



# wwPDB EM Validation Summary Report ⓘ

Jan 27, 2025 – 02:51 PM JST

PDB ID : 9J1W  
EMDB ID : EMD-61080  
Title : Endogenous dihydrolipoamide acetyltransferase (E2) core of pyruvate dehydrogenase complex from pig heart  
Authors : Wang, C.; Zhang, X.; Chang, Y.J.  
Deposited on : 2024-08-05  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

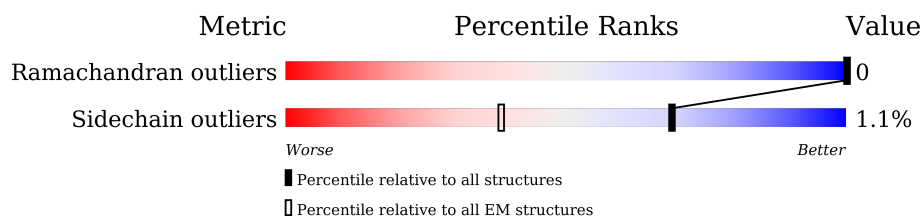
EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

# 1 Overall quality at a glance

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





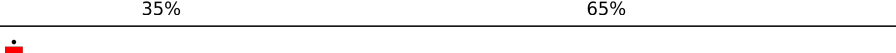

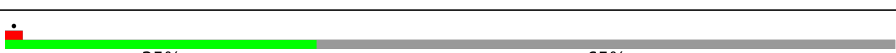


The reported resolution of this entry is 3.20 Å.

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.








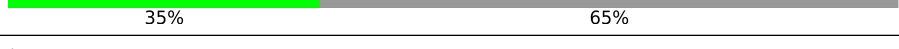

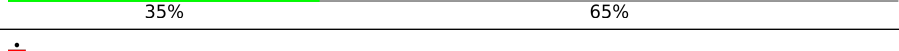
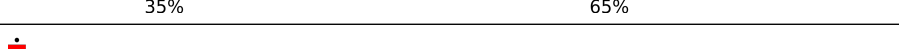
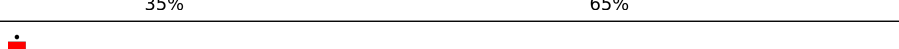















Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	647	 35% 65%
1	AA	647	 35% 65%
1	AB	647	 35% 65%
1	B	647	 35% 65%
1	BA	647	 35% 65%
1	BB	647	 35% 65%
1	C	647	 35% 65%
1	CA	647	 35% 65%
1	CB	647	 35% 65%




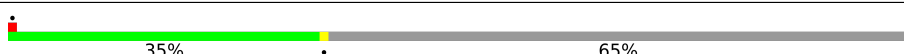

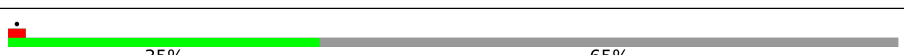
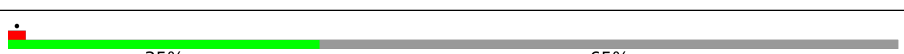


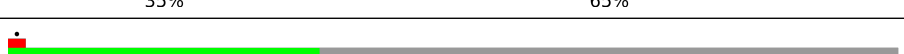


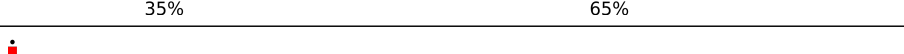












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Mol	Chain	Length	Quality of chain
1	D	647	
1	DA	647	
1	DB	647	
1	E	647	
1	EA	647	
1	EB	647	
1	F	647	
1	FA	647	
1	FB	647	
1	G	647	
1	GA	647	
1	GB	647	
1	H	647	
1	HA	647	
1	HB	647	
1	I	647	
1	IA	647	
1	J	647	
1	JA	647	
1	K	647	
1	KA	647	
1	L	647	
1	LA	647	
1	M	647	
1	MA	647	

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Mol	Chain	Length	Quality of chain
1	N	647	
1	NA	647	
1	O	647	
1	OA	647	
1	P	647	
1	PA	647	
1	Q	647	
1	QA	647	
1	R	647	
1	RA	647	
1	S	647	
1	SA	647	
1	T	647	
1	TA	647	
1	UA	647	
1	V	647	
1	VA	647	
1	W	647	
1	WA	647	
1	X	647	
1	XA	647	
1	Y	647	
1	YA	647	
1	Z	647	
1	ZA	647	

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Mol	Chain	Length	Quality of chain
1	a	647	<div><div></div><div>35%</div><div></div><div>65%</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 105420 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 Acetyltransferase component of pyruvate dehydrogenase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	228	Total	C	N	O	S	0	0
			1757	1120	303	324	10		
1	AA	228	Total	C	N	O	S	0	0
			1757	1120	303	324	10		
1	AB	228	Total	C	N	O	S	0	0
			1757	1120	303	324	10		
1	B	228	Total	C	N	O	S	0	0
			1757	1120	303	324	10		
1	BA	228	Total	C	N	O	S	0	0
			1757	1120	303	324	10		
1	BB	228	Total	C	N	O	S	0	0
			1757	1120	303	324	10		
1	C	228	Total	C	N	O	S	0	0
			1757	1120	303	324	10		
1	CA	228	Total	C	N	O	S	0	0
			1757	1120	303	324	10		
1	CB	228	Total	C	N	O	S	0	0
			1757	1120	303	324	10		
1	D	228	Total	C	N	O	S	0	0
			1757	1120	303	324	10		
1	DA	228	Total	C	N	O	S	0	0
			1757	1120	303	324	10		
1	DB	228	Total	C	N	O	S	0	0
			1757	1120	303	324	10		
1	E	228	Total	C	N	O	S	0	0
			1757	1120	303	324	10		
1	EA	228	Total	C	N	O	S	0	0
			1757	1120	303	324	10		
1	EB	228	Total	C	N	O	S	0	0
			1757	1120	303	324	10		
1	F	228	Total	C	N	O	S	0	0
			1757	1120	303	324	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	FA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	FB	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	G	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	GA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	GB	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	H	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	HA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	HB	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	I	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	IA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	J	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	JA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	K	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	KA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	L	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	LA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	M	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	MA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	N	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	NA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	O	228	Total 1757	C 1120	N 303	O 324	S 10	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	OA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	P	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	PA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	Q	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	QA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	R	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	RA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	S	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	SA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	T	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	TA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	UA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	V	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	VA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	W	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	WA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	X	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	XA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	Y	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	YA	228	Total 1757	C 1120	N 303	O 324	S 10	0	0
1	Z	228	Total 1757	C 1120	N 303	O 324	S 10	0	0

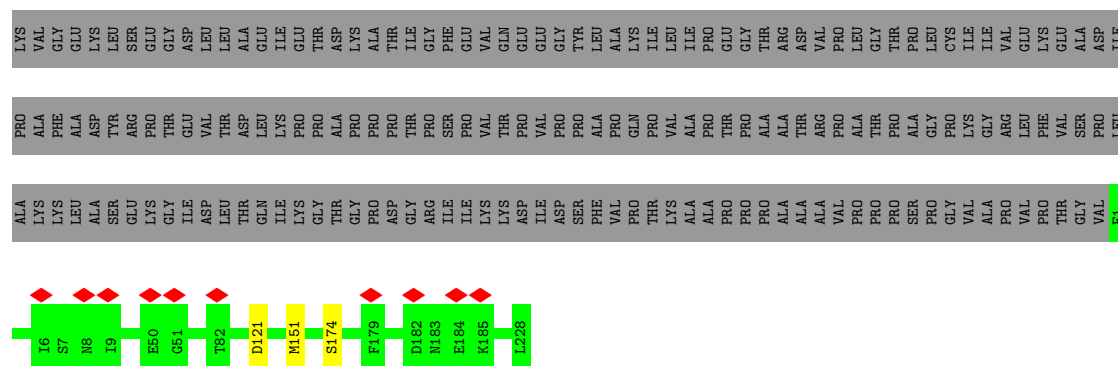
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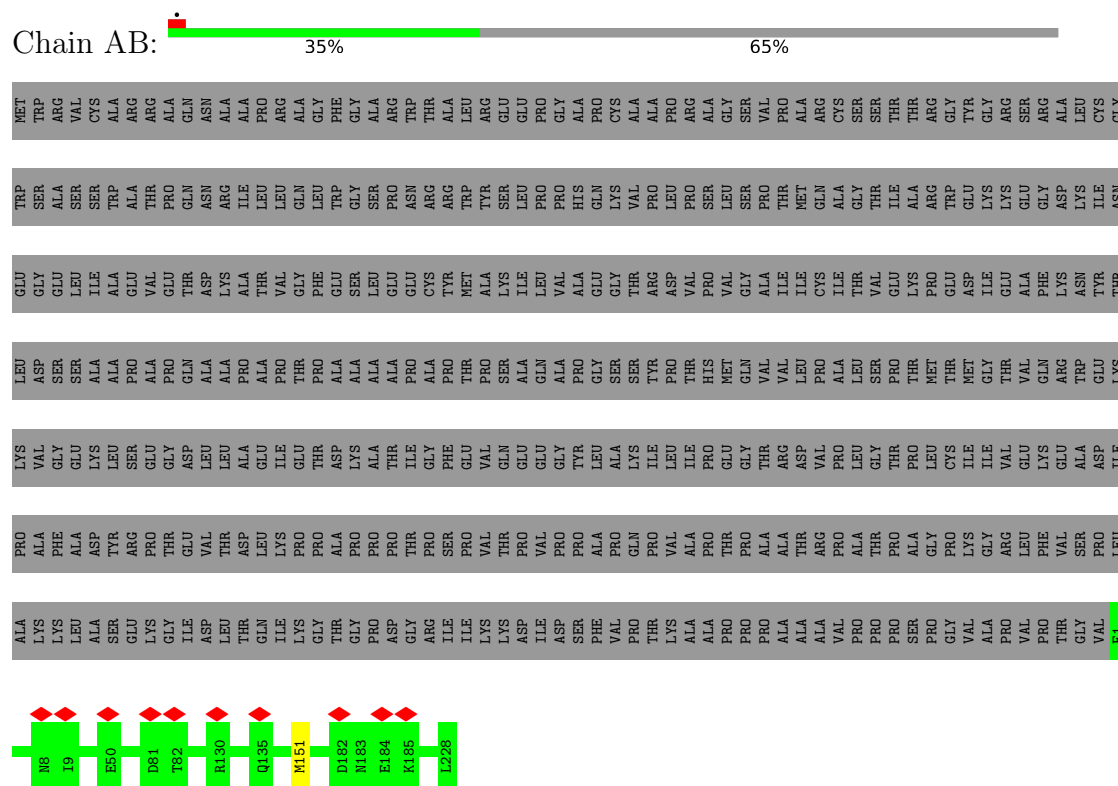
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ZA	228	Total	C	N	O	S	0	0
			1757	1120	303	324	10		
1	a	228	Total	C	N	O	S	0	0
			1757	1120	303	324	10		

