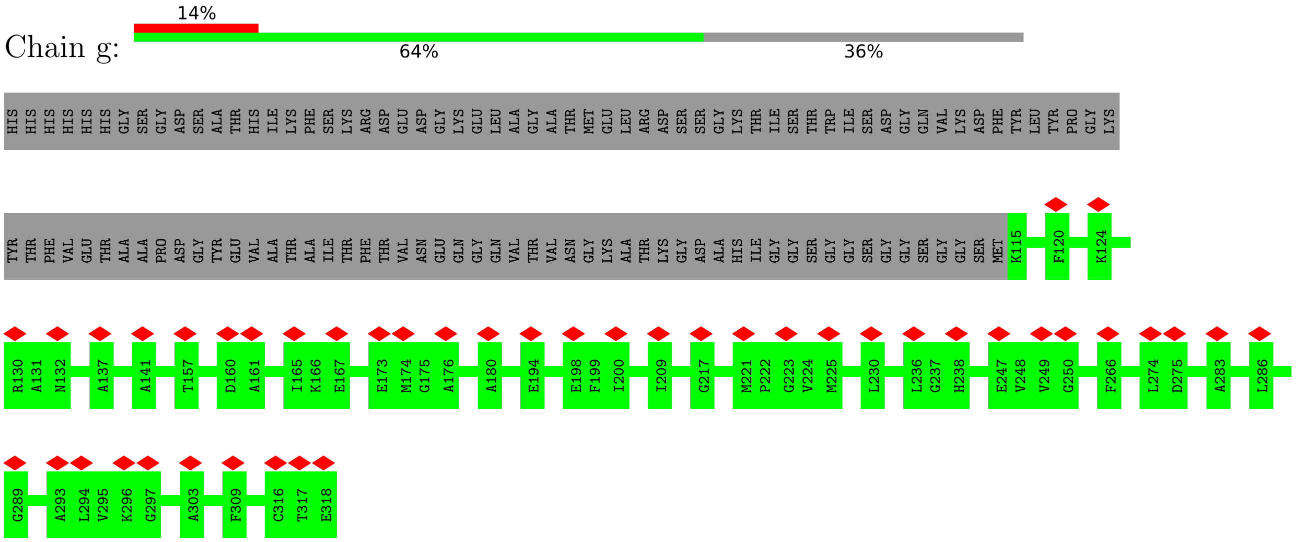
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain f:



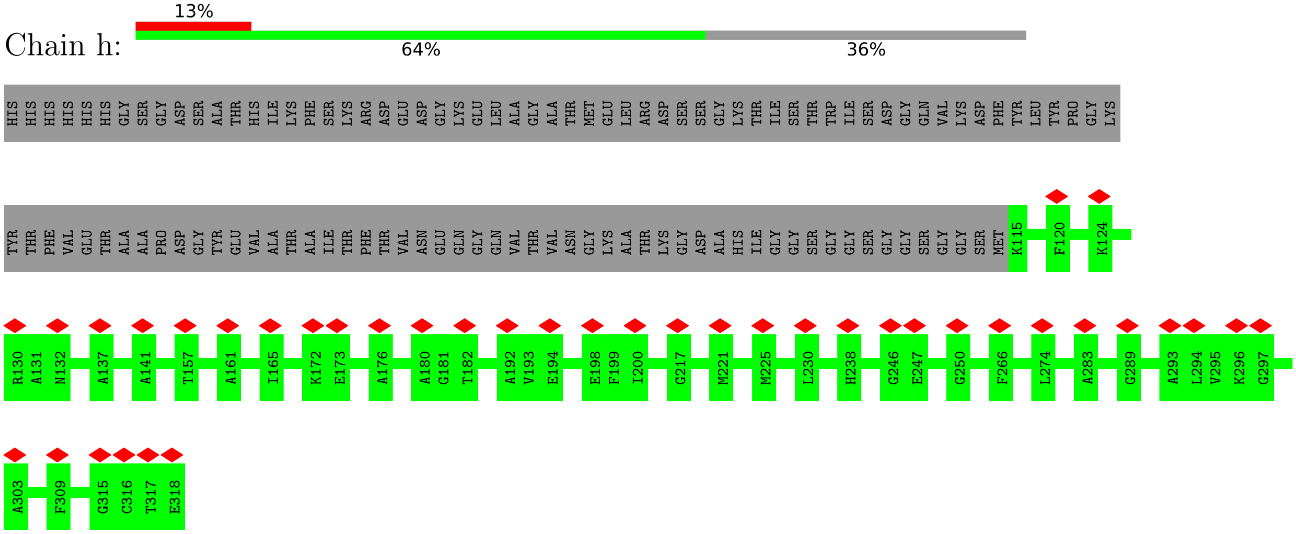
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain g:



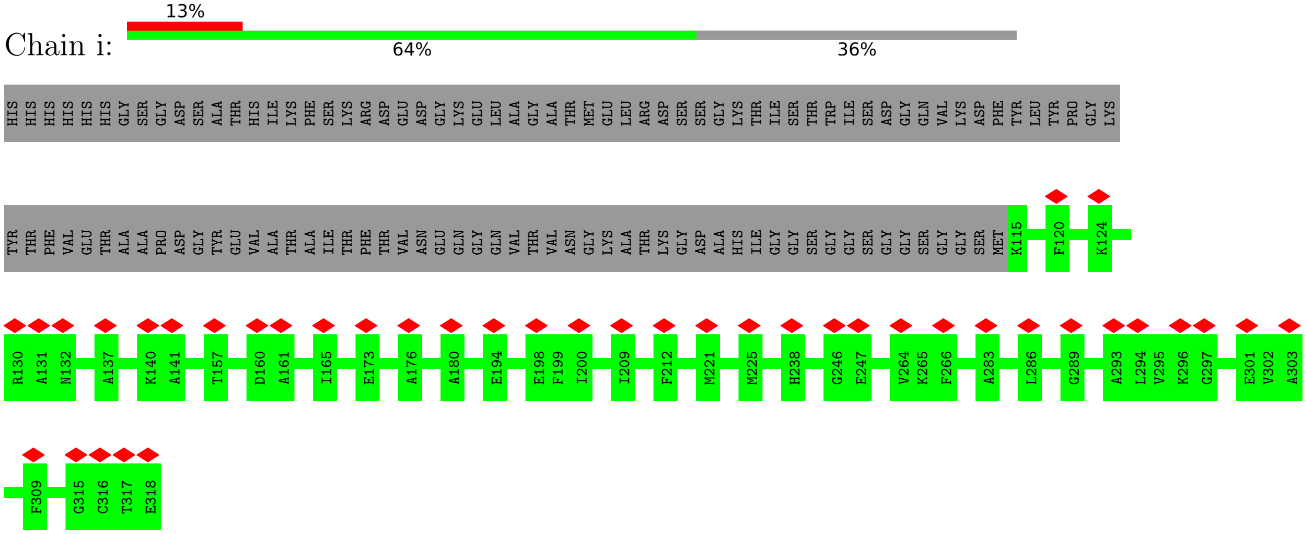
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain h:



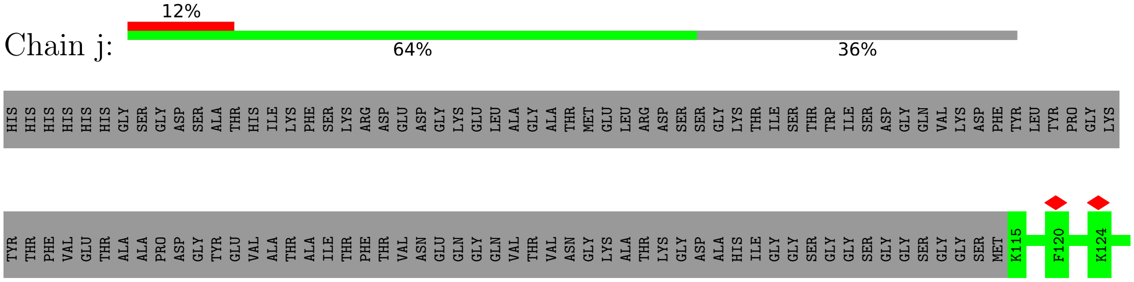
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

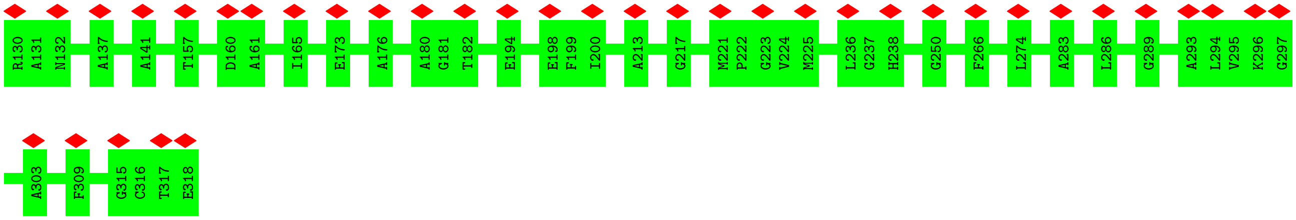
Chain i:



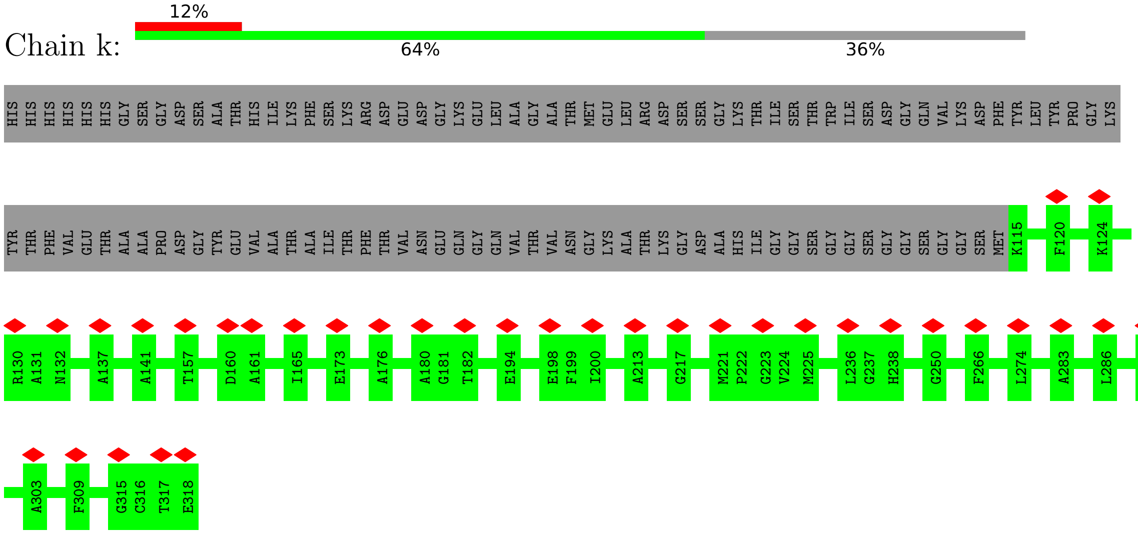
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain j:

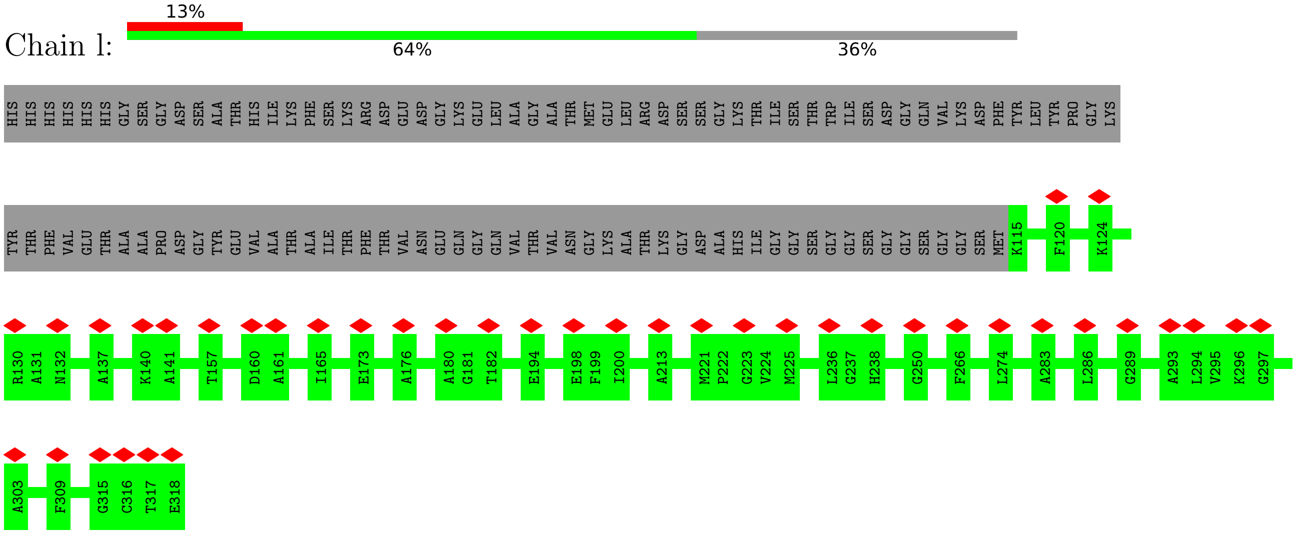




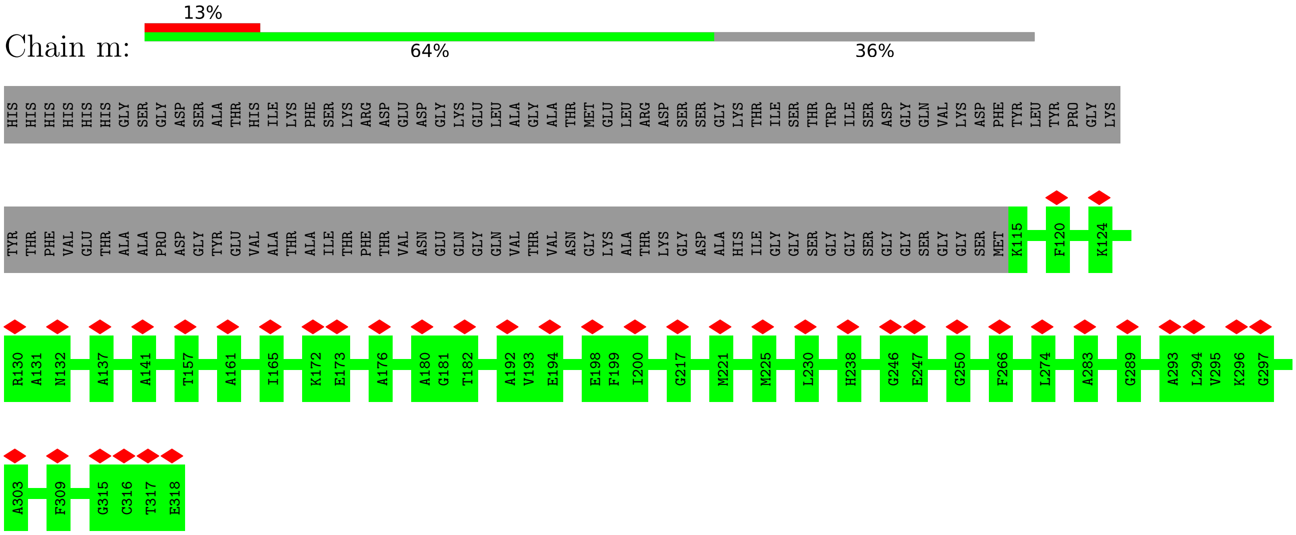
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase



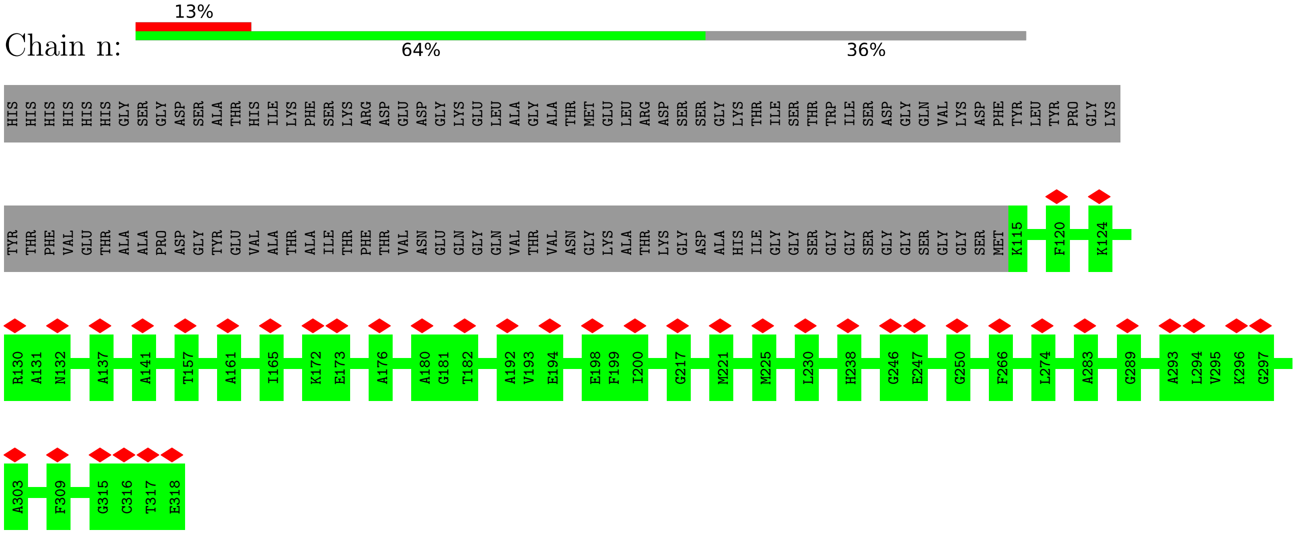
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase



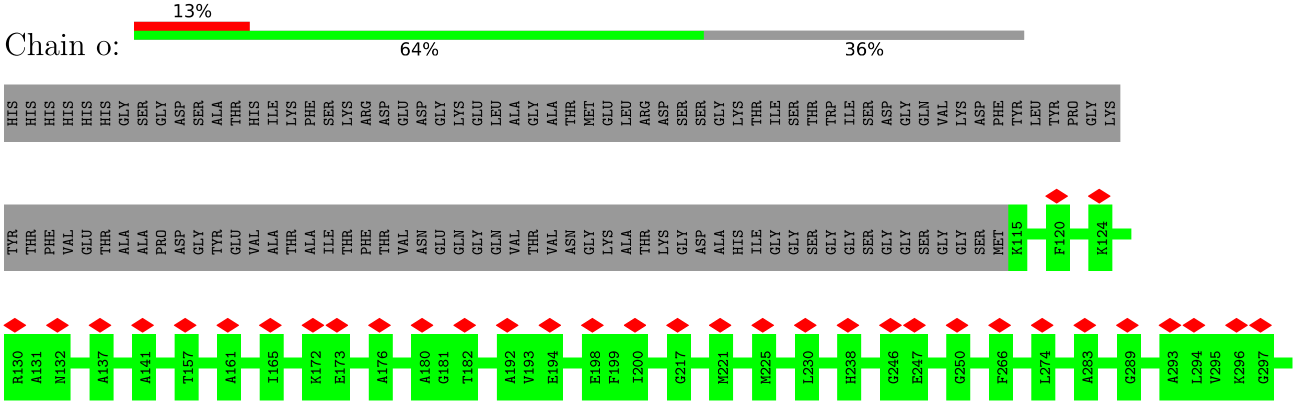
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

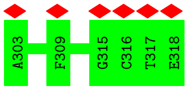


- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase



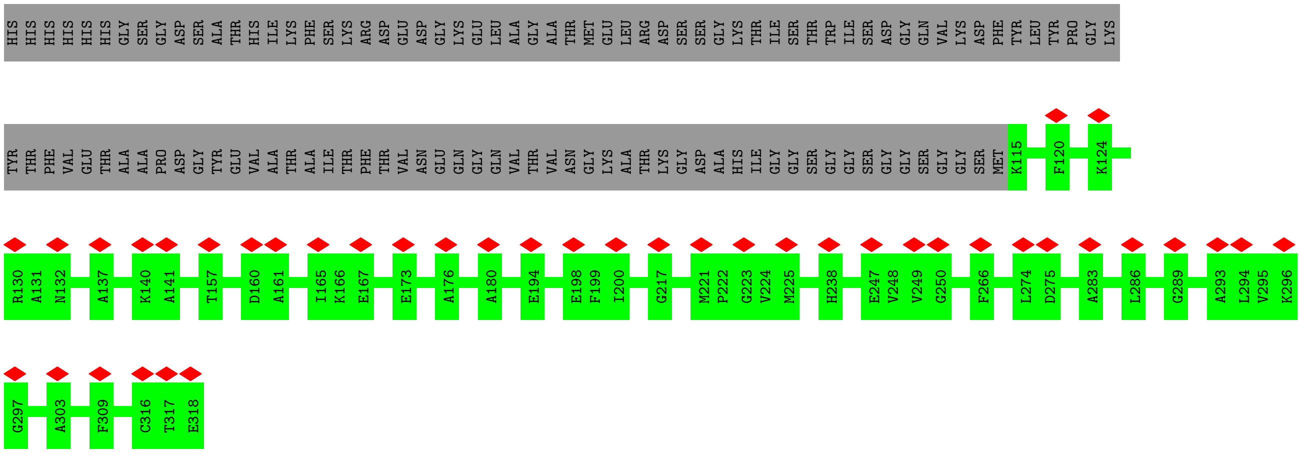
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase





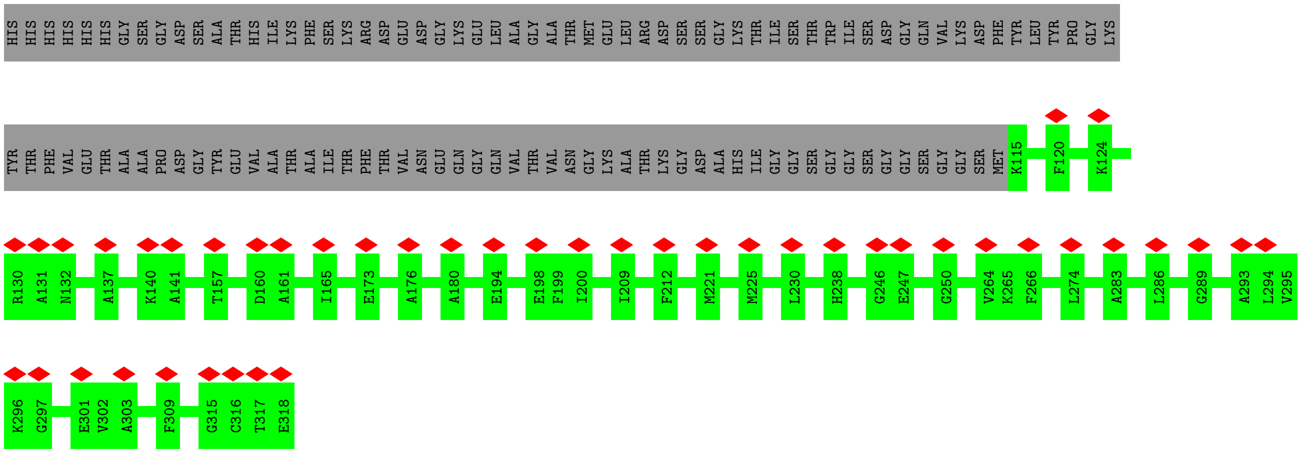
• Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain p:



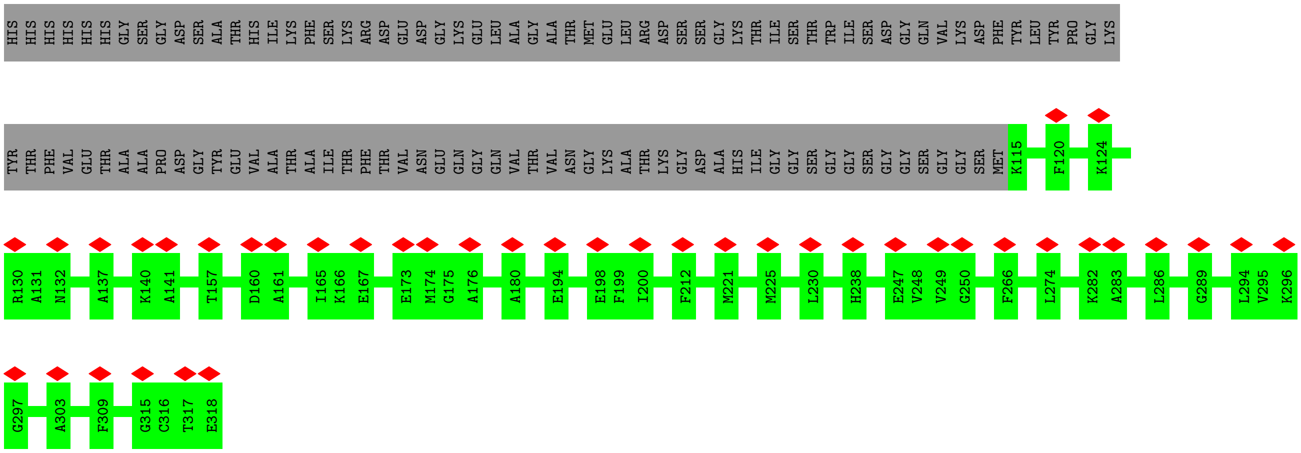
• Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain q:



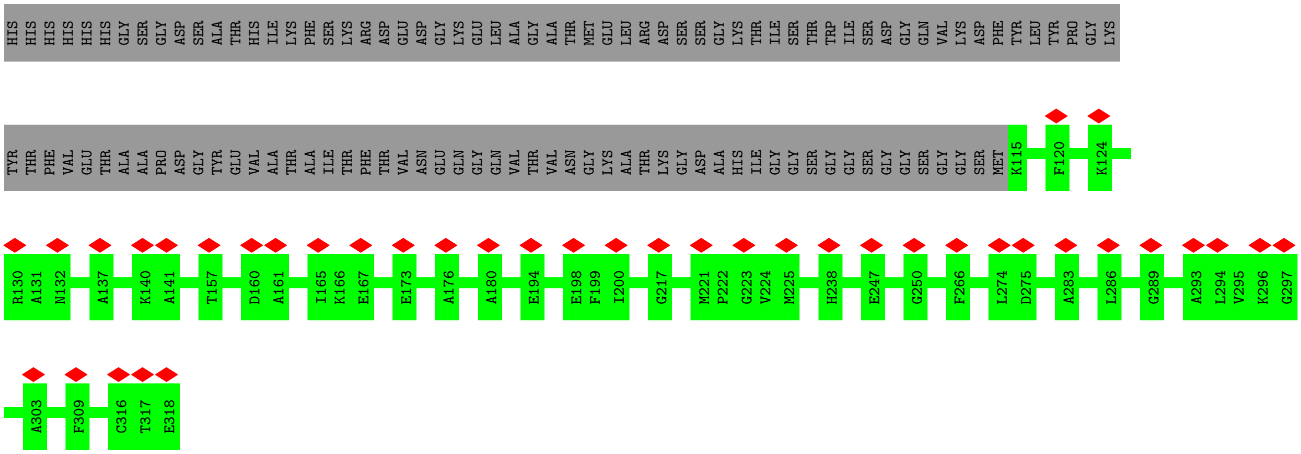
• Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain r:



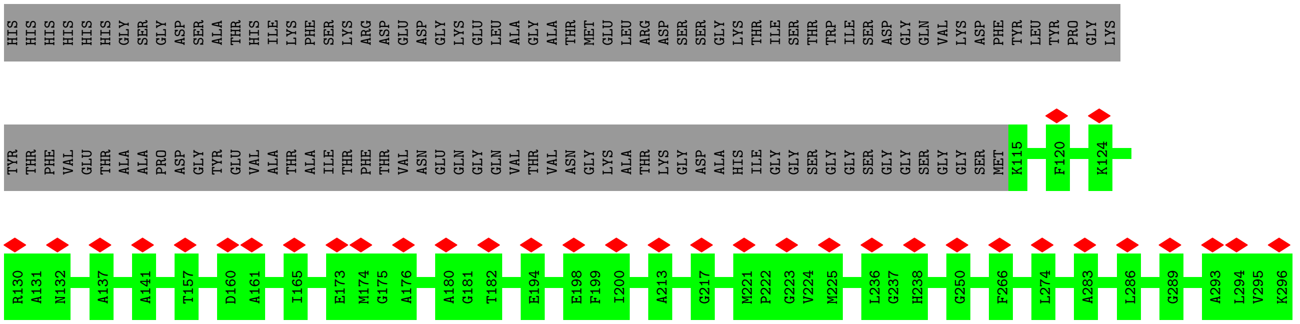
• Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

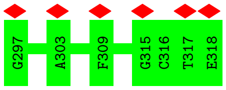
Chain s:



• Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

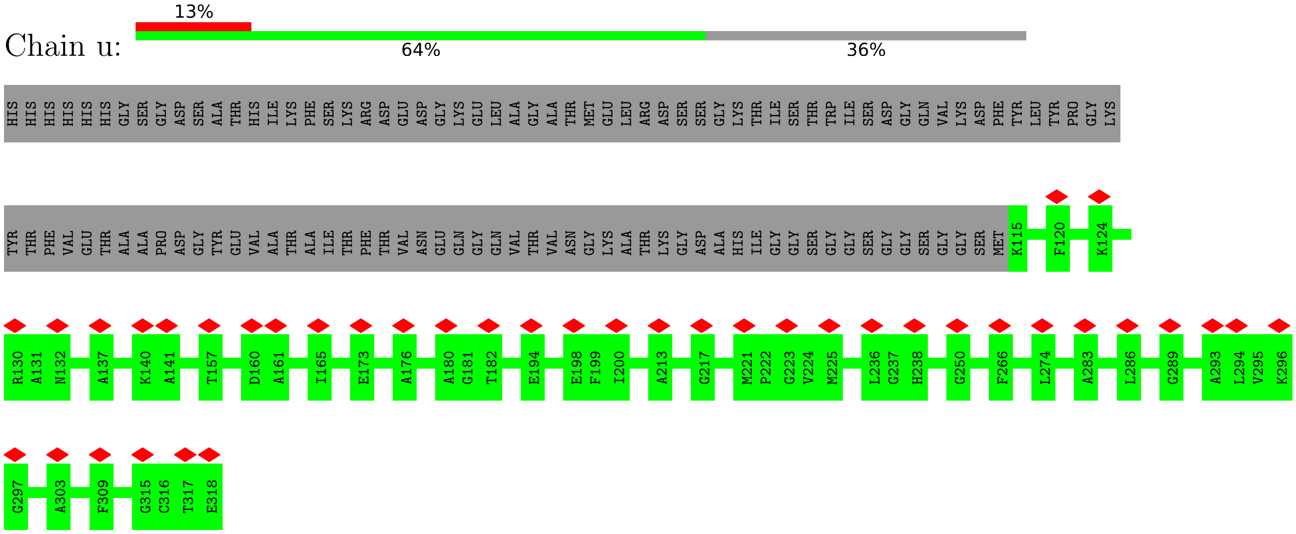
Chain t:





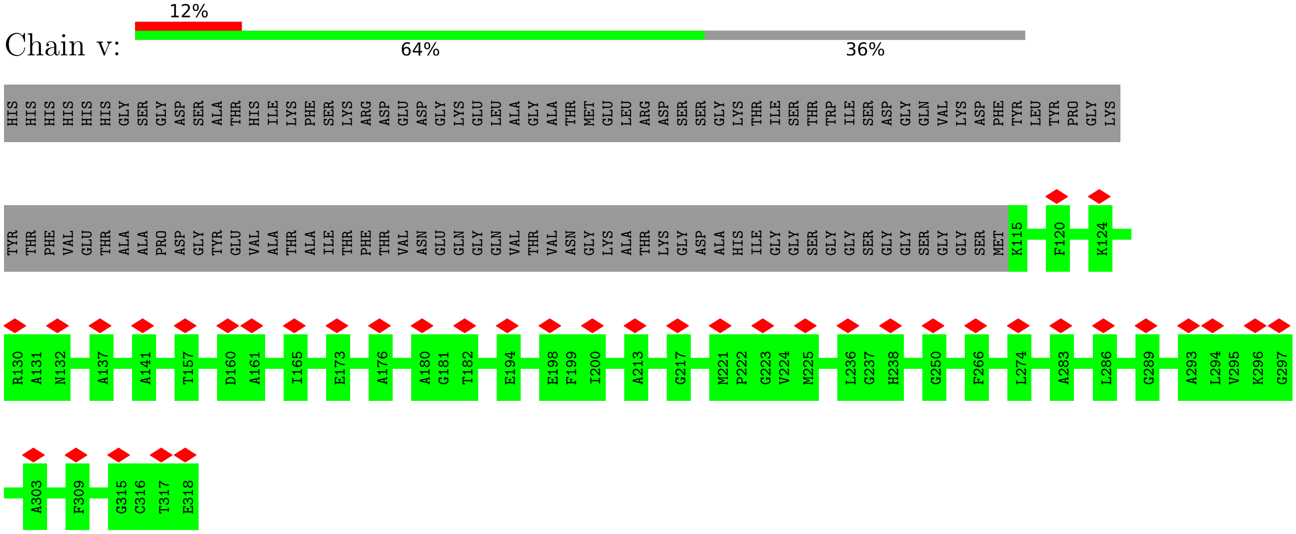
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain u:



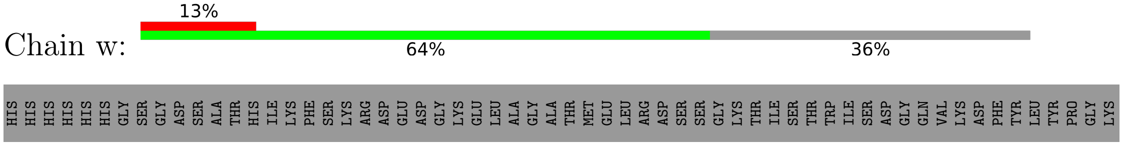
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

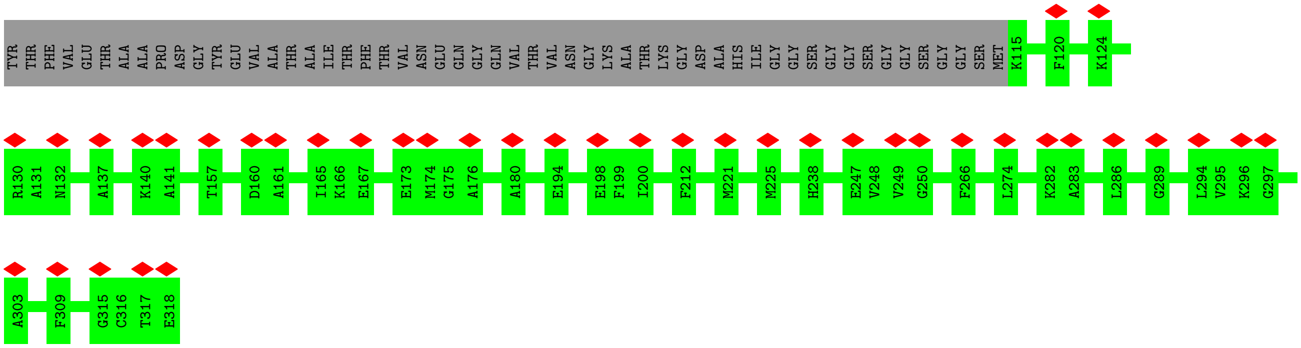
Chain v:



- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

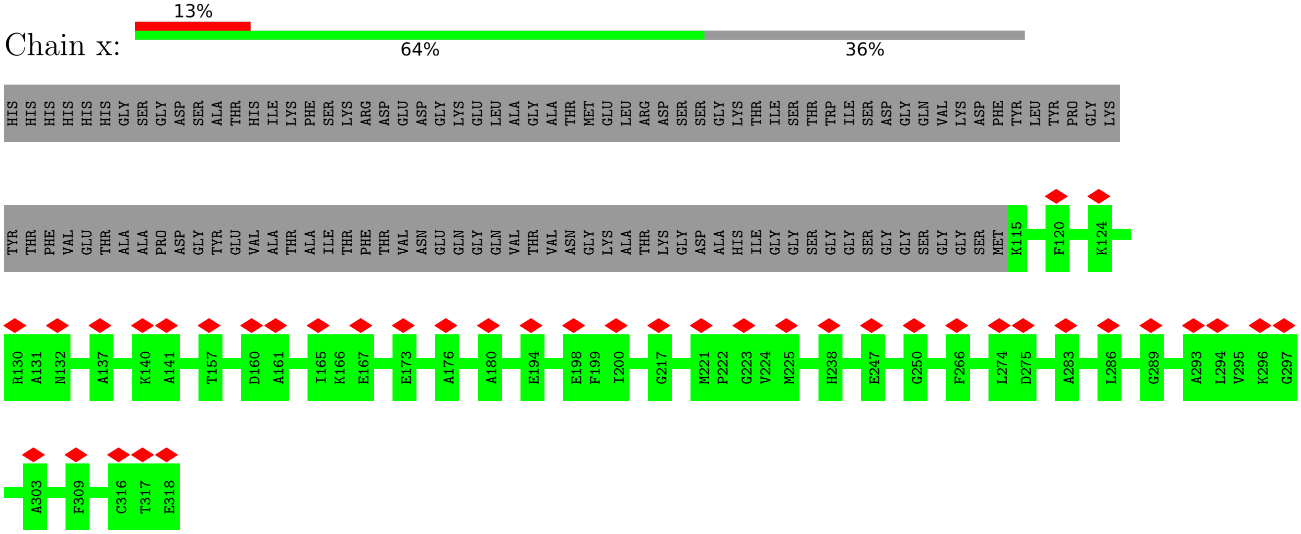
Chain w:





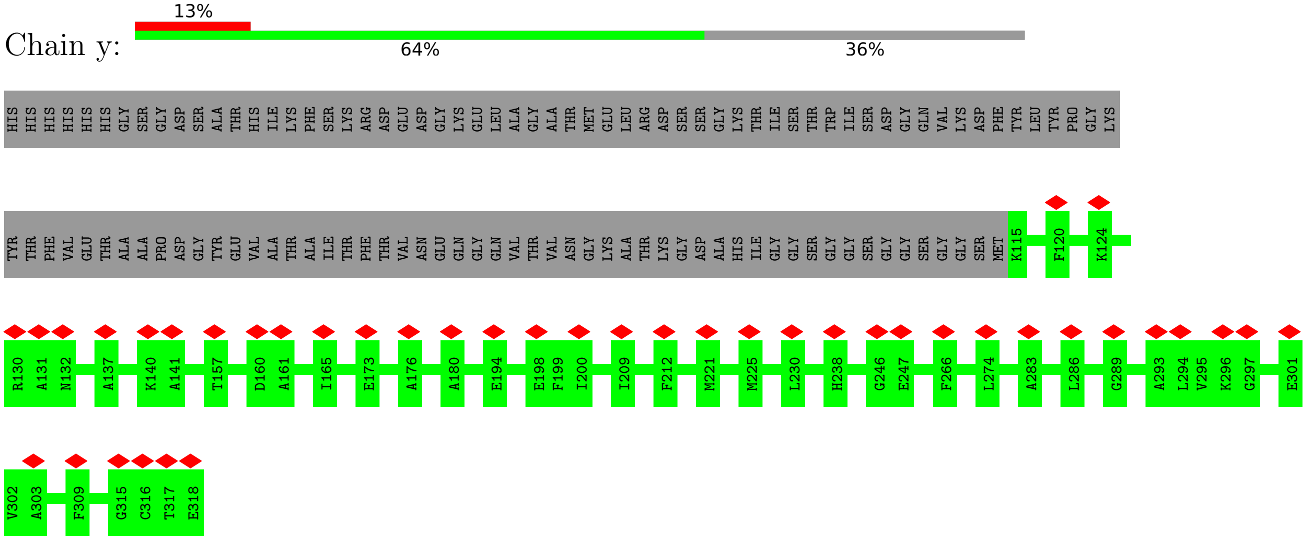
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain x:

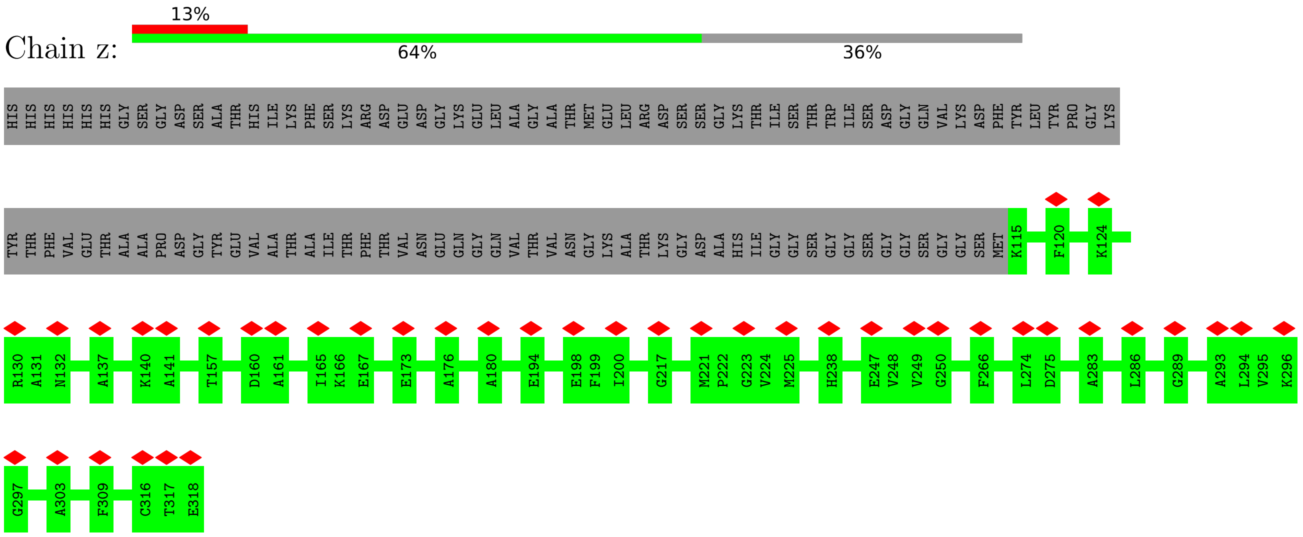


- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

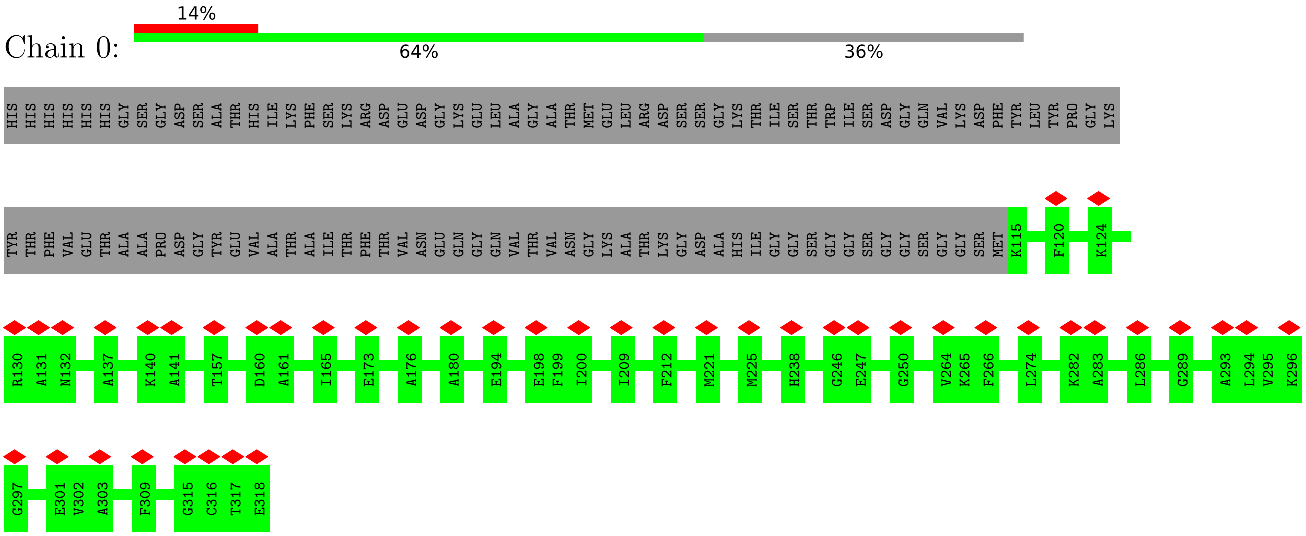
Chain y:



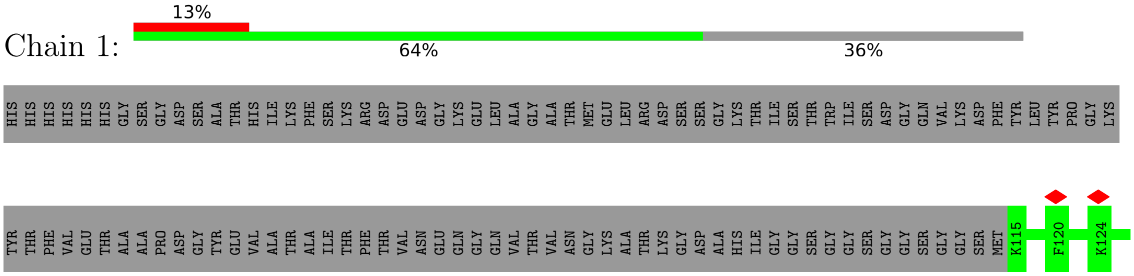
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

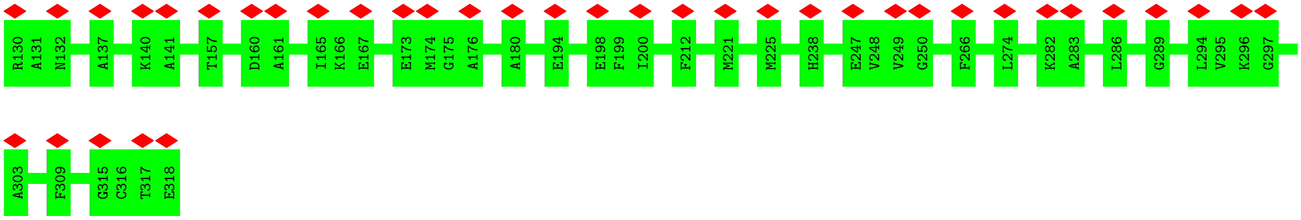


- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase



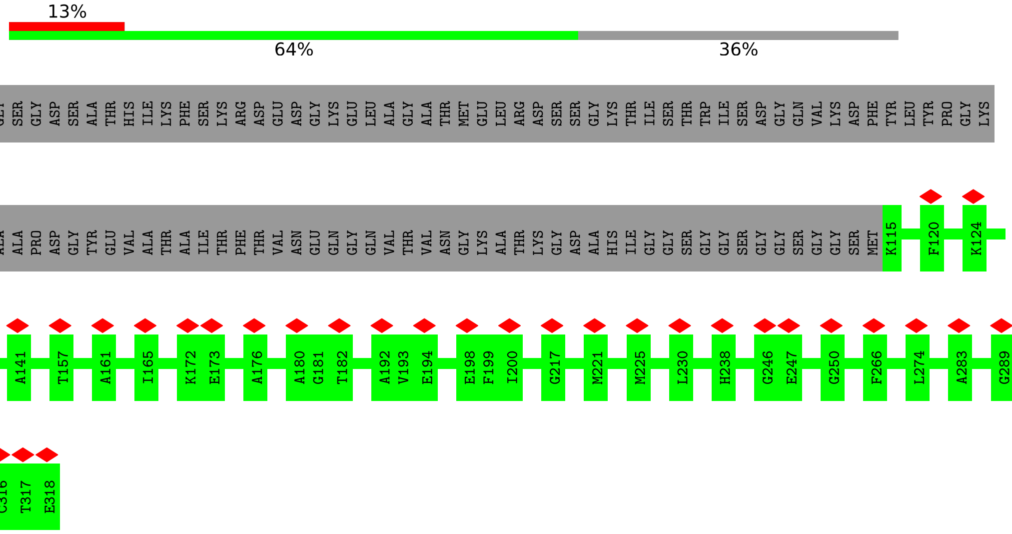
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase





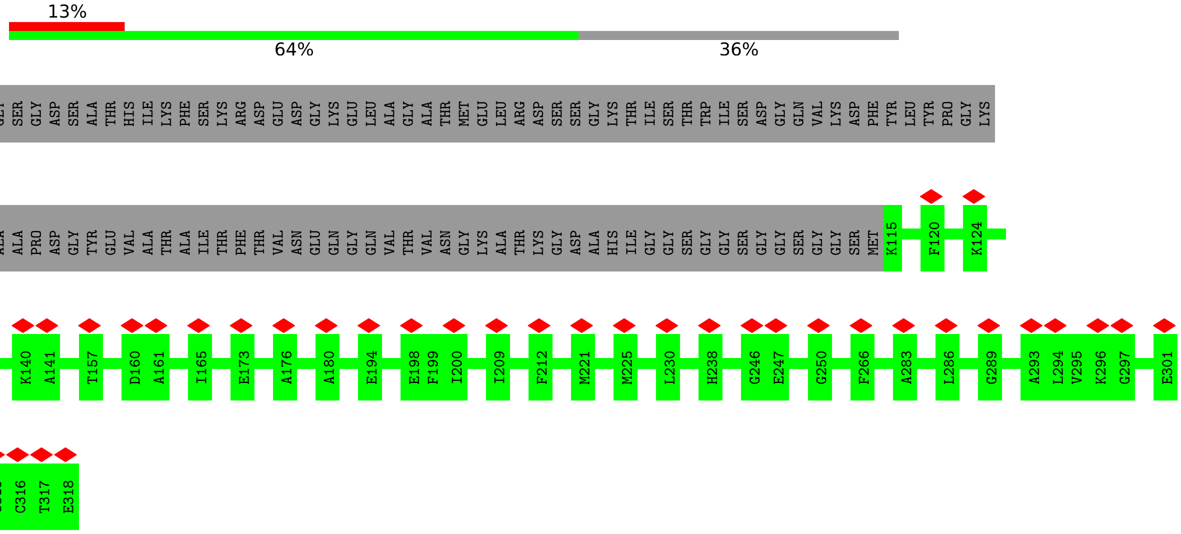
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain 2:



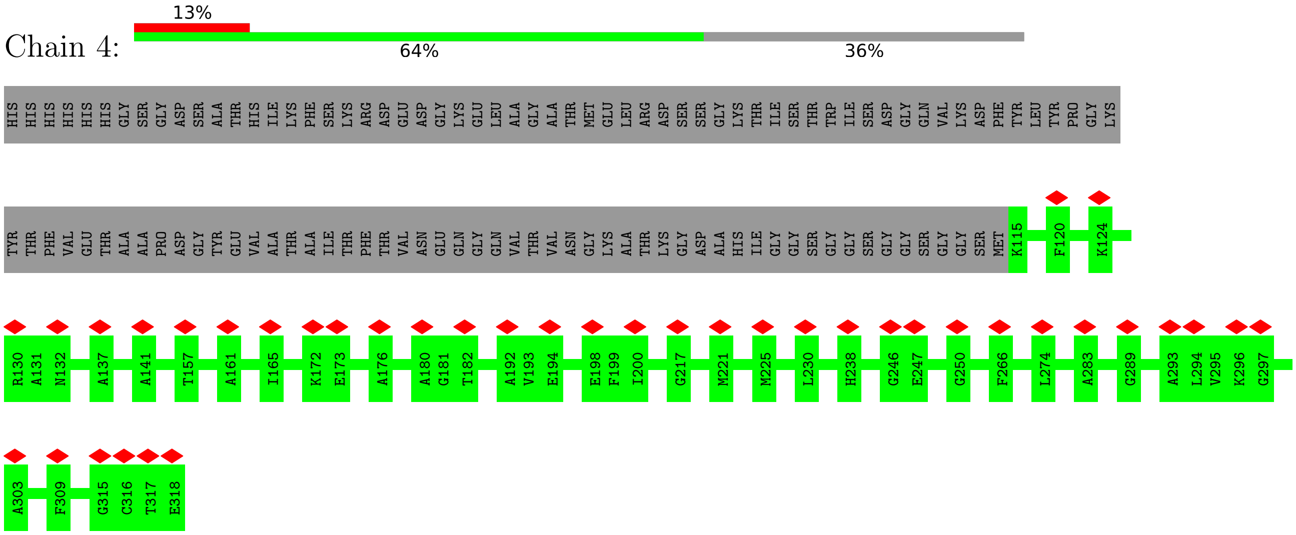
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain 3:



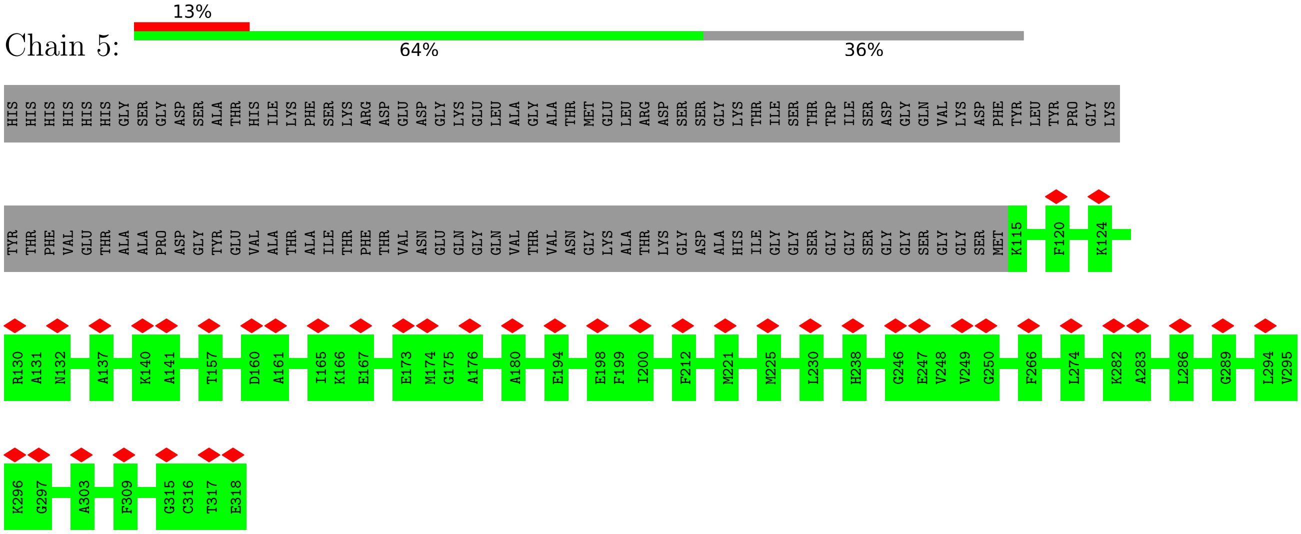
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain 4:



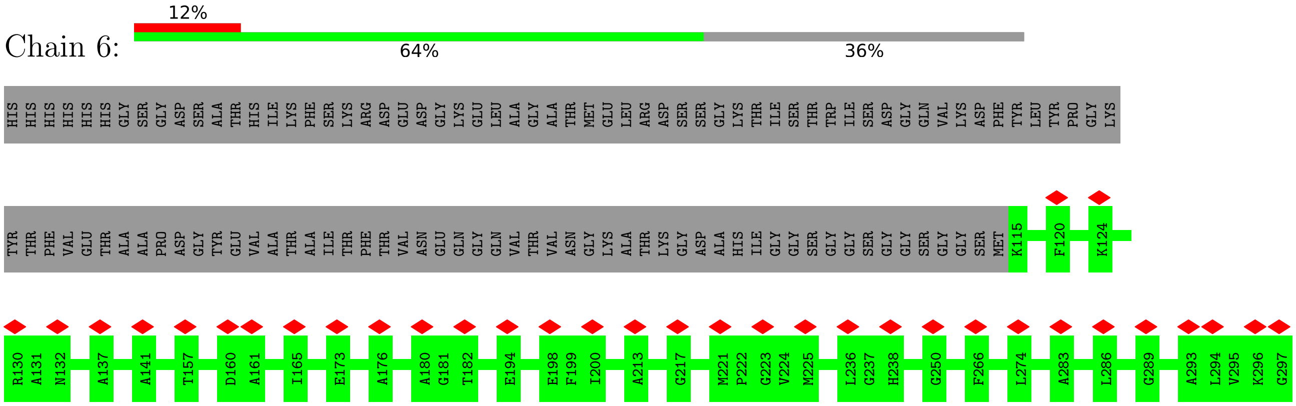
- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

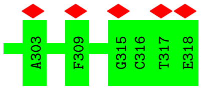
Chain 5:



- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

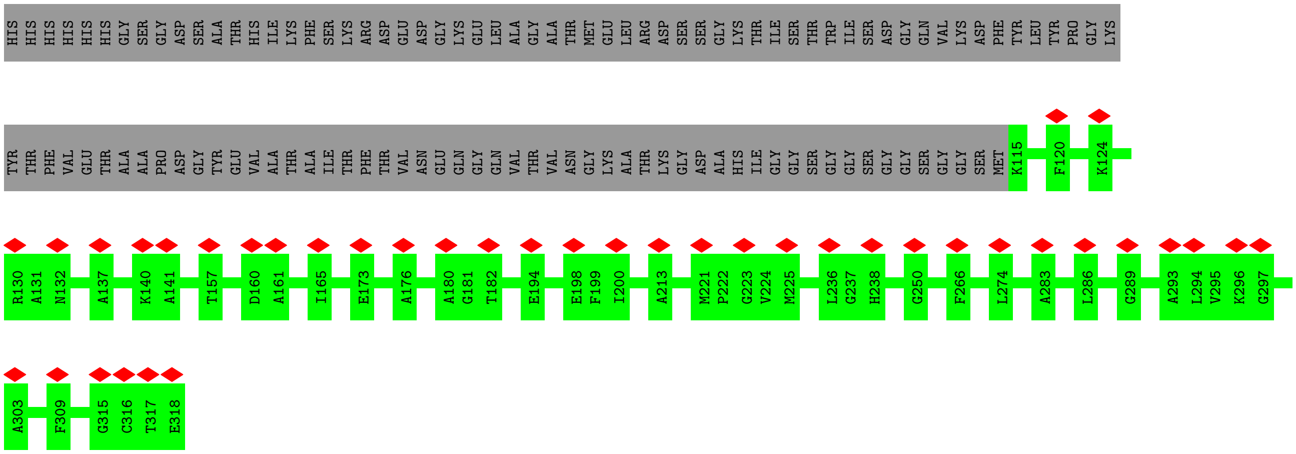
Chain 6:





- Molecule 1: CAP255 gp140 SpyTag-SpyCatcher mi3,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase

Chain 7:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1439	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^{-}/\text{Å}^2)$	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.077	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0292	Depositor
Map size (Å)	478.65598, 478.65598, 478.65598	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.662, 1.662, 1.662	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.60	0/1571	0.76	0/2117
1	1	0.60	0/1571	0.76	0/2117
1	2	0.60	0/1571	0.76	0/2117
1	3	0.60	0/1571	0.76	0/2117
1	4	0.60	0/1571	0.76	0/2117
1	5	0.60	0/1571	0.76	0/2117
1	6	0.60	0/1571	0.76	0/2117
1	7	0.60	0/1571	0.76	0/2117
1	A	0.60	0/1571	0.76	0/2117
1	B	0.60	0/1571	0.76	0/2117
1	C	0.60	0/1571	0.76	0/2117
1	D	0.60	0/1571	0.76	0/2117
1	E	0.60	0/1571	0.76	0/2117
1	F	0.60	0/1571	0.76	0/2117
1	G	0.60	0/1571	0.76	0/2117
1	H	0.60	0/1571	0.76	0/2117
1	I	0.60	0/1571	0.76	0/2117
1	J	0.60	0/1571	0.76	0/2117
1	K	0.60	0/1571	0.76	0/2117
1	L	0.60	0/1571	0.76	0/2117
1	M	0.60	0/1571	0.76	0/2117
1	N	0.60	0/1571	0.76	0/2117
1	O	0.60	0/1571	0.76	0/2117
1	P	0.60	0/1571	0.76	0/2117
1	Q	0.60	0/1571	0.76	0/2117
1	R	0.60	0/1571	0.76	0/2117
1	S	0.60	0/1571	0.76	0/2117
1	T	0.60	0/1571	0.76	0/2117
1	U	0.60	0/1571	0.76	0/2117
1	V	0.60	0/1571	0.76	0/2117
1	W	0.60	0/1571	0.76	0/2117
1	X	0.60	0/1571	0.76	0/2117
1	Y	0.60	0/1571	0.76	0/2117
1	Z	0.60	0/1571	0.76	0/2117

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	a	0.60	0/1571	0.76	0/2117
1	b	0.60	0/1571	0.76	0/2117
1	c	0.60	0/1571	0.76	0/2117
1	d	0.60	0/1571	0.76	0/2117
1	e	0.60	0/1571	0.76	0/2117
1	f	0.60	0/1571	0.76	0/2117
1	g	0.60	0/1571	0.76	0/2117
1	h	0.60	0/1571	0.76	0/2117
1	i	0.60	0/1571	0.76	0/2117
1	j	0.60	0/1571	0.76	0/2117
1	k	0.60	0/1571	0.76	0/2117
1	l	0.60	0/1571	0.76	0/2117
1	m	0.60	0/1571	0.76	0/2117
1	n	0.60	0/1571	0.76	0/2117
1	o	0.60	0/1571	0.76	0/2117
1	p	0.60	0/1571	0.76	0/2117
1	q	0.60	0/1571	0.76	0/2117
1	r	0.60	0/1571	0.76	0/2117
1	s	0.60	0/1571	0.76	0/2117
1	t	0.60	0/1571	0.76	0/2117
1	u	0.60	0/1571	0.76	0/2117
1	v	0.60	0/1571	0.76	0/2117
1	w	0.60	0/1571	0.76	0/2117
1	x	0.60	0/1571	0.76	0/2117
1	y	0.60	0/1571	0.76	0/2117
1	z	0.60	0/1571	0.76	0/2117
All	All	0.60	0/94260	0.76	0/127020

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 ⓘ

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	1	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	2	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	3	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	4	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	5	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	6	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	7	202/318 (64%)	201 (100%)	1 (0%)	0	100	100
1	A	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	B	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	C	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	D	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	E	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	F	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	G	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	H	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	I	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	J	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	K	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	L	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	M	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	N	202/318 (64%)	201 (100%)	1 (0%)	0	100	100
1	O	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	P	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	Q	202/318 (64%)	201 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	S	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	T	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	U	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	V	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	W	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	X	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	Y	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	Z	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	a	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	b	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	c	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	d	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	e	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	f	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	g	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	h	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	i	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	j	202/318 (64%)	201 (100%)	1 (0%)	0	100	100
1	k	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	l	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	m	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	n	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	o	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	p	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	q	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	r	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	s	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	t	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	u	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	v	202/318 (64%)	200 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	x	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	y	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
1	z	202/318 (64%)	200 (99%)	2 (1%)	0	100	100
All	All	12120/19080 (64%)	12004 (99%)	116 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	165/251 (66%)	165 (100%)	0	100	100
1	1	165/251 (66%)	165 (100%)	0	100	100
1	2	165/251 (66%)	165 (100%)	0	100	100
1	3	165/251 (66%)	165 (100%)	0	100	100
1	4	165/251 (66%)	165 (100%)	0	100	100
1	5	165/251 (66%)	165 (100%)	0	100	100
1	6	165/251 (66%)	165 (100%)	0	100	100
1	7	165/251 (66%)	165 (100%)	0	100	100
1	A	165/251 (66%)	165 (100%)	0	100	100
1	B	165/251 (66%)	165 (100%)	0	100	100
1	C	165/251 (66%)	165 (100%)	0	100	100
1	D	165/251 (66%)	165 (100%)	0	100	100
1	E	165/251 (66%)	165 (100%)	0	100	100
1	F	165/251 (66%)	165 (100%)	0	100	100
1	G	165/251 (66%)	165 (100%)	0	100	100
1	H	165/251 (66%)	165 (100%)	0	100	100
1	I	165/251 (66%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	165/251 (66%)	165 (100%)	0	100	100
1	K	165/251 (66%)	165 (100%)	0	100	100
1	L	165/251 (66%)	165 (100%)	0	100	100
1	M	165/251 (66%)	165 (100%)	0	100	100
1	N	165/251 (66%)	165 (100%)	0	100	100
1	O	165/251 (66%)	165 (100%)	0	100	100
1	P	165/251 (66%)	165 (100%)	0	100	100
1	Q	165/251 (66%)	165 (100%)	0	100	100
1	R	165/251 (66%)	165 (100%)	0	100	100
1	S	165/251 (66%)	165 (100%)	0	100	100
1	T	165/251 (66%)	165 (100%)	0	100	100
1	U	165/251 (66%)	165 (100%)	0	100	100
1	V	165/251 (66%)	165 (100%)	0	100	100
1	W	165/251 (66%)	165 (100%)	0	100	100
1	X	165/251 (66%)	165 (100%)	0	100	100
1	Y	165/251 (66%)	165 (100%)	0	100	100
1	Z	165/251 (66%)	165 (100%)	0	100	100
1	a	165/251 (66%)	165 (100%)	0	100	100
1	b	165/251 (66%)	165 (100%)	0	100	100
1	c	165/251 (66%)	165 (100%)	0	100	100
1	d	165/251 (66%)	165 (100%)	0	100	100
1	e	165/251 (66%)	165 (100%)	0	100	100
1	f	165/251 (66%)	165 (100%)	0	100	100
1	g	165/251 (66%)	165 (100%)	0	100	100
1	h	165/251 (66%)	165 (100%)	0	100	100
1	i	165/251 (66%)	165 (100%)	0	100	100
1	j	165/251 (66%)	165 (100%)	0	100	100
1	k	165/251 (66%)	165 (100%)	0	100	100
1	l	165/251 (66%)	165 (100%)	0	100	100
1	m	165/251 (66%)	165 (100%)	0	100	100
1	n	165/251 (66%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	165/251 (66%)	165 (100%)	0	100	100
1	p	165/251 (66%)	165 (100%)	0	100	100
1	q	165/251 (66%)	165 (100%)	0	100	100
1	r	165/251 (66%)	165 (100%)	0	100	100
1	s	165/251 (66%)	165 (100%)	0	100	100
1	t	165/251 (66%)	165 (100%)	0	100	100
1	u	165/251 (66%)	165 (100%)	0	100	100
1	v	165/251 (66%)	165 (100%)	0	100	100
1	w	165/251 (66%)	165 (100%)	0	100	100
1	x	165/251 (66%)	165 (100%)	0	100	100
1	y	165/251 (66%)	165 (100%)	0	100	100
1	z	165/251 (66%)	165 (100%)	0	100	100
All	All	9900/15060 (66%)	9900 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

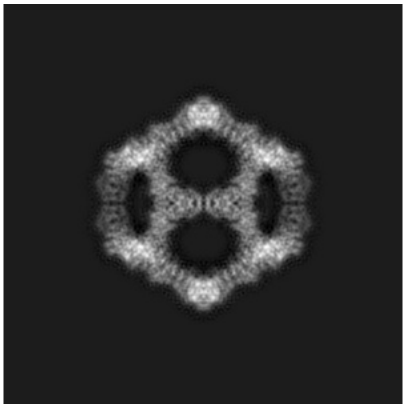
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50615. These allow visual inspection of the internal detail of the map and identification of artifacts.