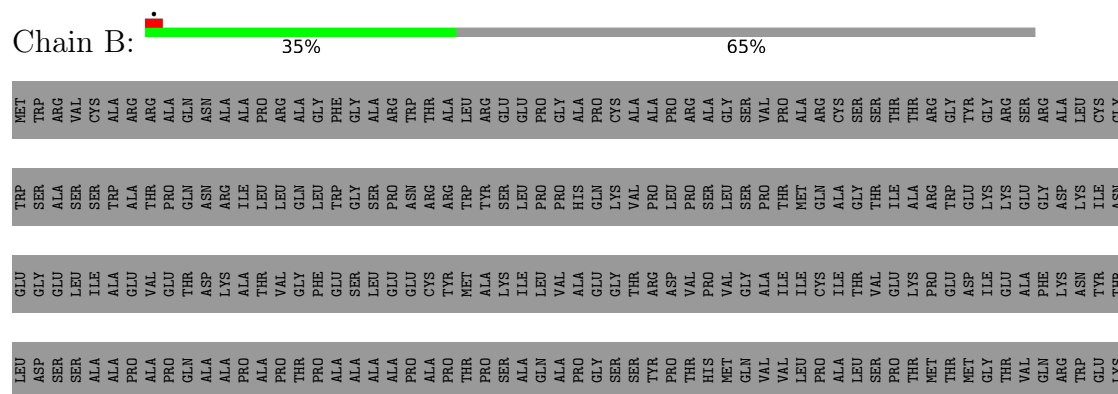


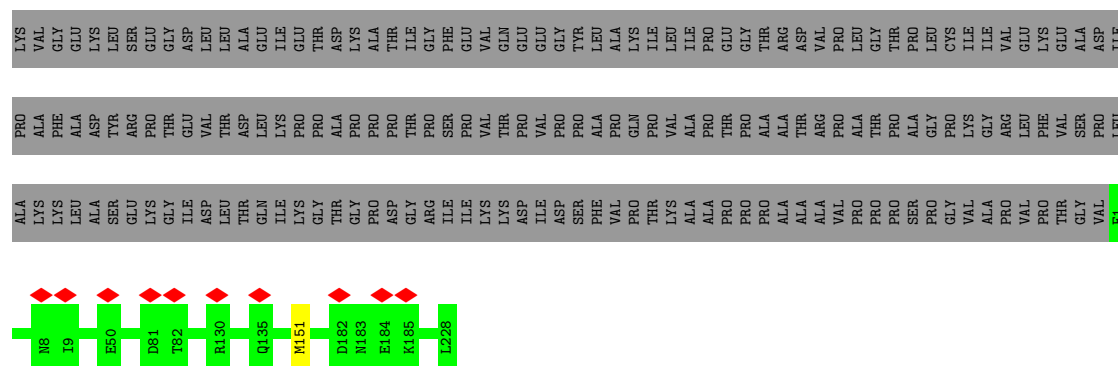


- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

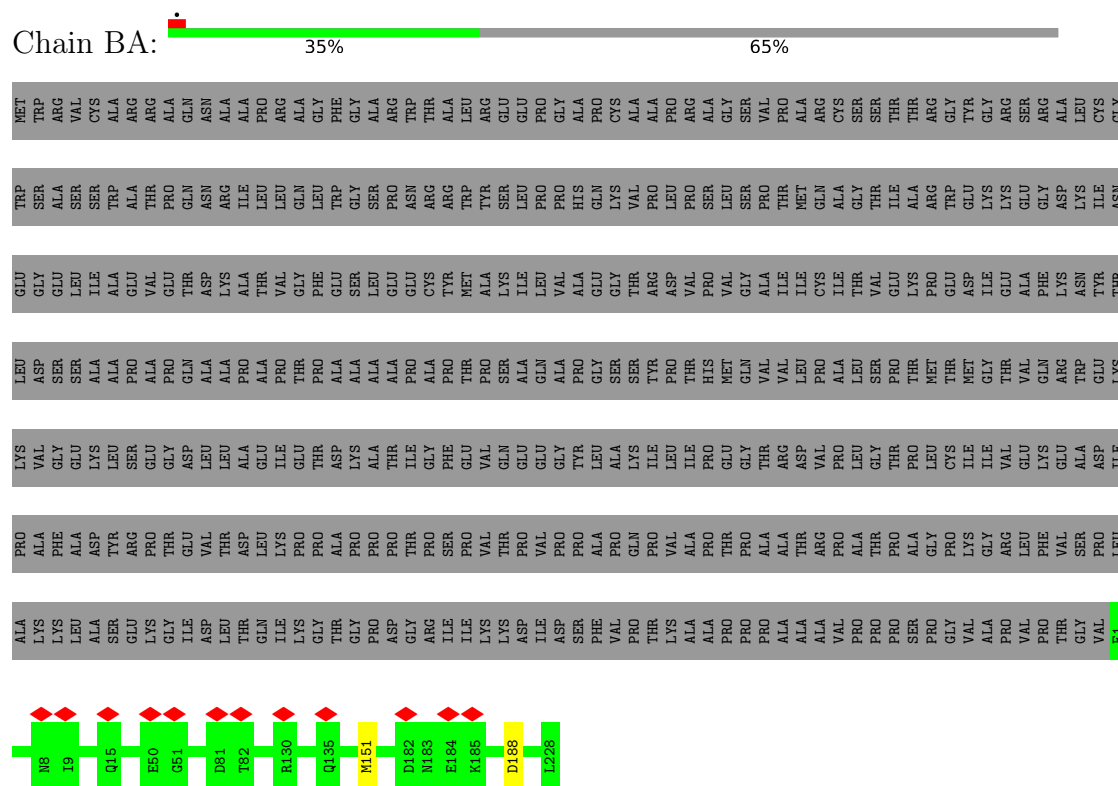


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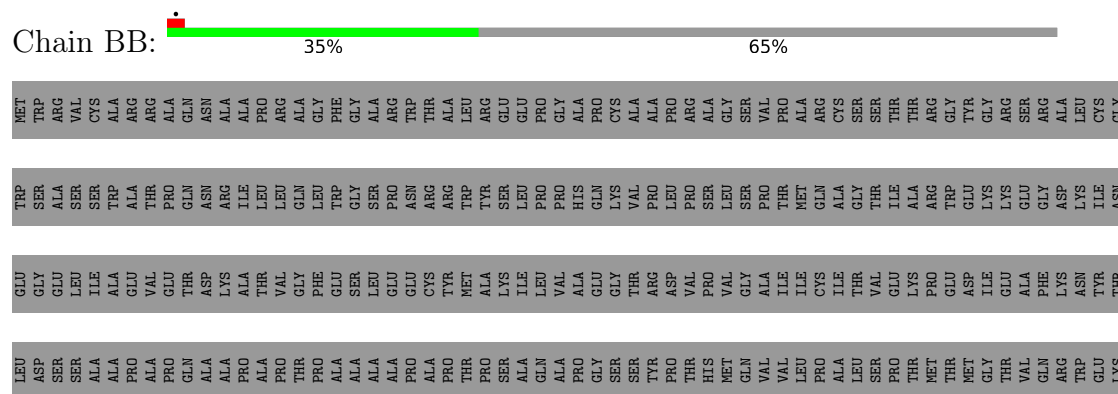


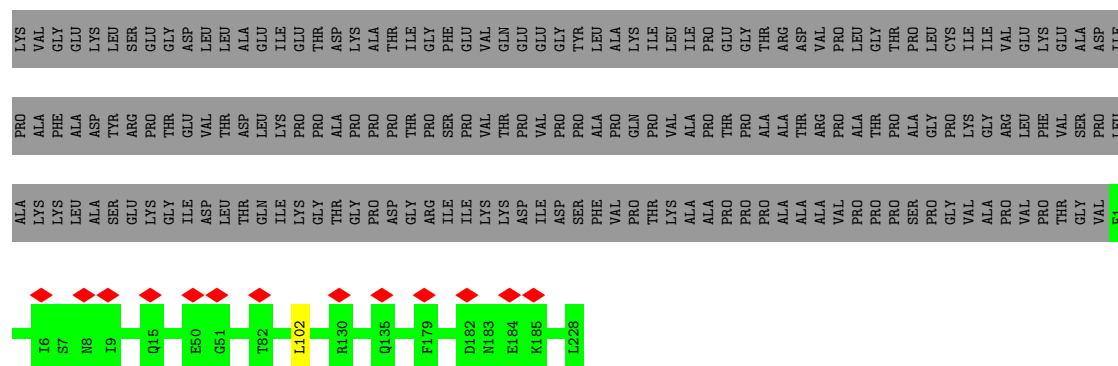


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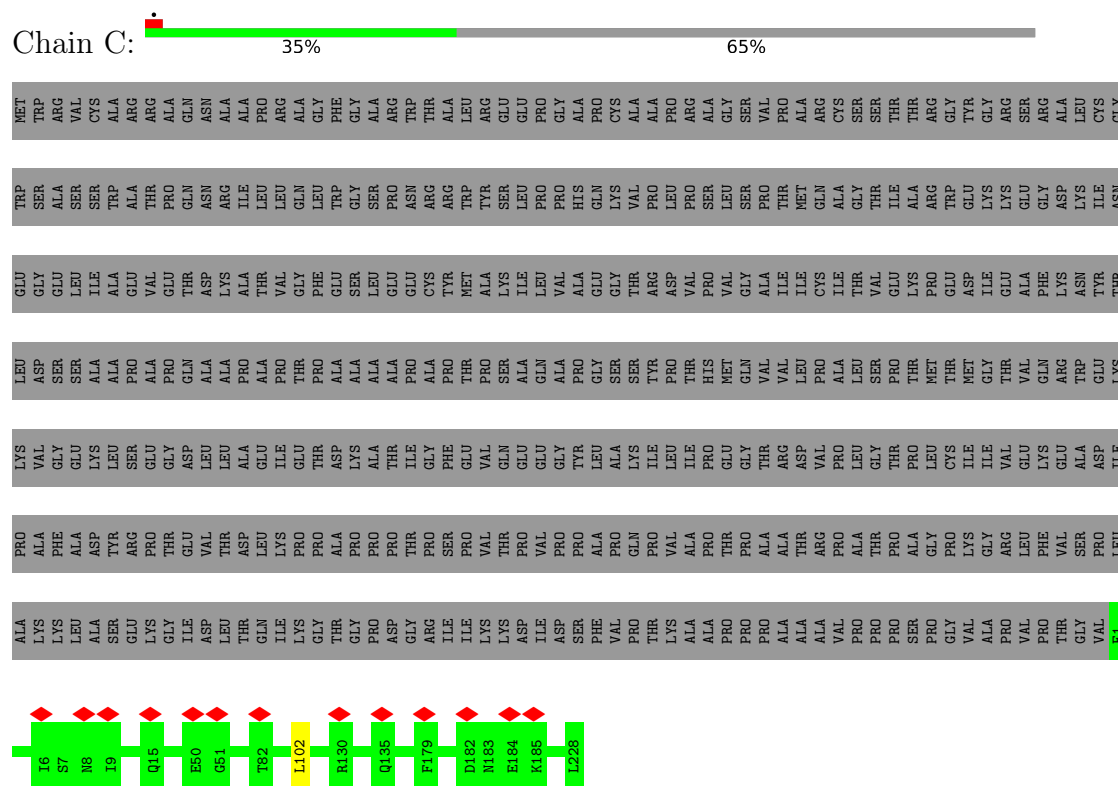


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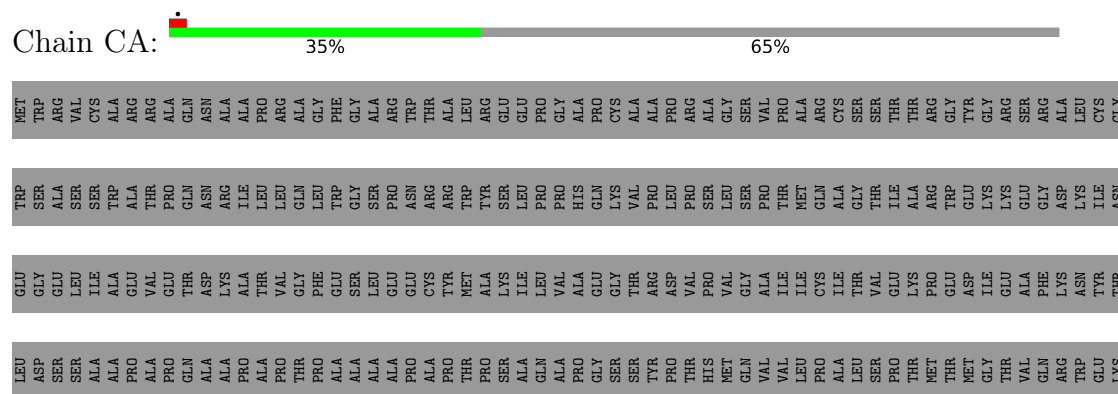


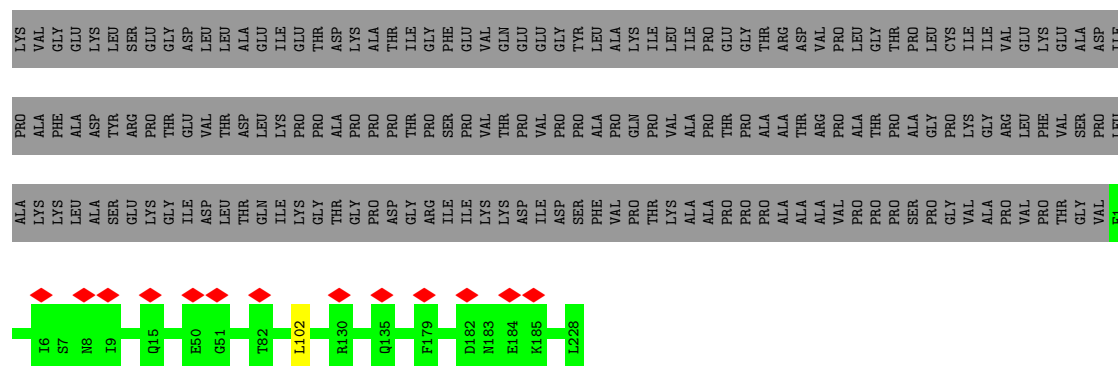


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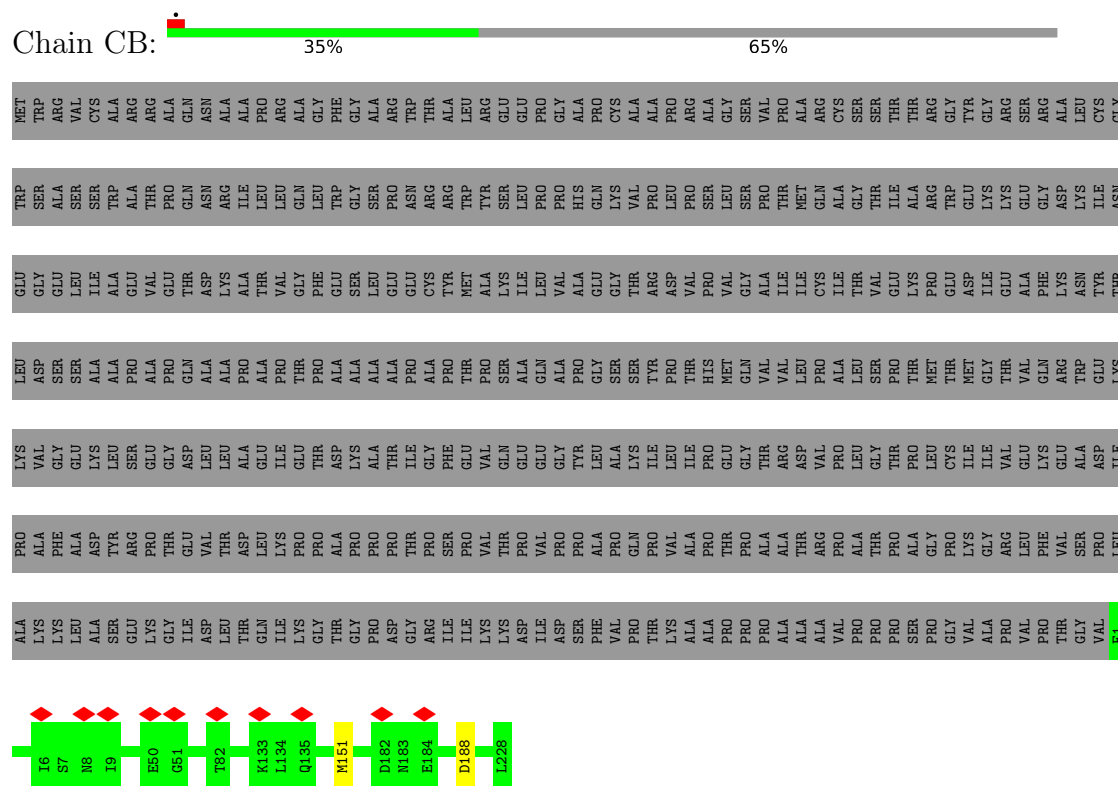


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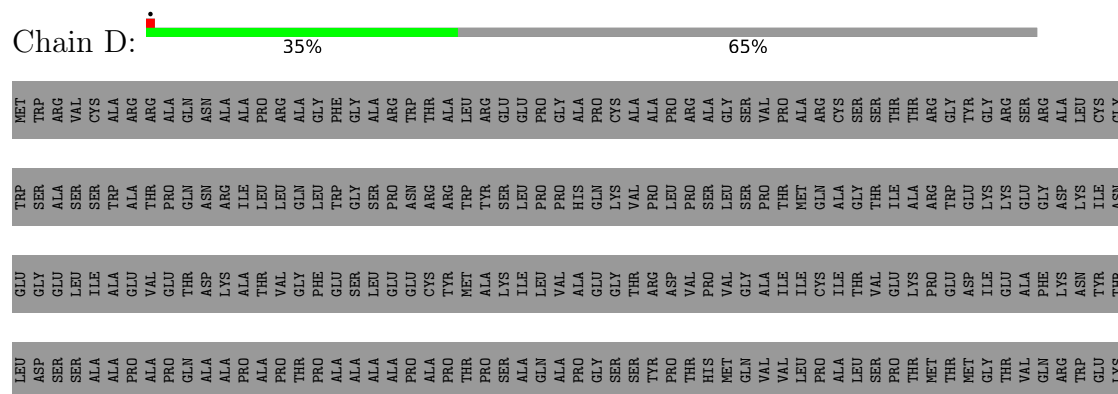




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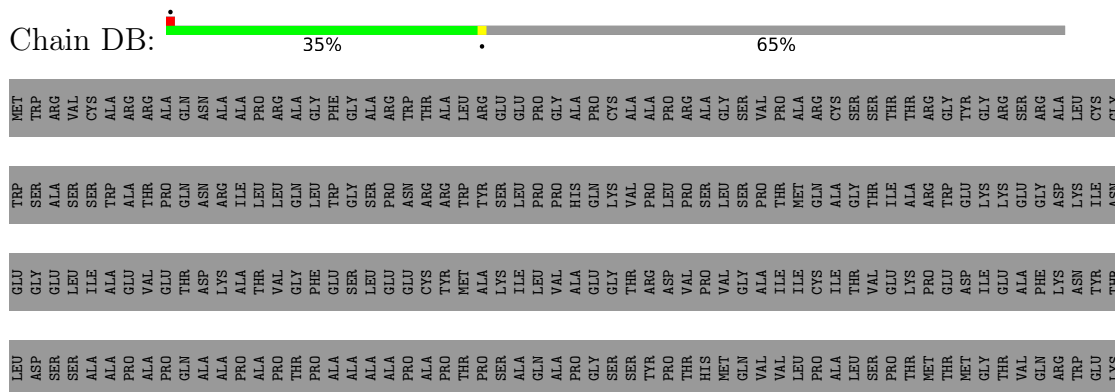


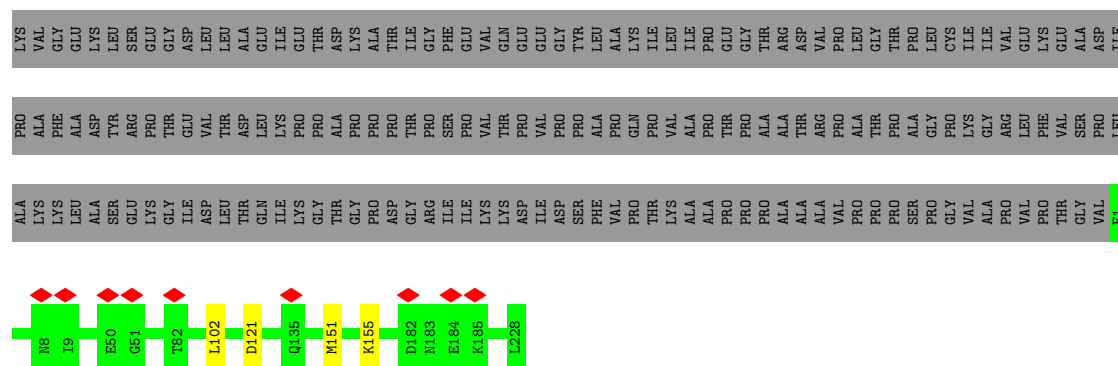
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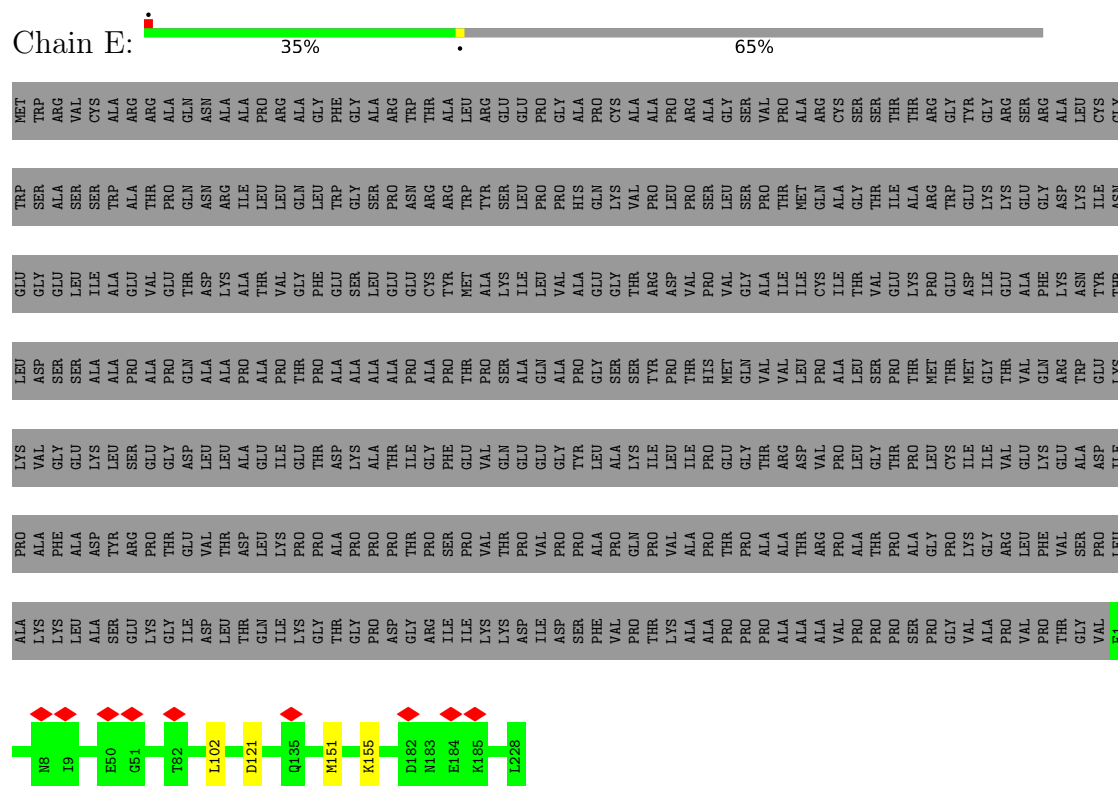
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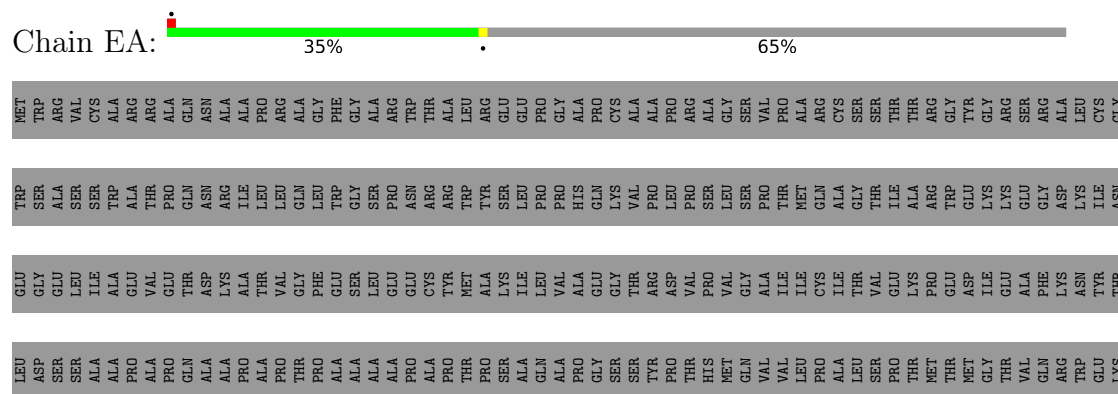




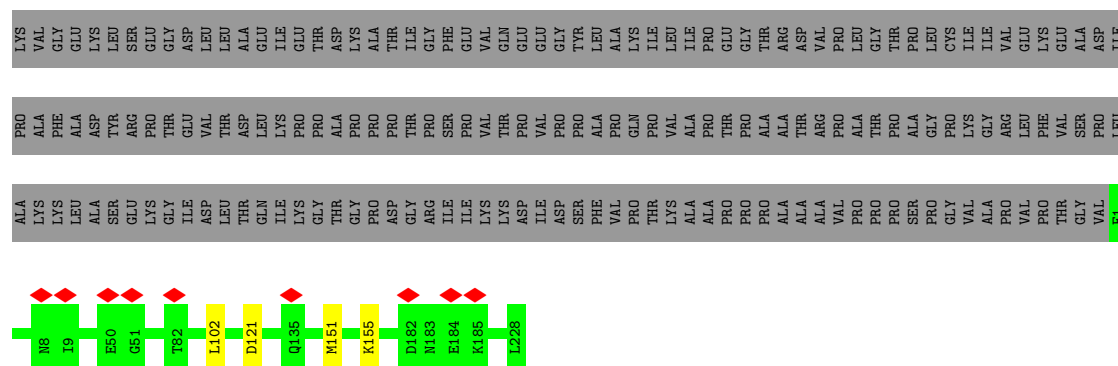
- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



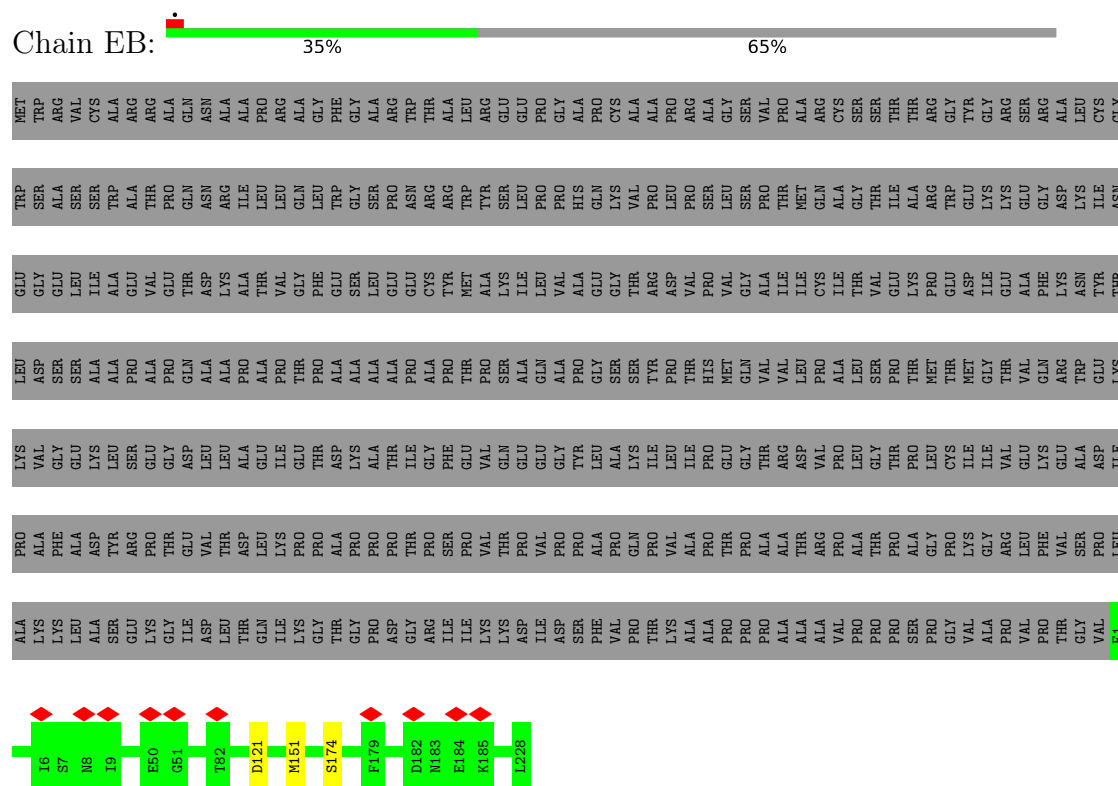
- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



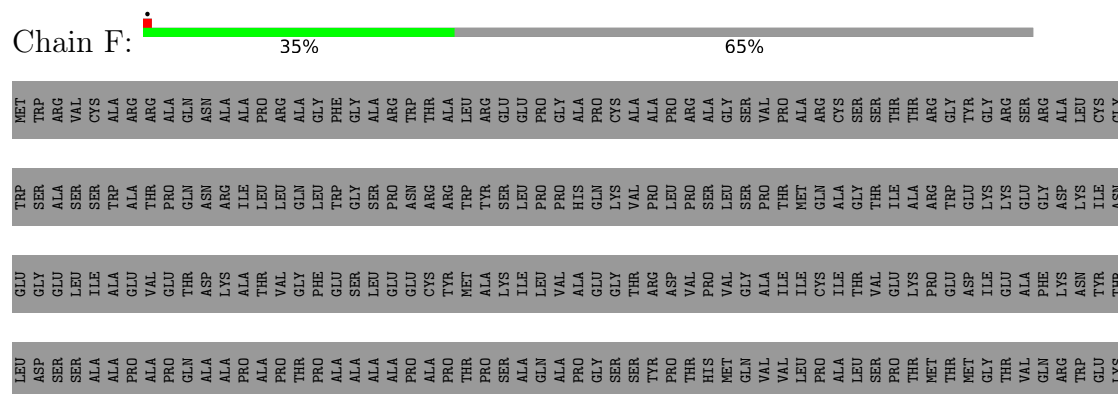


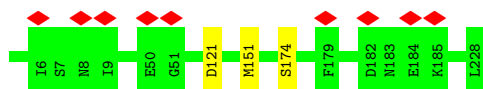


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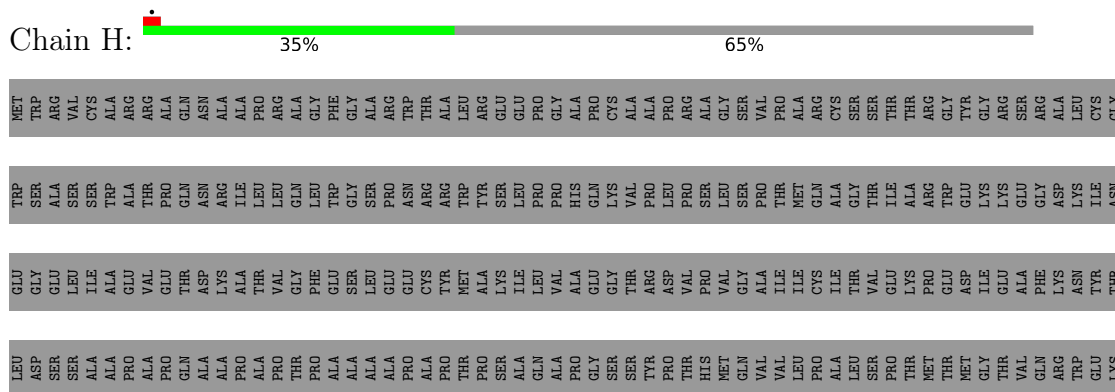