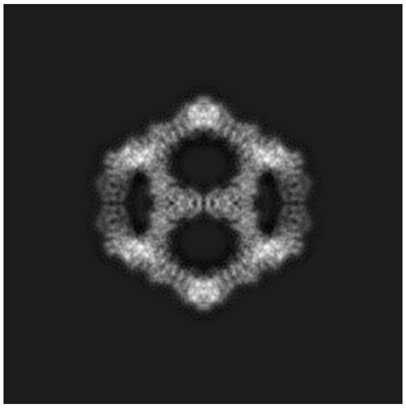
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

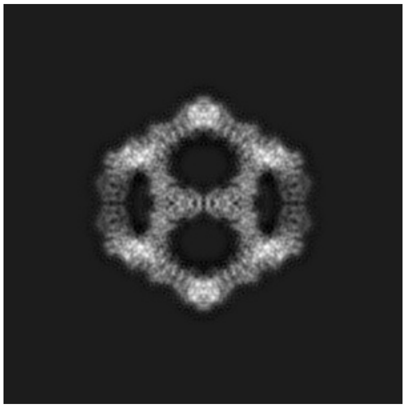
6.1.1 Primary map



X

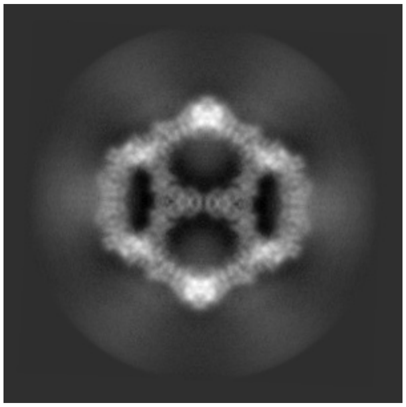


Y

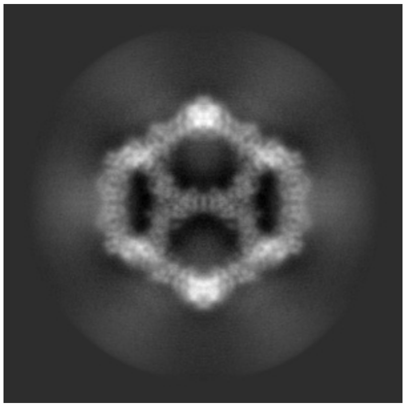


Z

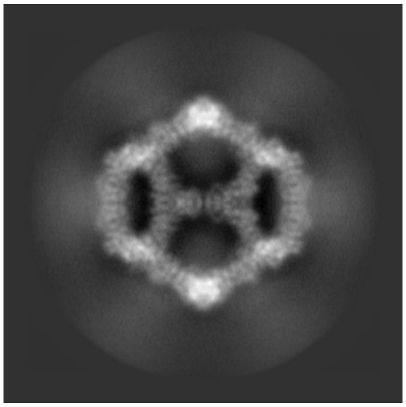
6.1.2 Raw map



X



Y

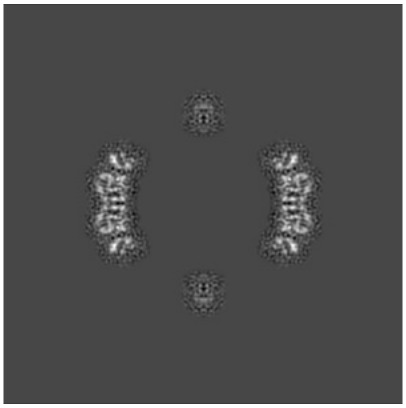


Z

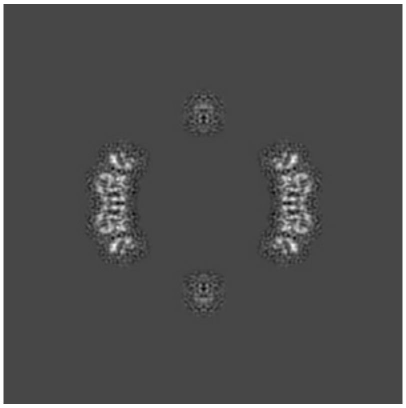
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

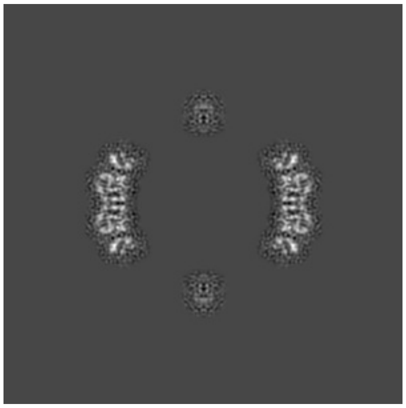
6.2.1 Primary map



X Index: 144

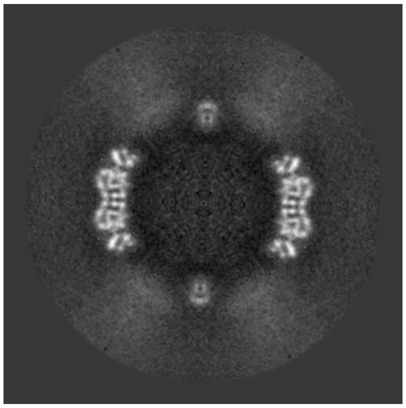


Y Index: 144

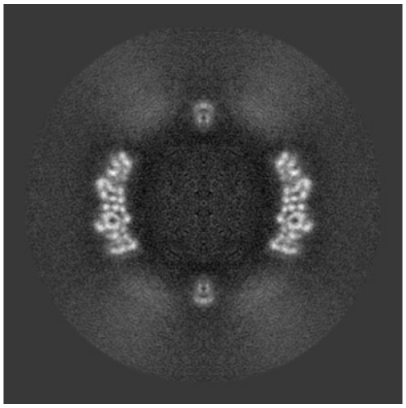


Z Index: 144

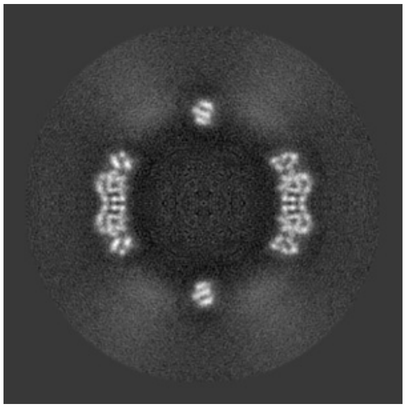
6.2.2 Raw map



X Index: 144



Y Index: 144

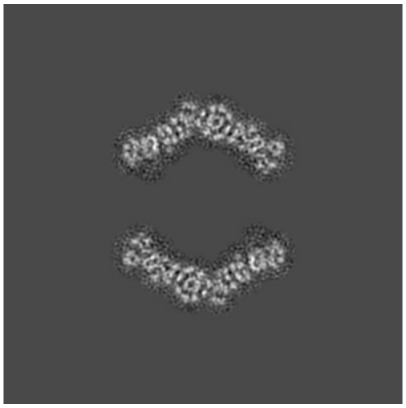


Z Index: 144

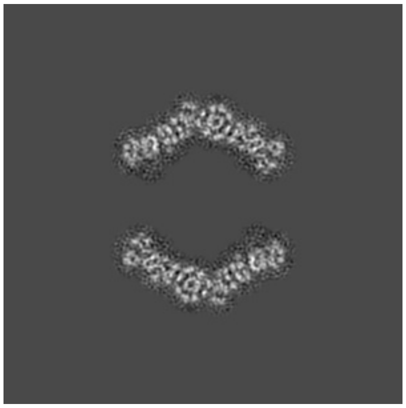
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

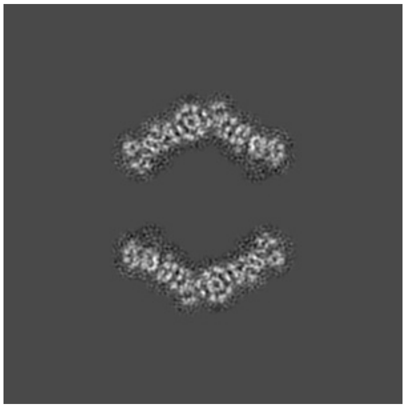
6.3.1 Primary map



X Index: 113

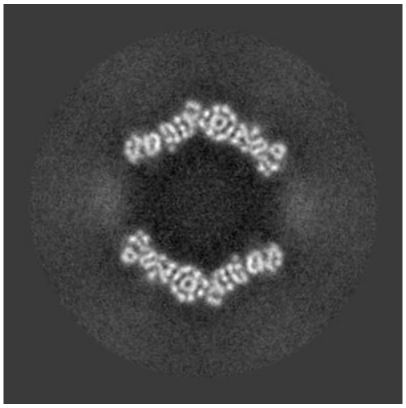


Y Index: 113

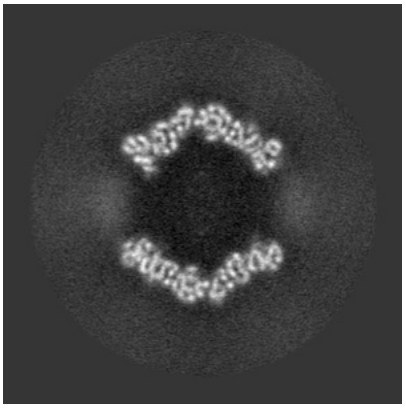


Z Index: 175

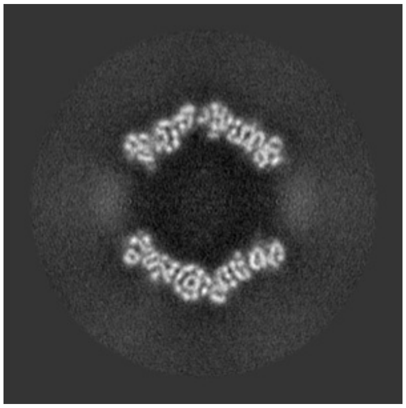
6.3.2 Raw map



X Index: 175



Y Index: 178

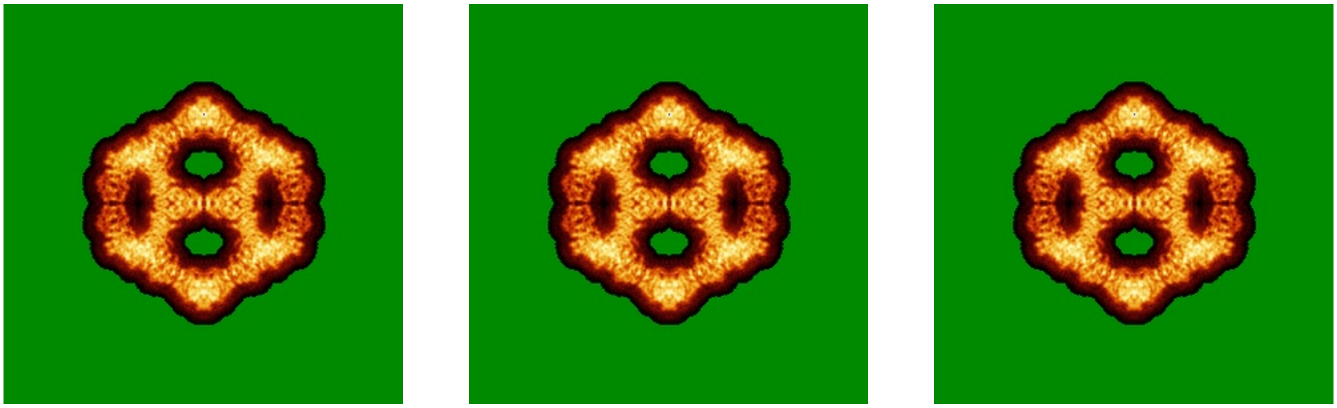


Z Index: 177

The images above show the largest variance slices of the map in three orthogonal directions.