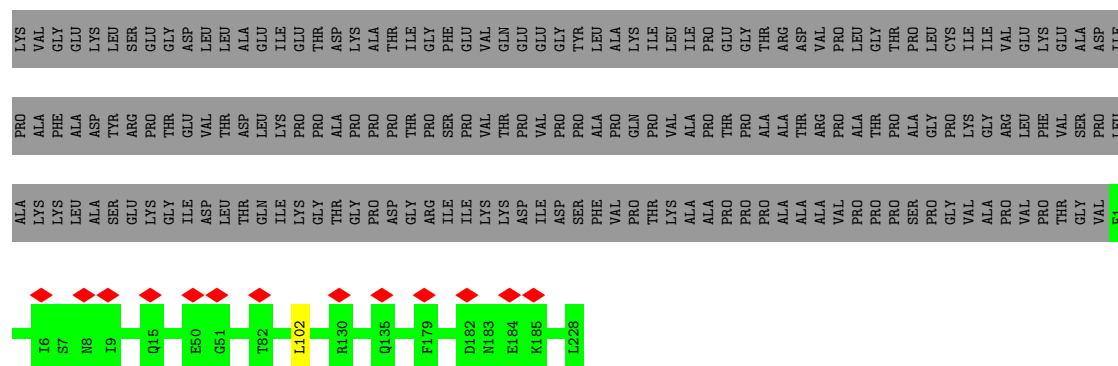
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ASP	SER	GLU	SER	TRP
SER	SER	LEU	SER	VAL
ALA	ALA	ILE	SER	CYS
ALA	ALA	ALA	TRP	ALA
PRO	PRO	GLU	ALA	ARG
ALA	ALA	VAL	THR	ARG
PRO	PRO	GLU	PRO	GLN
GLN	GLN	THR	ASN	ASN
ALA	ALA	ASP	ALA	ALA
ALA	ALA	LYS	ARG	ALA
PRO	PRO	ALA	ILE	ALA
ALA	ALA	THR	LEU	PRO
PRO	PRO	VAL	LEU	ARG
THR	THR	GLY	GLN	ALA
PRO	PRO	PHE	LEU	GLY
ALA	ALA	GLU	TRP	PHE
ALA	ALA	SER	GLY	GLY
ALA	ALA	LEU	SER	ALA
ALA	ALA	GLU	PRO	ARG
PRO	PRO	GLU	ASN	TRP
ALA	ALA	CYS	ARG	THR
PRO	PRO	TYR	ARG	ALA
THR	THR	MET	TRP	LEU
PRO	PRO	ALA	TYR	ARG
SER	SER	LYS	SER	GLU
ALA	ALA	ILE	LEU	GLU
GLN	GLN	LEU	PRO	PRO
ALA	ALA	VAL	PRO	GLY
PRO	PRO	ALA	HIS	ALA
GLY	GLY	GLU	GLN	PRO
SER	SER	GLY	LYS	CYS
SER	SER	THR	VAL	ALA
TYR	TYR	ARG	PRO	ALA
PRO	PRO	ASP	LEU	PRO
THR	THR	VAL	PRO	ARG
HIS	HIS	PRO	SER	ALA
MET	MET	VAL	LEU	GLY
GLN	GLN	GLY	SER	SER
VAL	VAL	ALA	PRO	VAL
VAL	VAL	ILE	THR	PRO
LEU	LEU	ILE	THR	ALA
PRO	PRO	CYS	GLN	ARG
MET	MET	PRO	MET	ALA
THR	THR	PRO	GLY	CYS
LEU	LEU	THR	GLY	SER
SER	SER	VAL	THR	THR
PRO	PRO	GLU	ILE	THR
THR	THR	LYS	ALA	THR
VAL	VAL	ALA	ARG	GLY
GLN	GLN	PHE	GLY	TYR
THR	THR	LYS	GLU	GLY
ARG	ARG	ASN	LYS	ARG
PRO	PRO	ASP	ASP	SER
TRP	TRP	ASN	LYS	ALA
GLY	GLY	TYR	ILE	LEU
GLU	GLU	THR	ASN	CYS



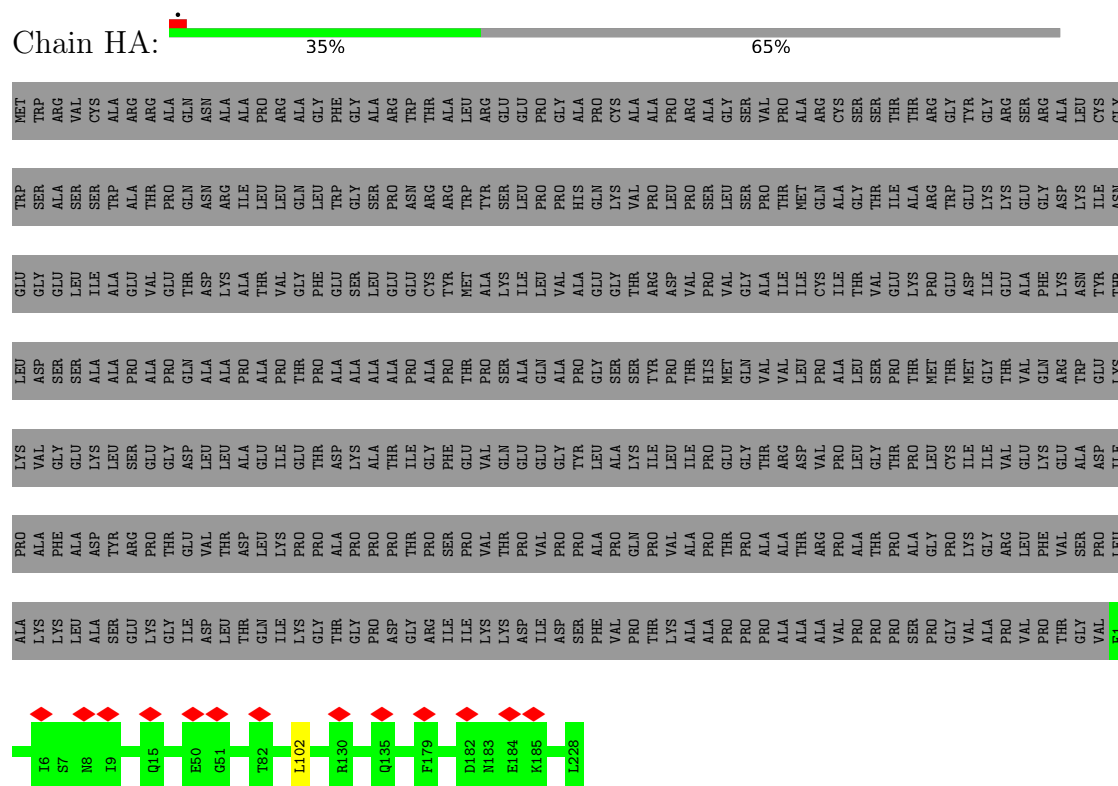
- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

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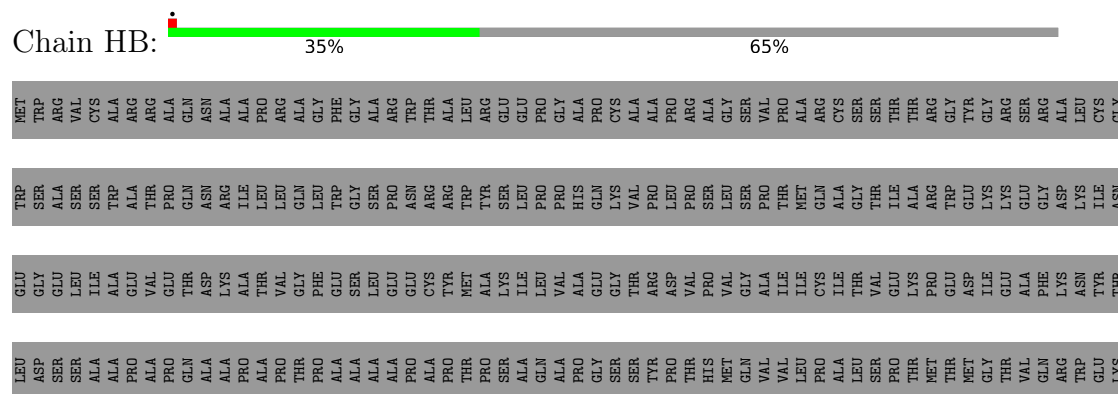


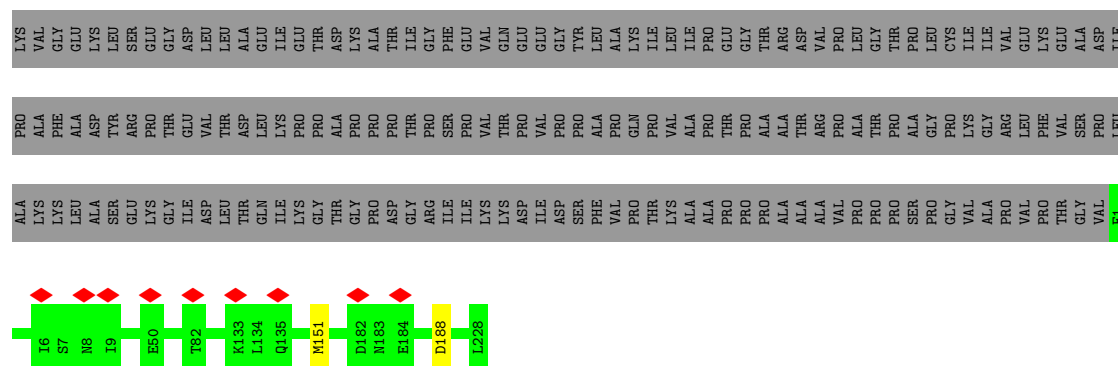


- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

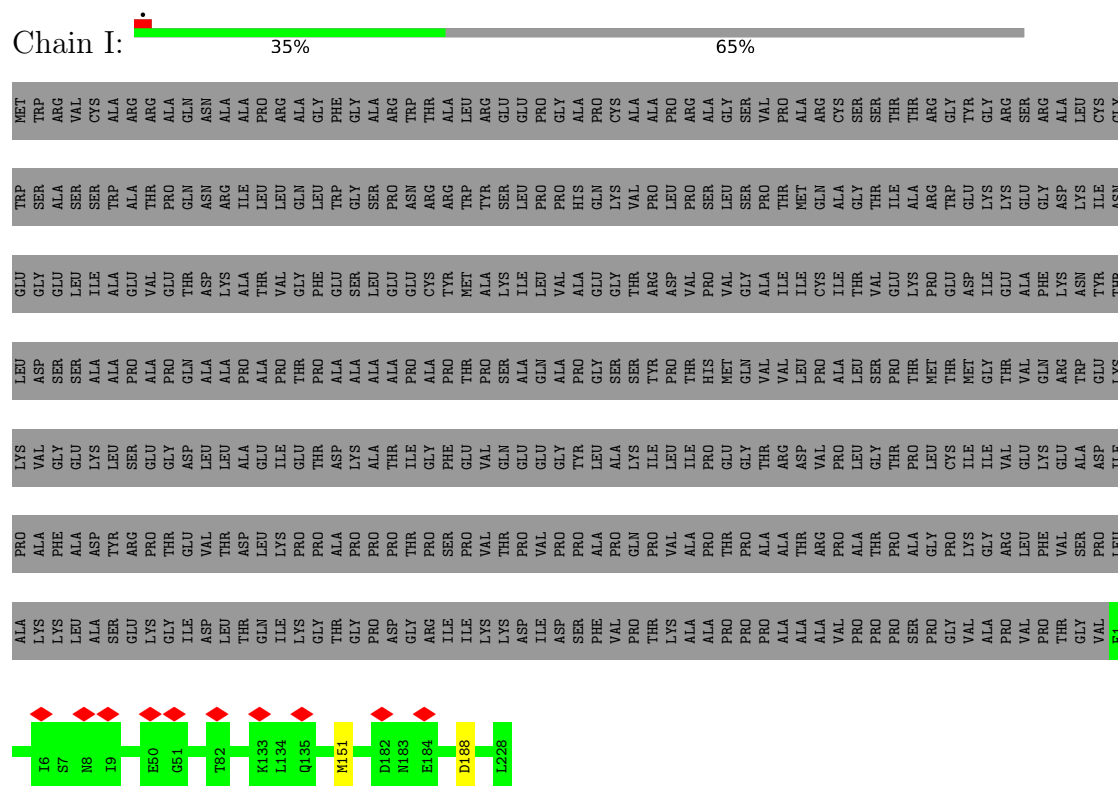


- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

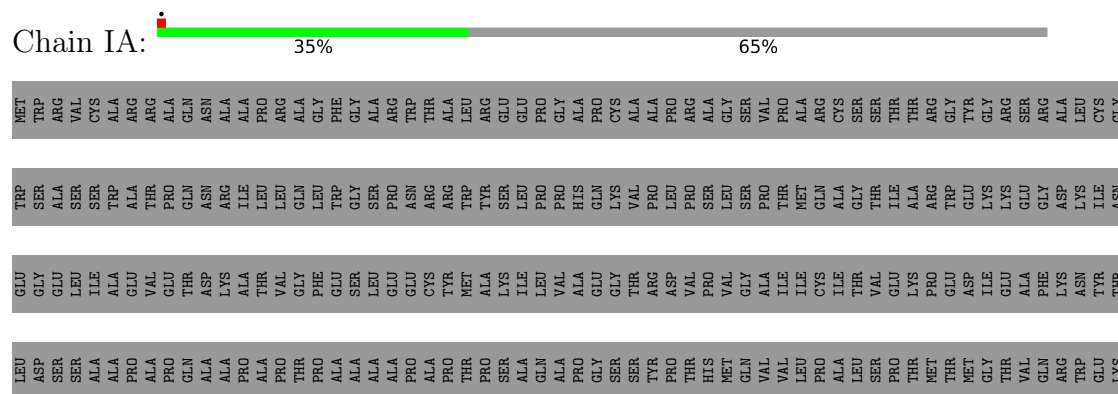


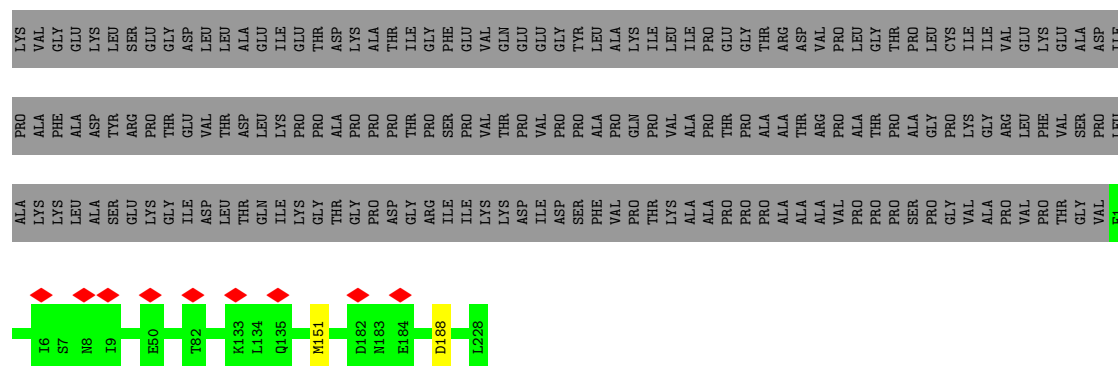


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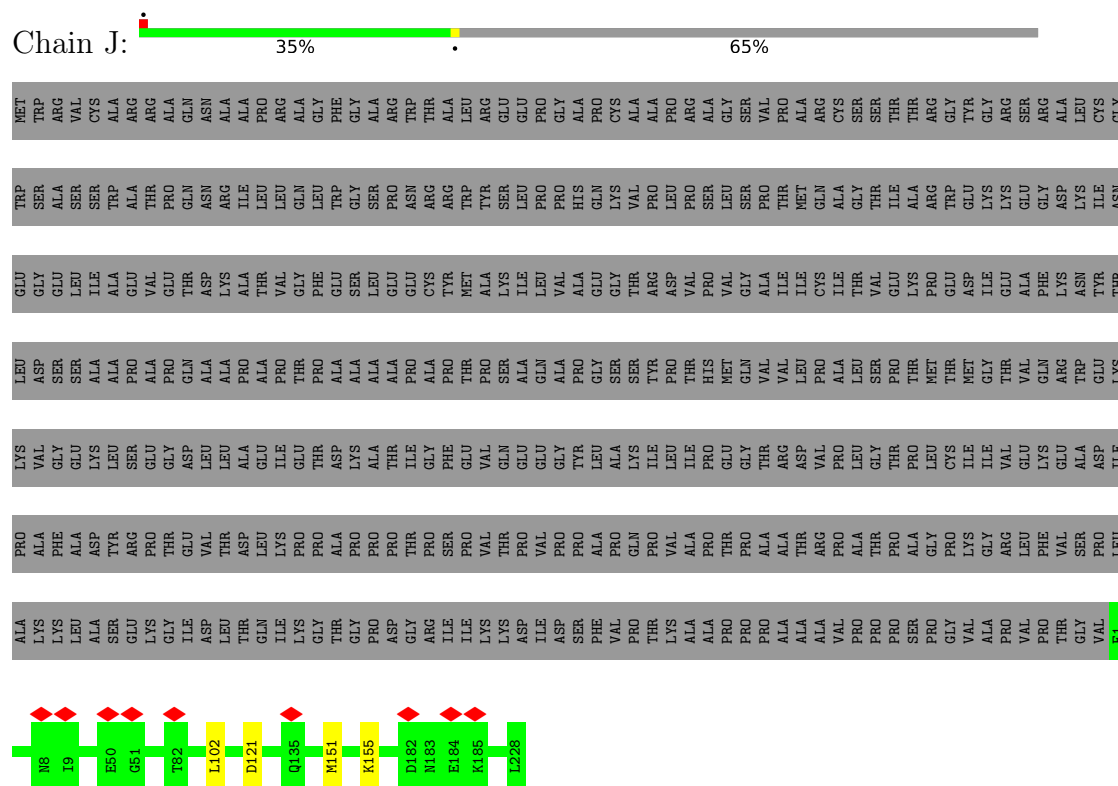


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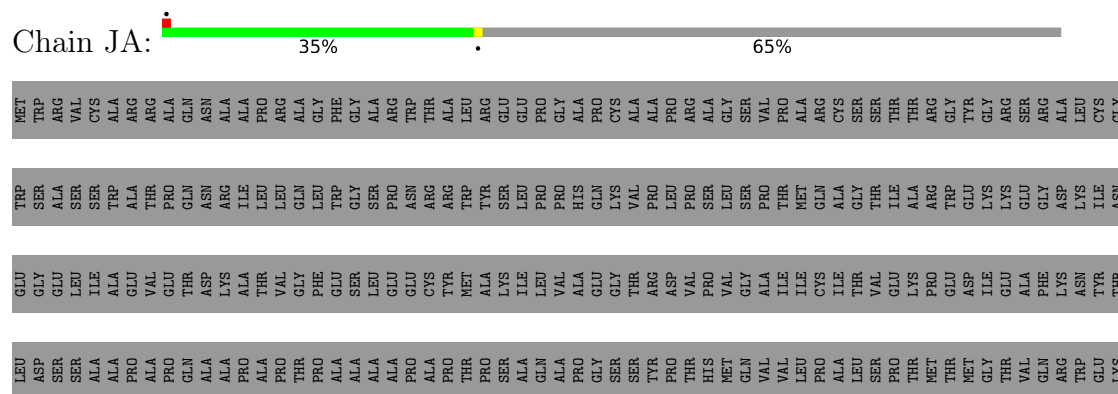


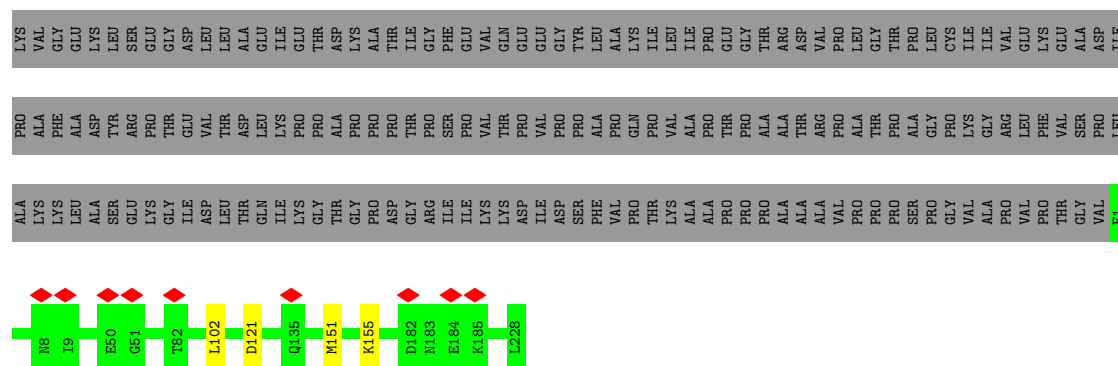


- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

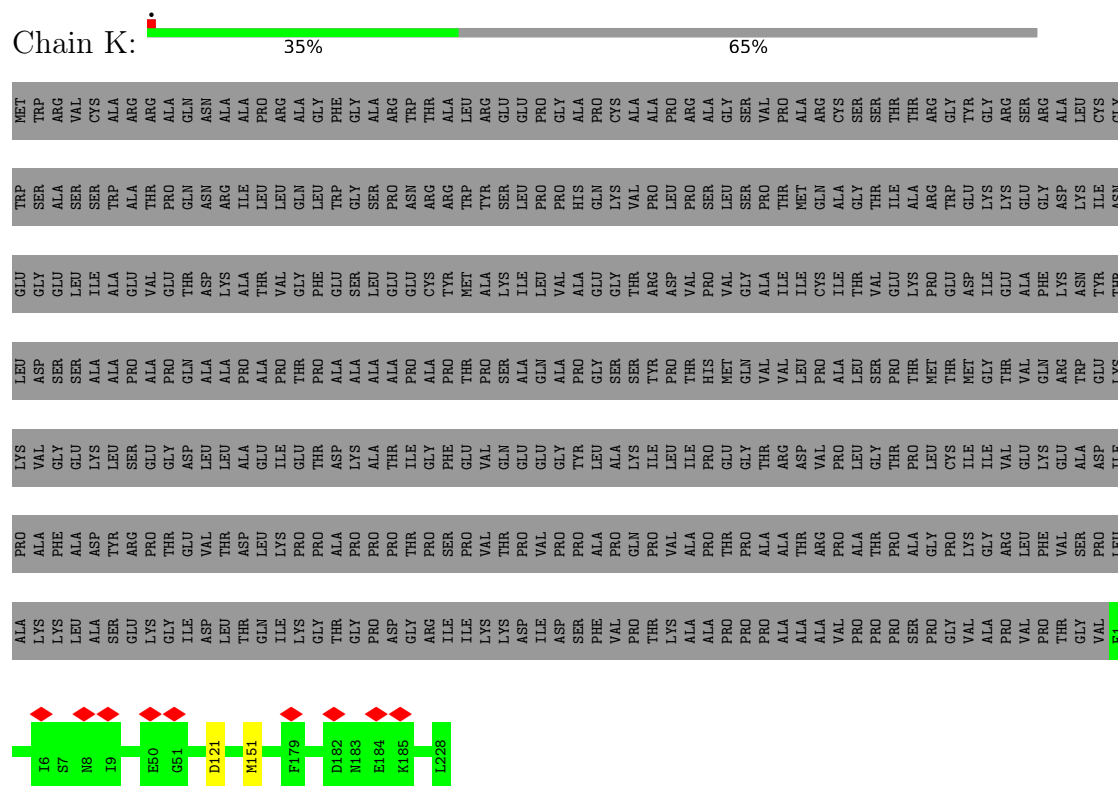


- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

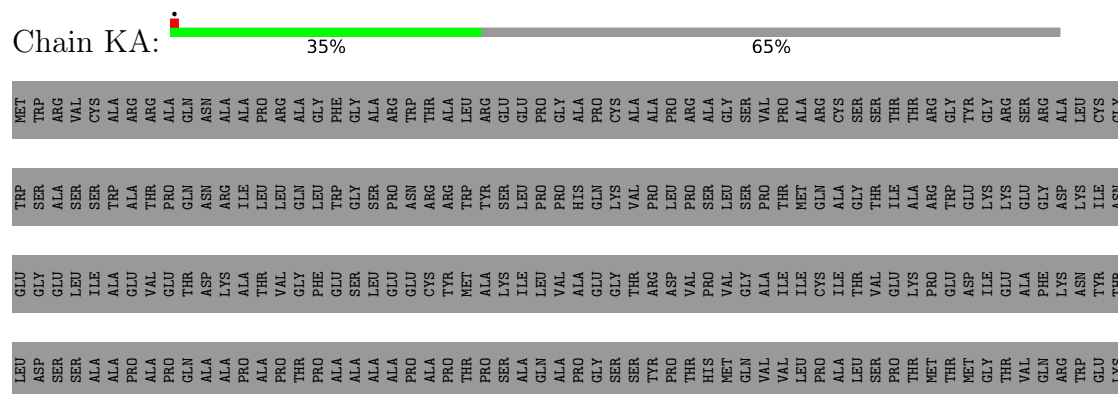




- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



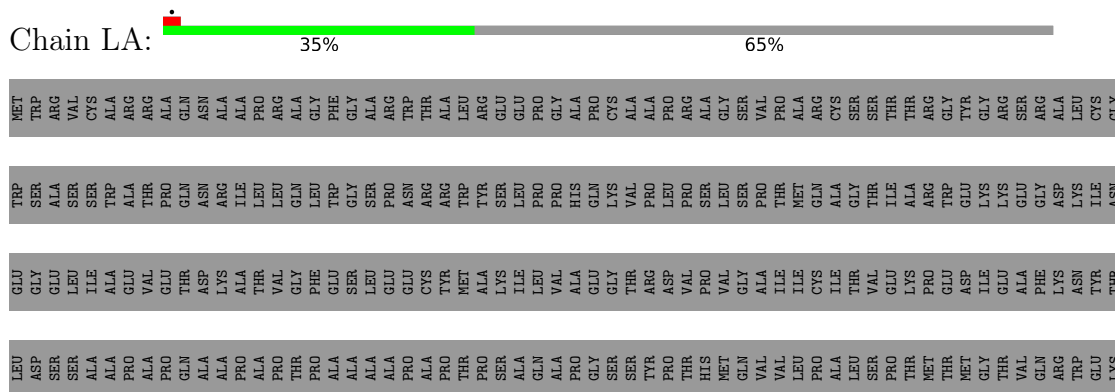
- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