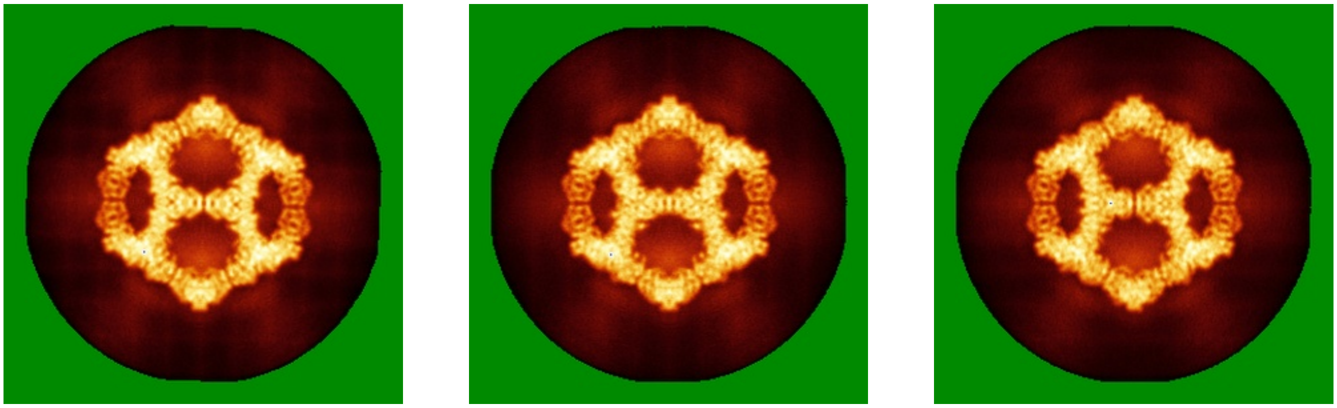
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0292. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_50615_msk_1.map

X

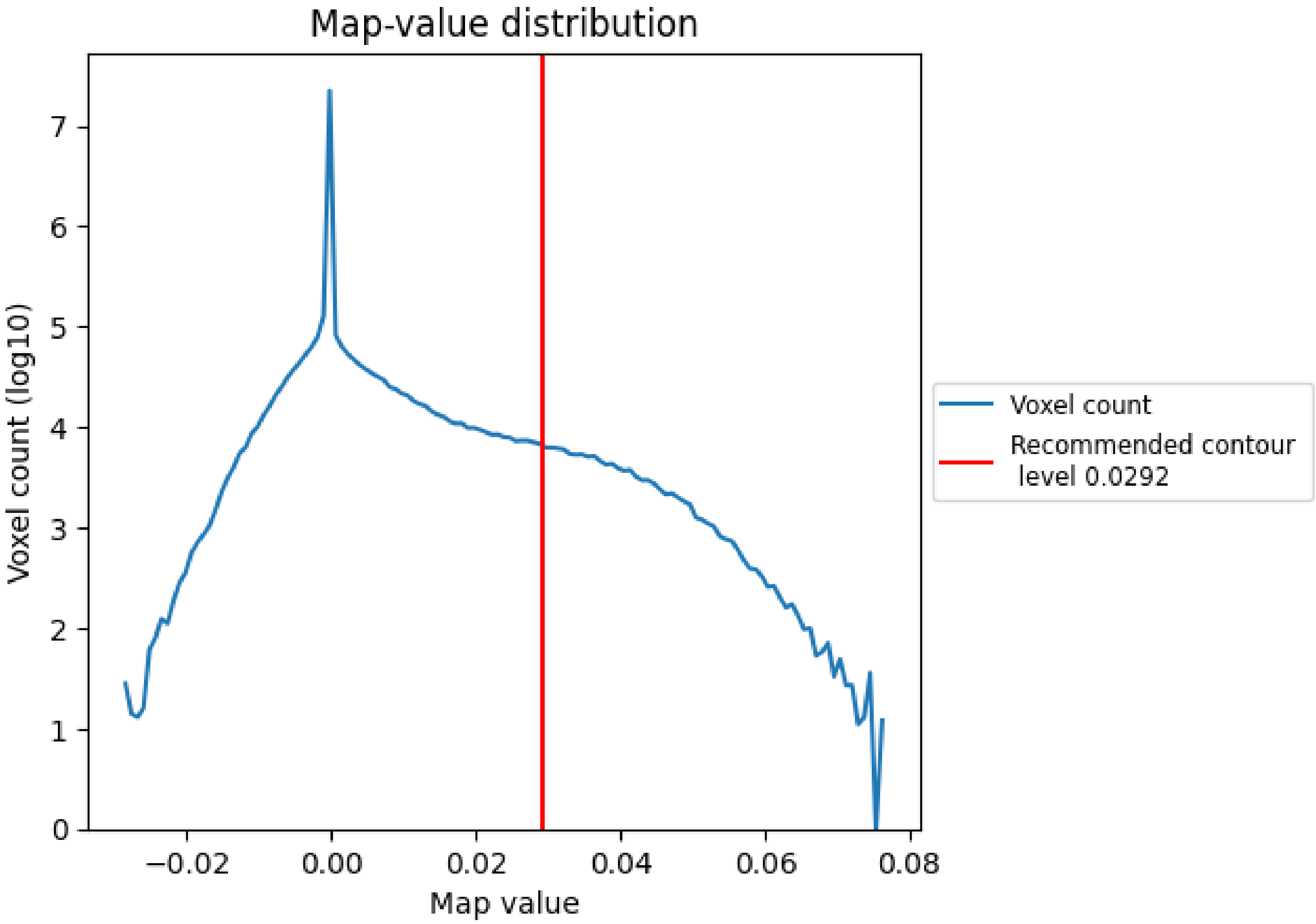
Y

Z

7 Map analysis ⓘ

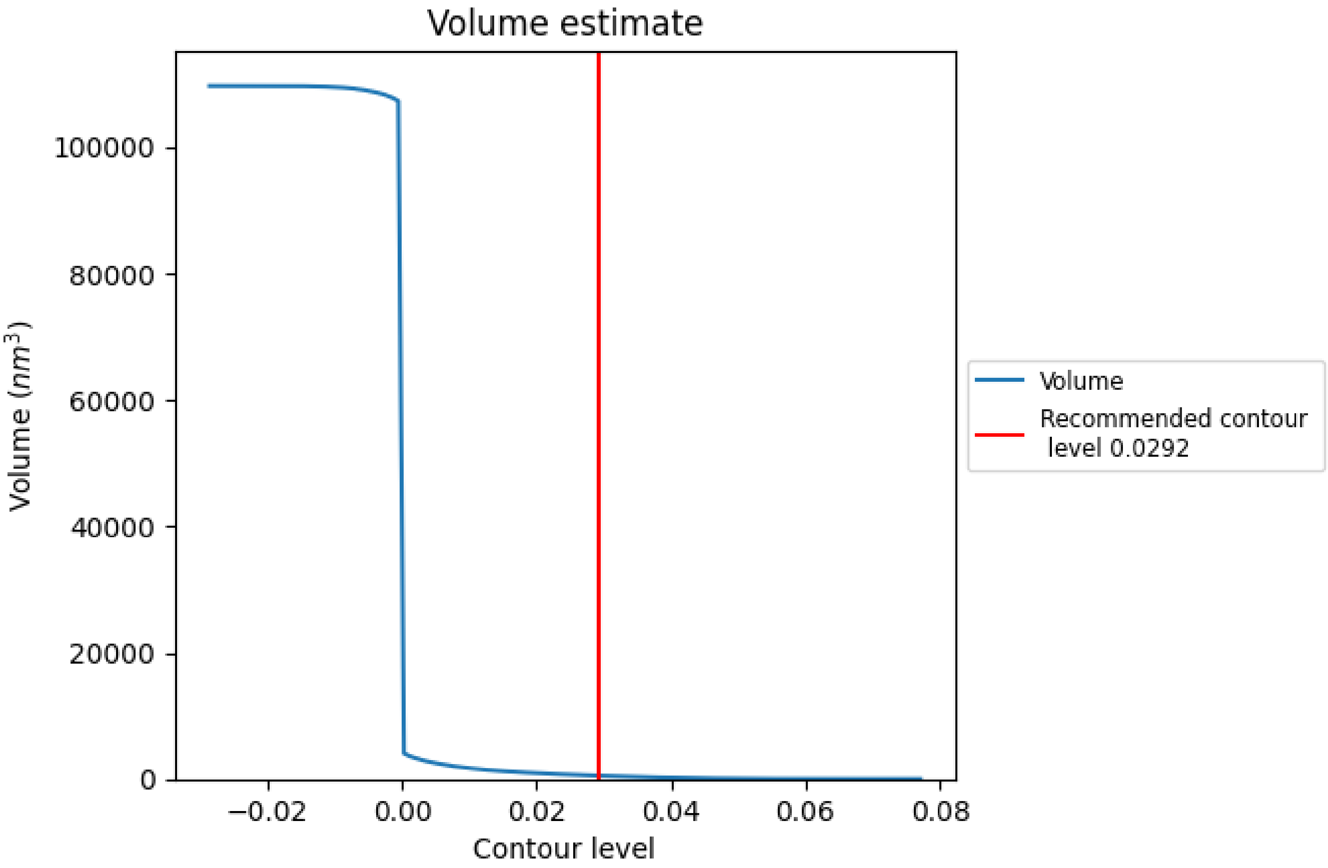
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

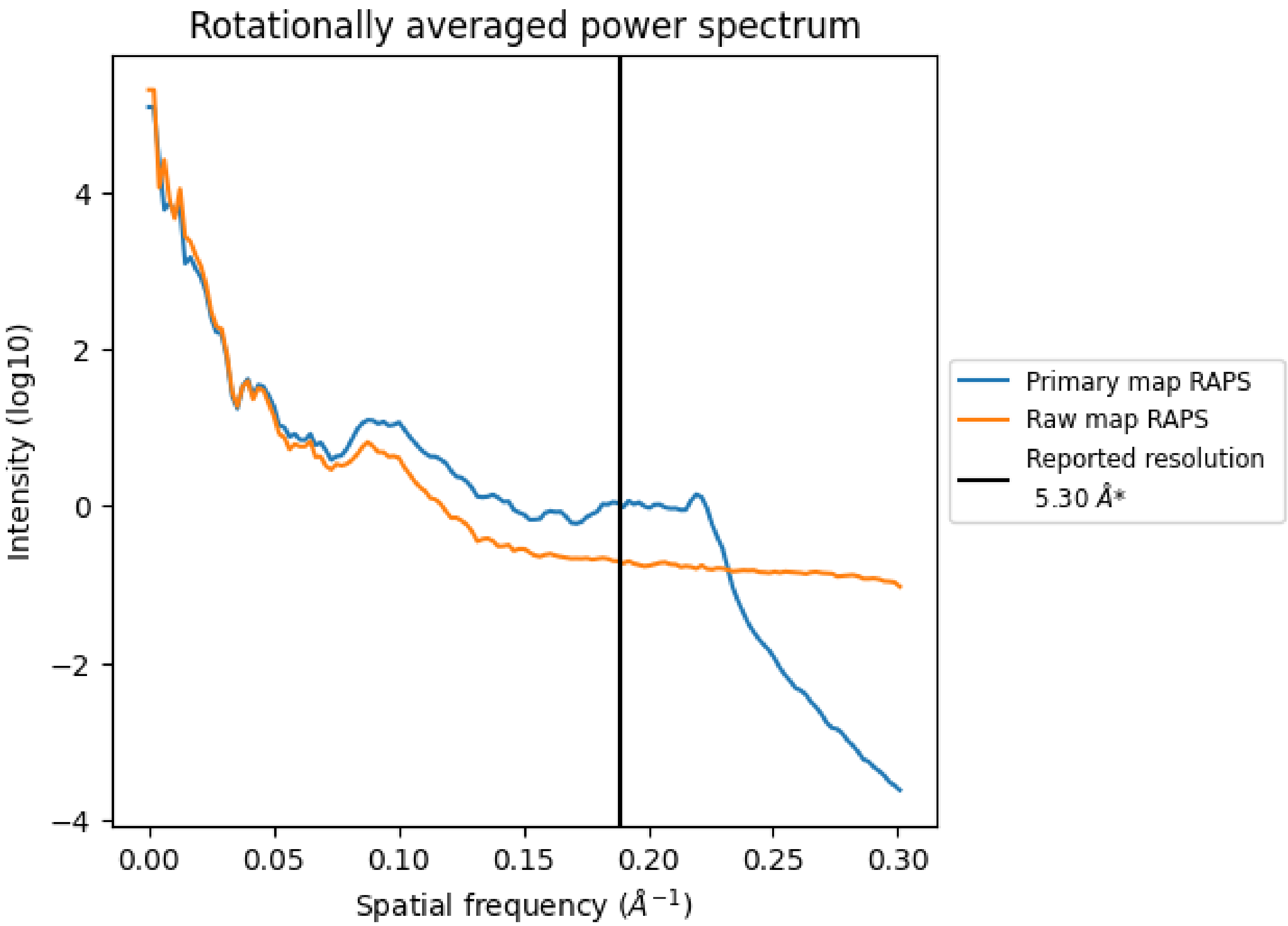
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 526 nm^3; this corresponds to an approximate mass of 475 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