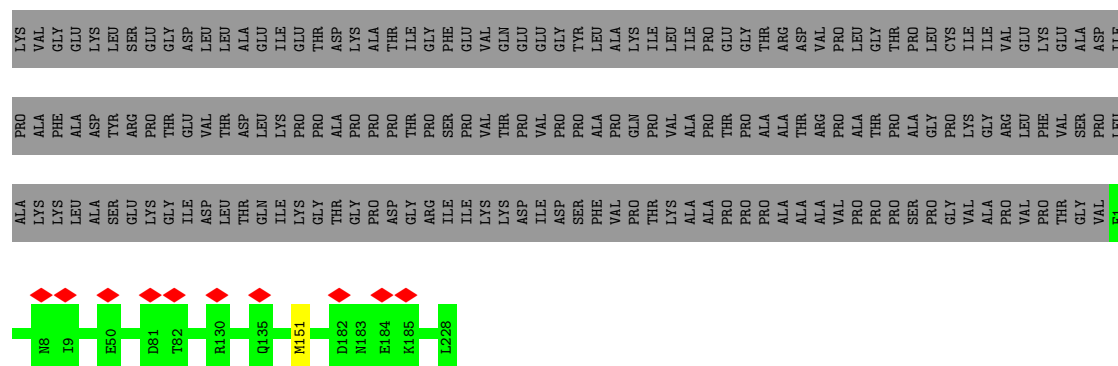




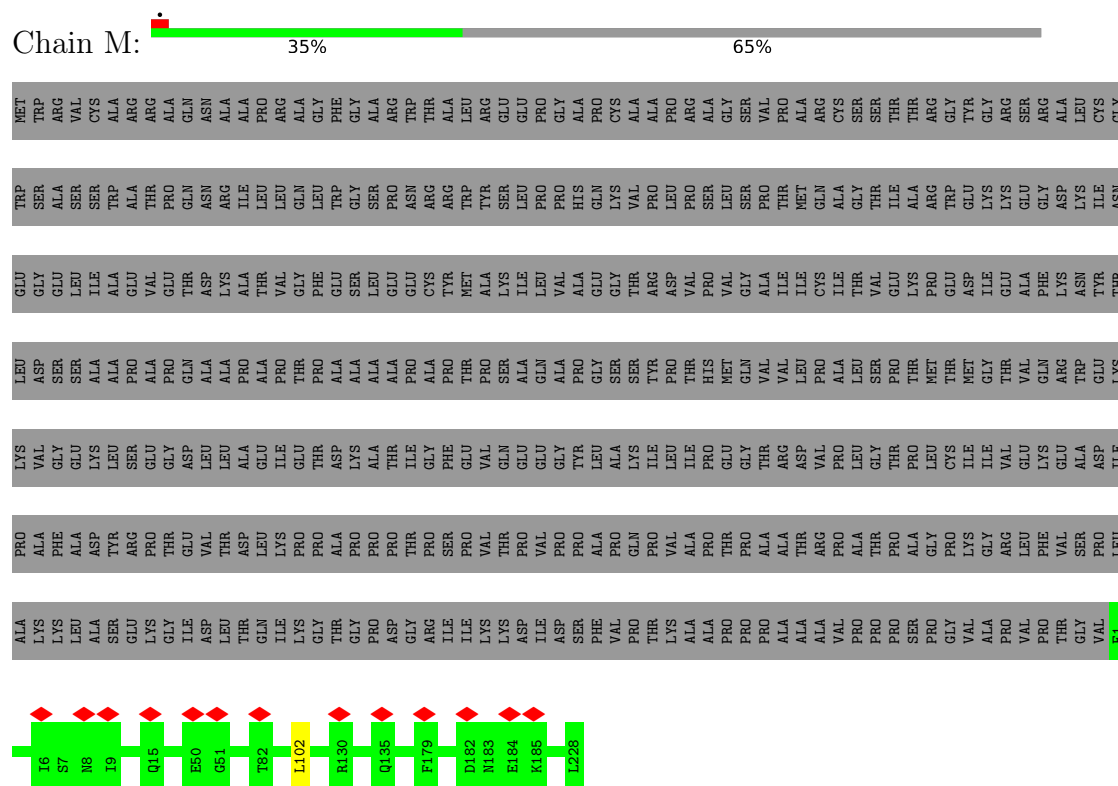
- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

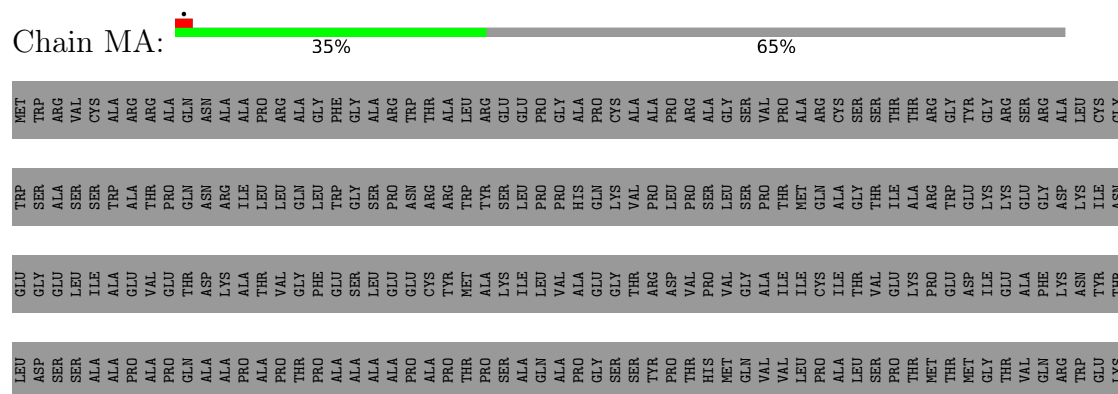


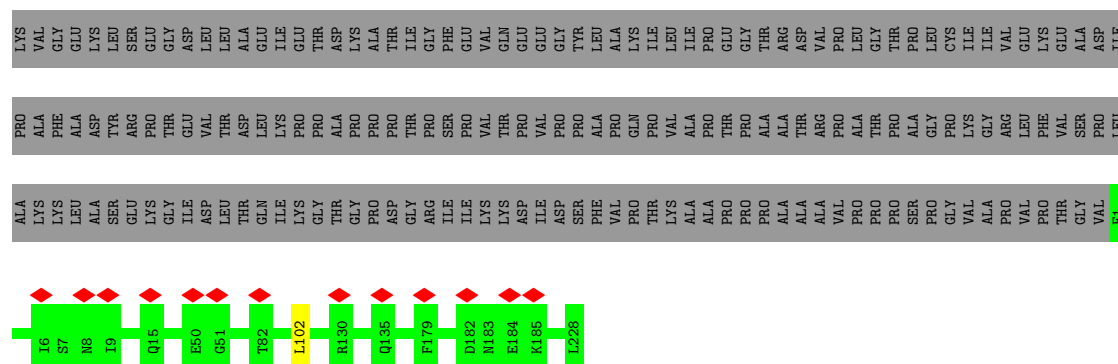


- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

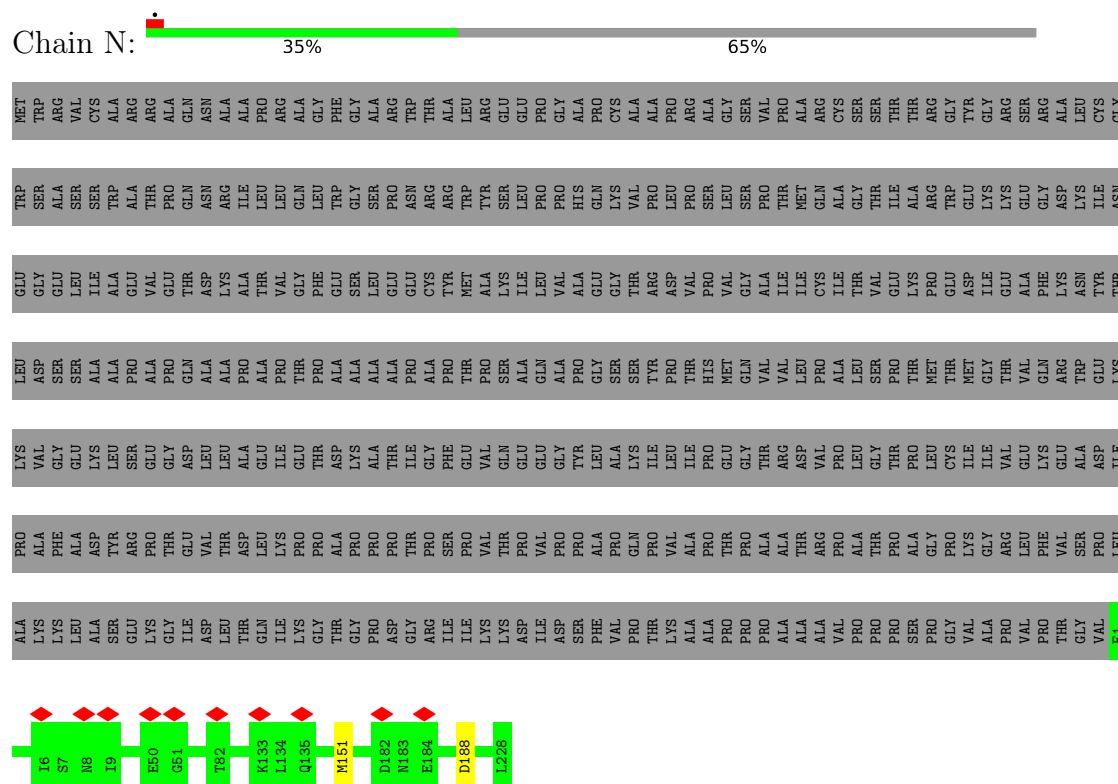


- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

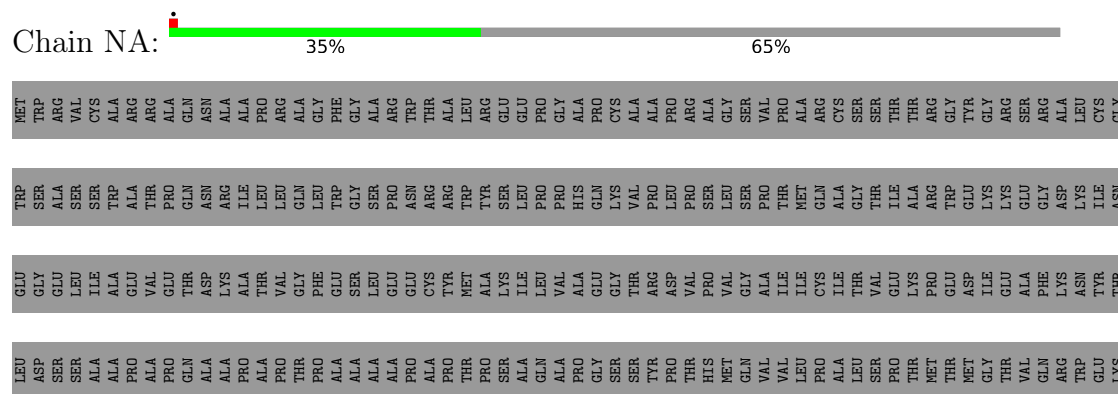


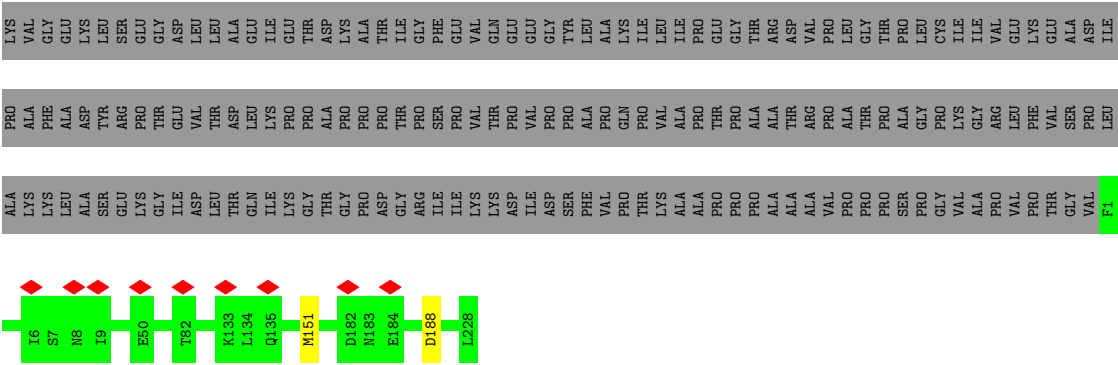


- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

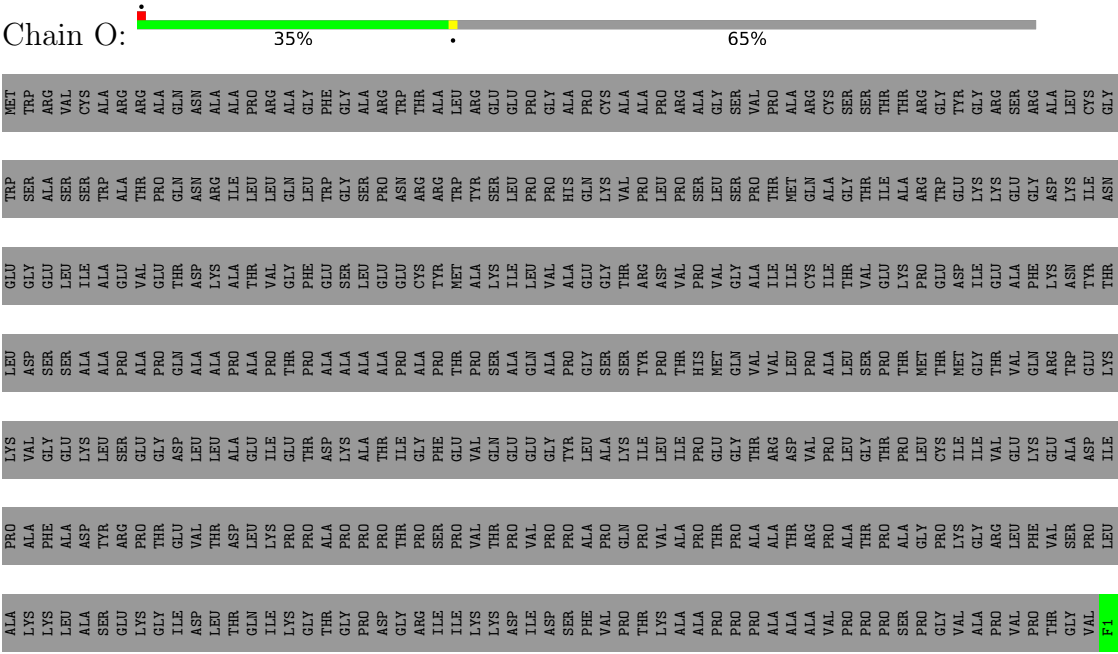


- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

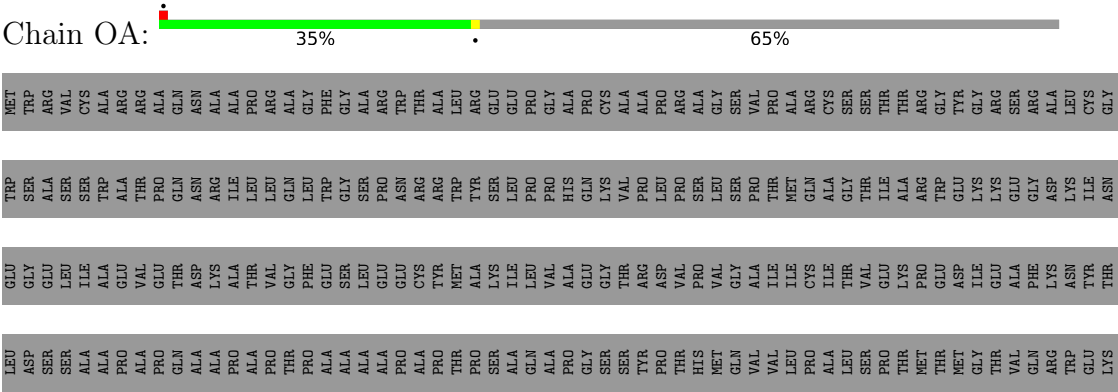




● Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

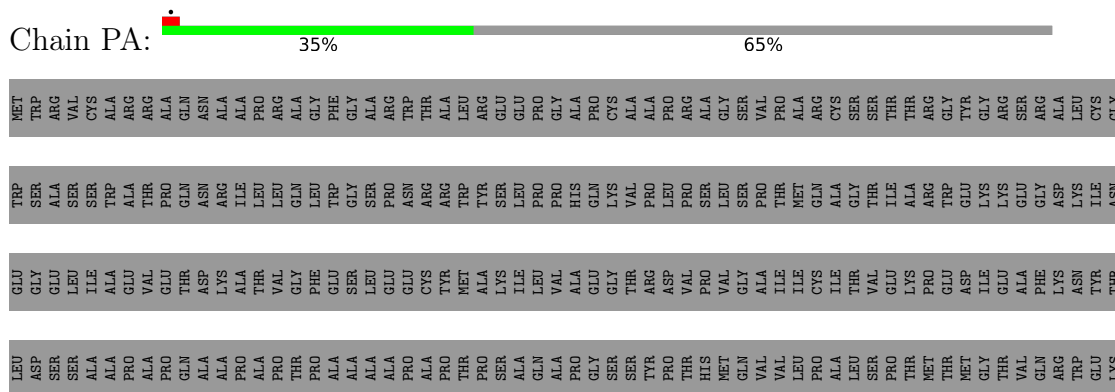


● Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



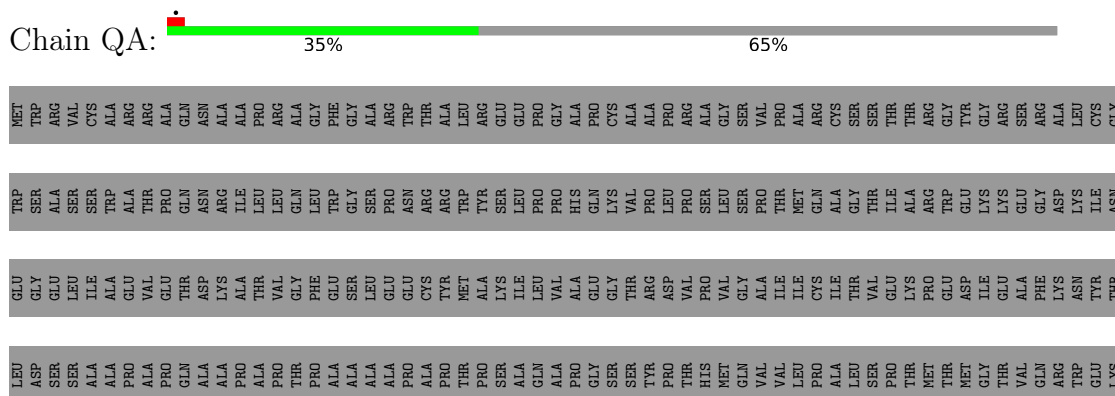
- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

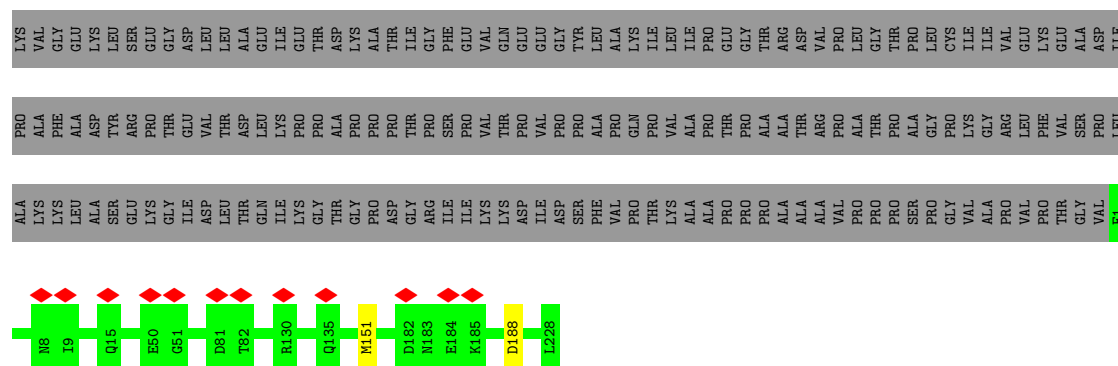
- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



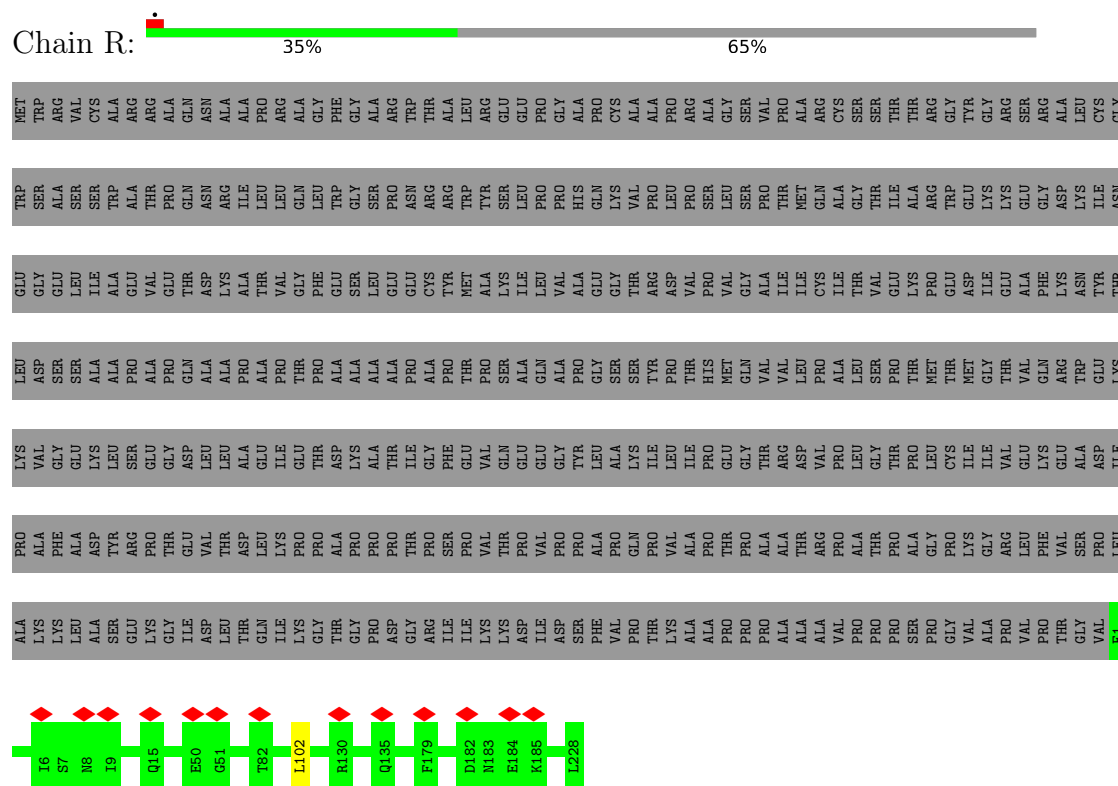
- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

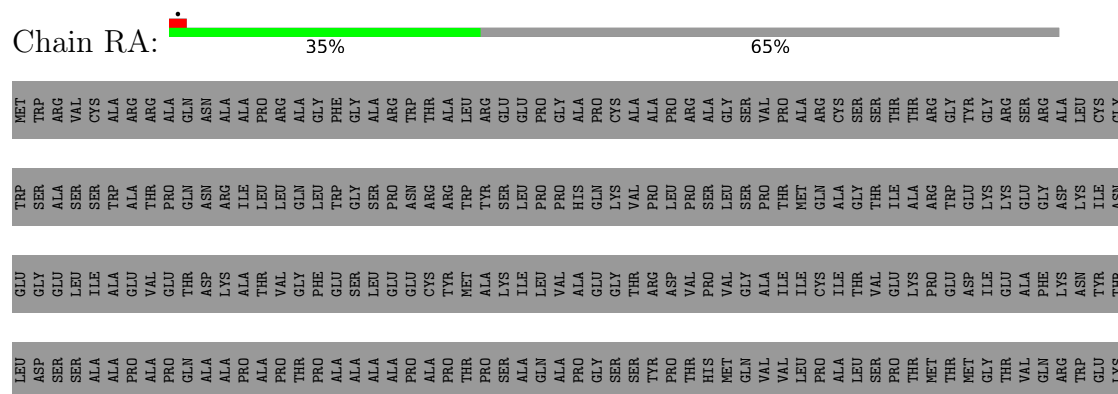




- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



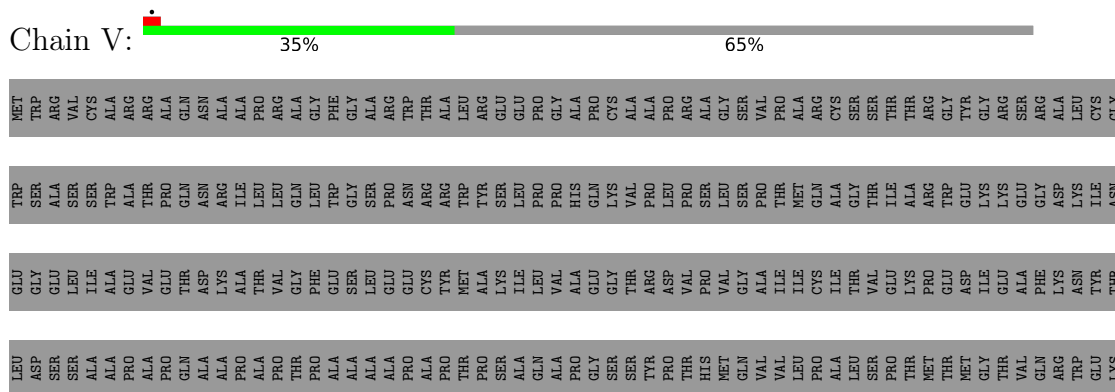


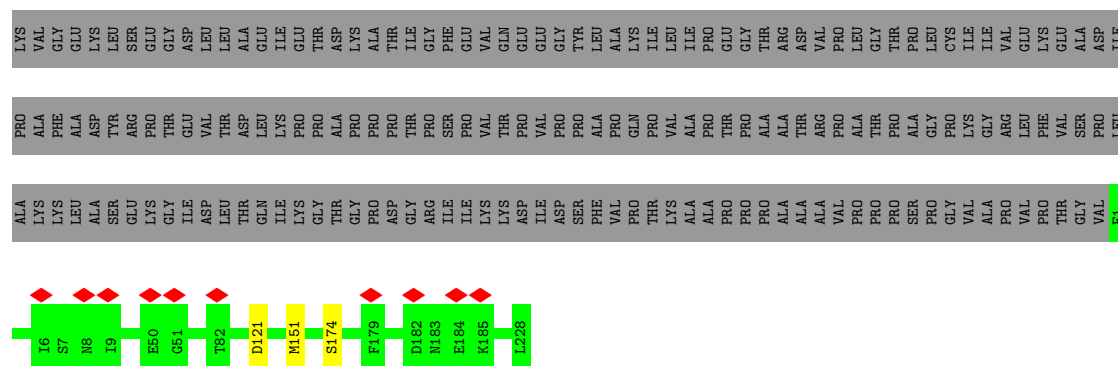




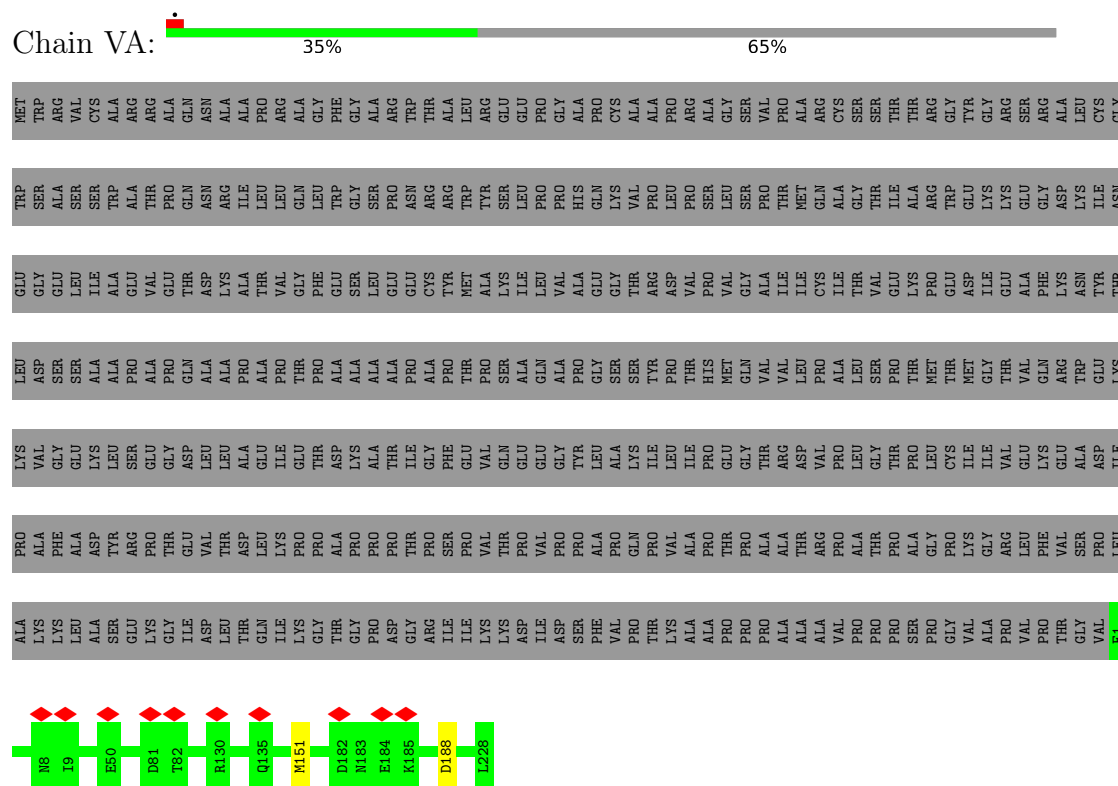
- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