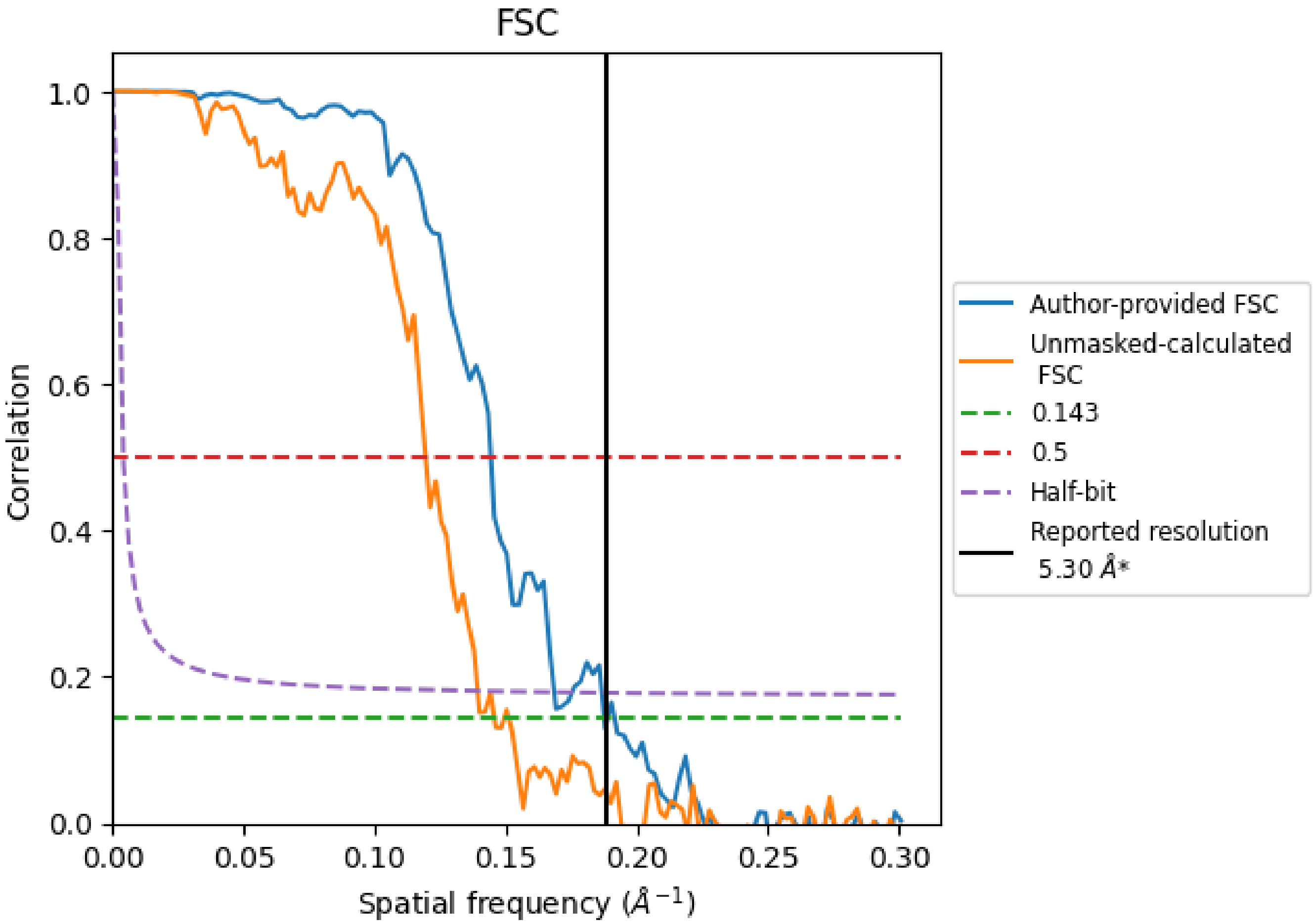


*Reported resolution corresponds to spatial frequency of 0.189 Å^{-1}

8 Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.189 Å^{-1}

8.2 Resolution estimates ⓘ

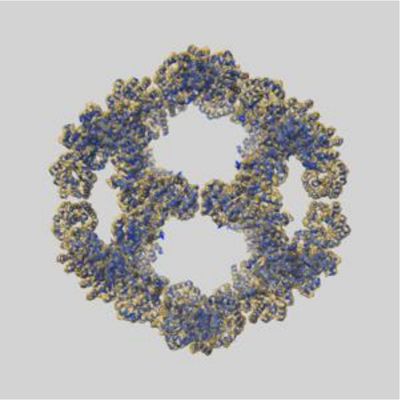
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	5.30	-	-
Author-provided FSC curve	5.33	6.93	5.93
Unmasked-calculated*	6.86	8.37	7.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.86 differs from the reported value 5.3 by more than 10 %

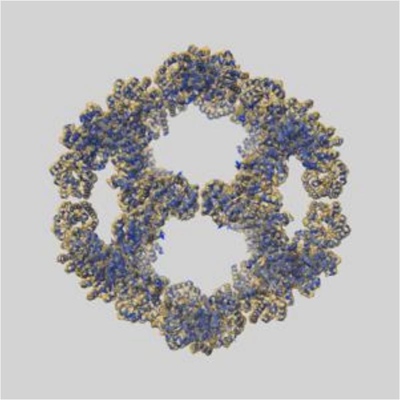
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-50615 and PDB model 9FO3. Per-residue inclusion information can be found in section 3 on page 20.

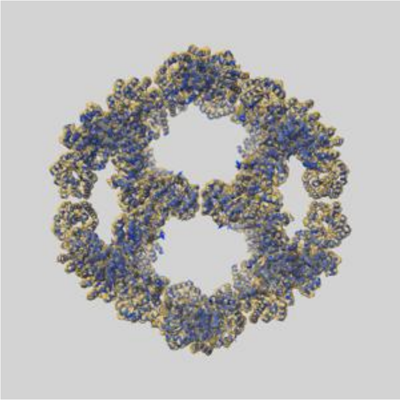
9.1 Map-model overlay ⓘ



X



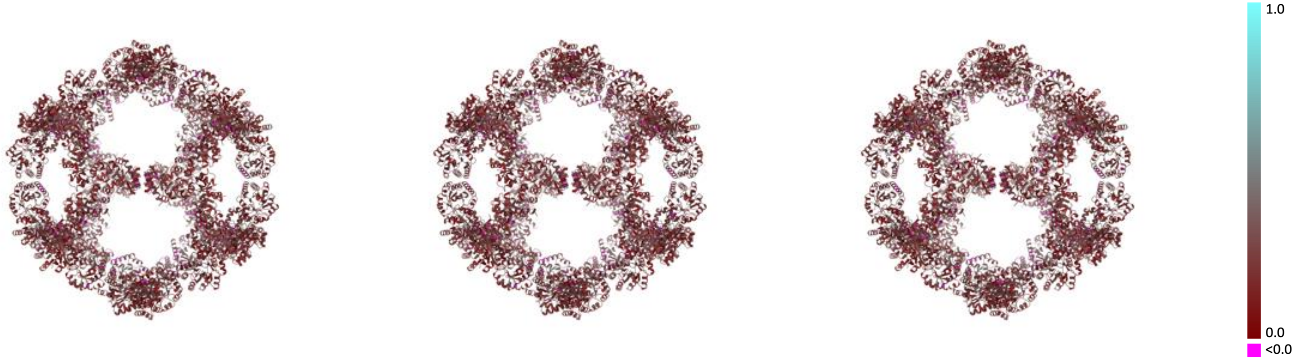
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0292 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

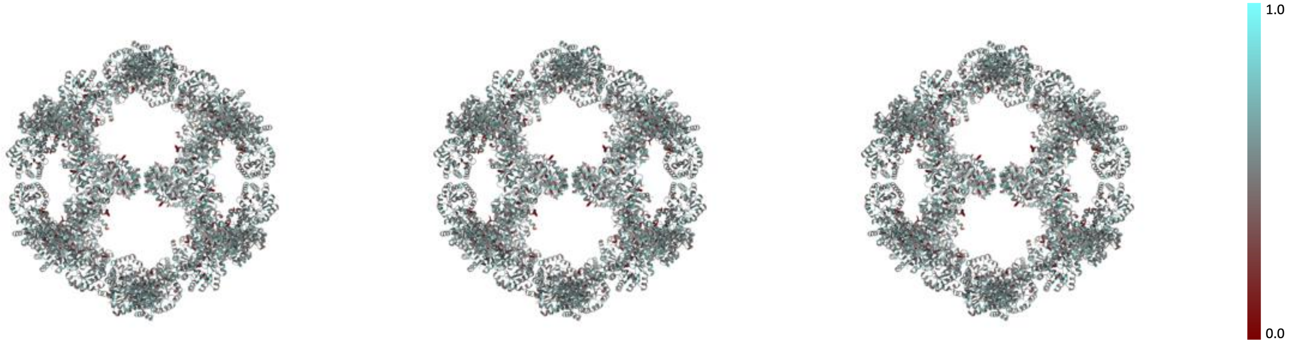
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

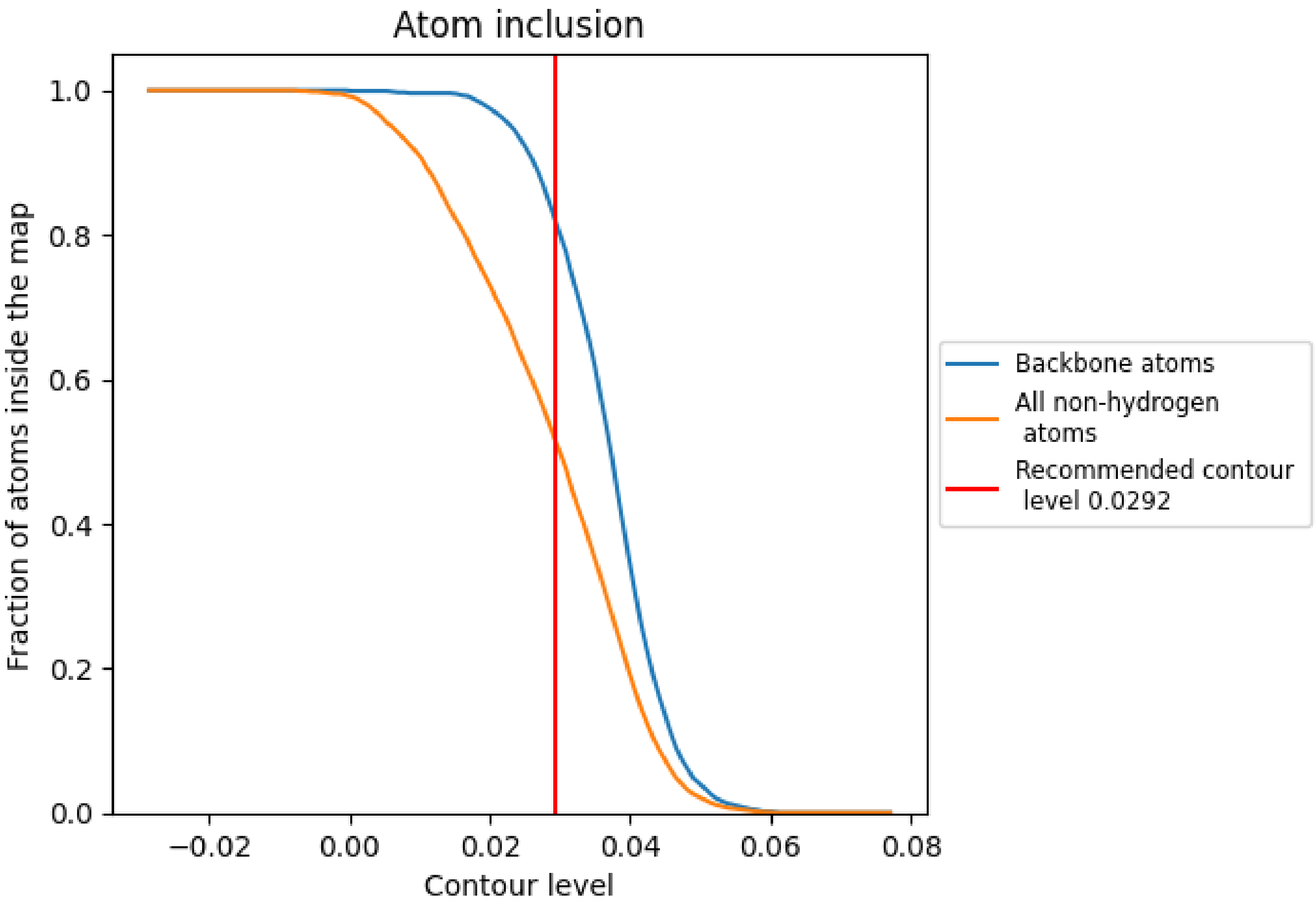
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0292).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0292) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5190	0.2310
0	0.5140	0.2290
1	0.5200	0.2310
2	0.5210	0.2310
3	0.5160	0.2310
4	0.5210	0.2290
5	0.5170	0.2300
6	0.5200	0.2310
7	0.5200	0.2340
A	0.5230	0.2310
B	0.5180	0.2330
C	0.5180	0.2310
D	0.5210	0.2320
E	0.5150	0.2310
F	0.5200	0.2320
G	0.5140	0.2300
H	0.5170	0.2310
I	0.5220	0.2290
J	0.5210	0.2290
K	0.5200	0.2320
L	0.5210	0.2300
M	0.5140	0.2310
N	0.5190	0.2300
O	0.5200	0.2300
P	0.5170	0.2300
Q	0.5200	0.2310
R	0.5200	0.2320
S	0.5180	0.2300
T	0.5200	0.2320
U	0.5160	0.2310
V	0.5200	0.2320
W	0.5210	0.2280
X	0.5200	0.2330
Y	0.5190	0.2320
Z	0.5150	0.2320

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Chain	Atom inclusion	Q-score
a	0.5180	0.2330
b	0.5210	0.2340
c	0.5140	0.2310
d	0.5180	0.2320
e	0.5190	0.2310
f	0.5180	0.2310
g	0.5190	0.2330
h	0.5210	0.2310
i	0.5160	0.2320
j	0.5190	0.2340
k	0.5200	0.2320
l	0.5200	0.2310
m	0.5210	0.2300
n	0.5210	0.2290
o	0.5210	0.2320
p	0.5200	0.2330
q	0.5140	0.2310
r	0.5180	0.2300
s	0.5190	0.2330
t	0.5200	0.2310
u	0.5200	0.2300
v	0.5210	0.2350
w	0.5200	0.2300
x	0.5200	0.2320
y	0.5160	0.2290
z	0.5200	0.2320