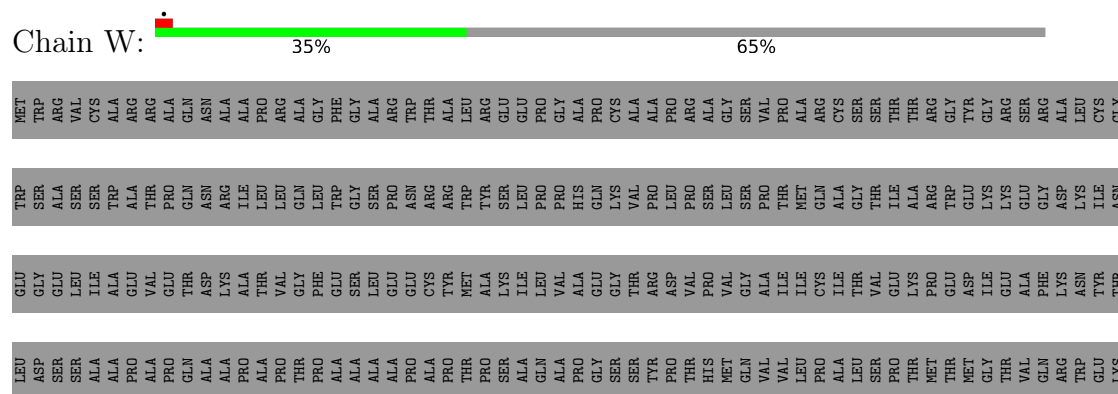




- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

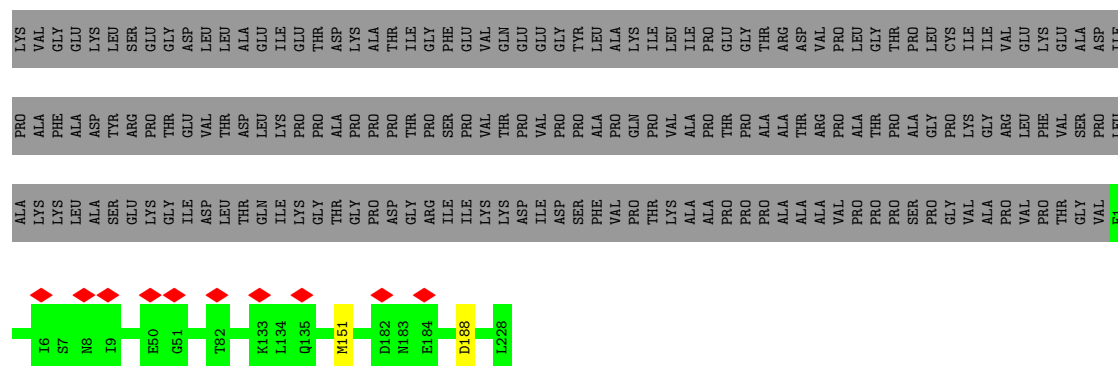


- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

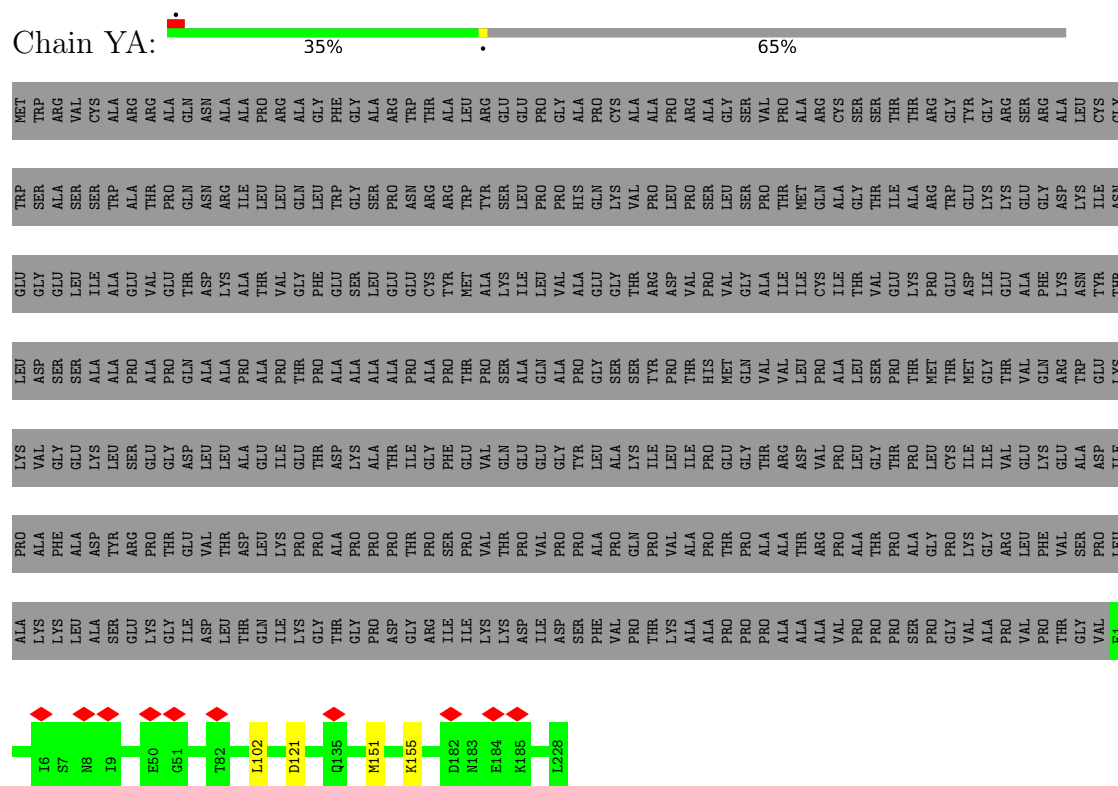




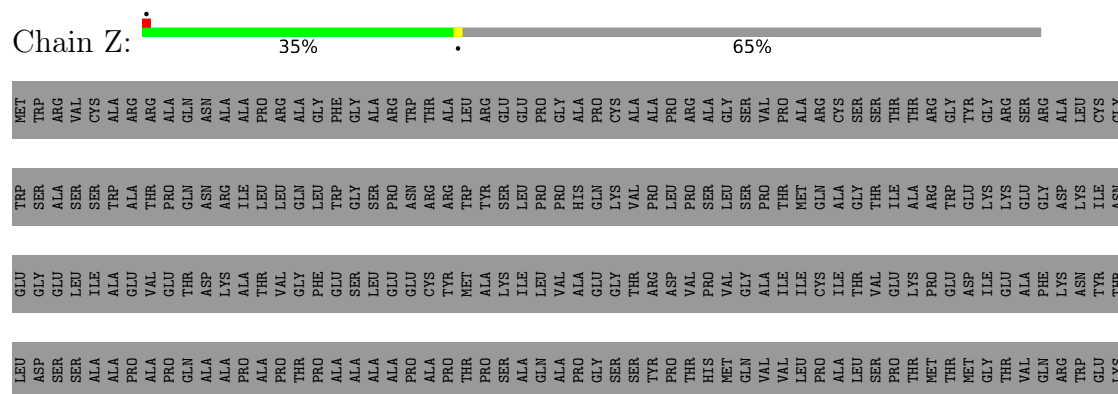




- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

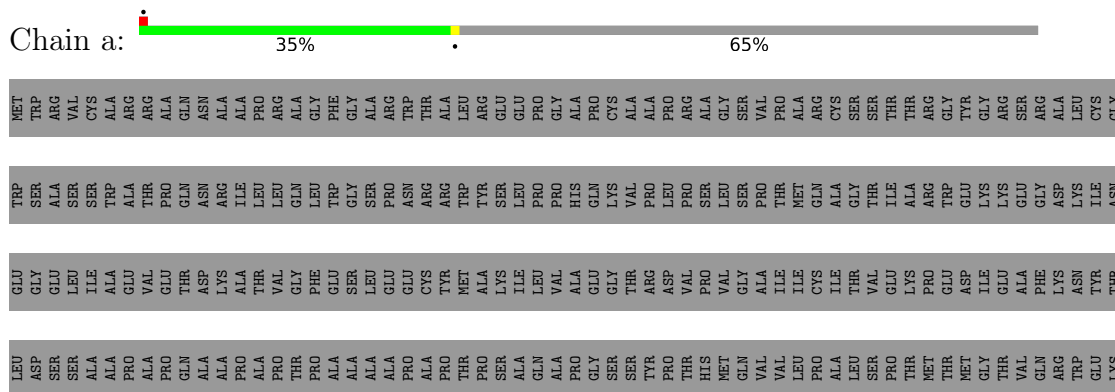


- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



ALA	LYS	LYS	LEU	ALA	SER	GLU	LYS	ILE	ASP	LEU	THR	GLN	ILE	LYS	GLY	THR	PRO	ASP	GLY	ILE	ILE	GLY	VAL	LYS	ASP	ILE	SER	PHE	VAL	PRO	PRO	THR	PRO	ALA	ALA	ALA	VAL	VAL	PRO	PRO	THR	GLY	VAL	VAL	PRO	THR	GLY	VAL	PRO	GLY	F1
PRO	ALA	PHE	ALA	ASP	TYR	ARG	PRO	THR	GLU	VAL	THR	ASP	LEU	LYS	PRO	PRO	PRO	THR	THR	PRO	PRO	VAL	THR	PRO	GLN	PRO	PRO	VAL	THR	VAL	PRO	ALA	ALA	THR	ARG	PRO	ALA	THR	PRO	GLY	PRO	LYS	GLY	ALA	THR	SER	PRO	LEU			
LYS	VAL	GLY	LYS	LEU	SER	GLY	GLY	ILE	ASP	LEU	THR	ASP	LEU	LYS	PRO	PRO	PRO	THR	THR	PRO	PRO	VAL	THR	PRO	GLN	PRO	PRO	VAL	THR	VAL	PRO	ALA	ALA	THR	ARG	PRO	ALA	THR	PRO	GLY	PRO	LYS	GLY	ALA	THR	SER	PRO	LEU			





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68914	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	52	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.424	Depositor
Minimum map value	-1.451	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.34	Depositor
Map size ( $\text{\AA}$ )	614.4, 614.4, 614.4	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.2, 1.2, 1.2	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.25	0/1788	0.46	0/2422
1	AA	0.26	0/1788	0.47	0/2422
1	AB	0.26	0/1788	0.48	0/2422
1	B	0.26	0/1788	0.48	0/2422
1	BA	0.26	0/1788	0.47	0/2422
1	BB	0.26	0/1788	0.48	0/2422
1	C	0.26	0/1788	0.48	0/2422
1	CA	0.26	0/1788	0.48	0/2422
1	CB	0.26	0/1788	0.47	0/2422
1	D	0.25	0/1788	0.47	0/2422
1	DA	0.25	0/1788	0.48	0/2422
1	DB	0.26	0/1788	0.46	0/2422
1	E	0.26	0/1788	0.46	0/2422
1	EA	0.26	0/1788	0.46	0/2422
1	EB	0.25	0/1788	0.47	0/2422
1	F	0.26	0/1788	0.47	0/2422
1	FA	0.25	0/1788	0.47	0/2422
1	FB	0.26	0/1788	0.47	0/2422
1	G	0.26	0/1788	0.47	0/2422
1	GA	0.26	0/1788	0.47	0/2422
1	GB	0.26	0/1788	0.48	0/2422
1	H	0.26	0/1788	0.48	0/2422
1	HA	0.26	0/1788	0.48	0/2422
1	HB	0.25	0/1788	0.47	0/2422
1	I	0.26	0/1788	0.47	0/2422
1	IA	0.26	0/1788	0.47	0/2422
1	J	0.26	0/1788	0.46	0/2422
1	JA	0.26	0/1788	0.46	0/2422
1	K	0.26	0/1788	0.47	0/2422
1	KA	0.25	0/1788	0.46	0/2422
1	L	0.25	0/1788	0.46	0/2422
1	LA	0.26	0/1788	0.48	0/2422
1	M	0.26	0/1788	0.48	0/2422
1	MA	0.26	0/1788	0.48	0/2422

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	N	0.25	0/1788	0.49	0/2422
1	NA	0.26	0/1788	0.47	0/2422
1	O	0.26	0/1788	0.46	0/2422
1	OA	0.26	0/1788	0.46	0/2422
1	P	0.26	0/1788	0.47	0/2422
1	PA	0.26	0/1788	0.47	0/2422
1	Q	0.26	0/1788	0.48	0/2422
1	QA	0.26	0/1788	0.47	0/2422
1	R	0.26	0/1788	0.48	0/2422
1	RA	0.26	0/1788	0.49	0/2422
1	S	0.25	0/1788	0.47	0/2422
1	SA	0.25	0/1788	0.48	0/2422
1	T	0.26	0/1788	0.46	0/2422
1	TA	0.26	0/1788	0.46	0/2422
1	UA	0.26	0/1788	0.47	0/2422
1	V	0.25	0/1788	0.47	0/2422
1	VA	0.26	0/1788	0.48	0/2422
1	W	0.26	0/1788	0.48	0/2422
1	WA	0.26	0/1788	0.48	0/2422
1	X	0.26	0/1788	0.48	0/2422
1	XA	0.26	0/1788	0.49	0/2422
1	Y	0.26	0/1788	0.49	0/2422
1	YA	0.26	0/1788	0.46	0/2422
1	Z	0.26	0/1788	0.47	0/2422
1	ZA	0.25	0/1788	0.46	0/2422
1	a	0.26	0/1788	0.46	0/2422
All	All	0.26	0/107280	0.47	0/145320

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	A	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	AA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	AB	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	B	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	BA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	BB	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	C	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	CA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	CB	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	D	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	DA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	DB	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	E	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	EA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	EB	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	F	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	FA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	FB	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	G	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	GA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	GB	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	H	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	HA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	HB	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	I	226/647 (35%)	222 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	IA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	J	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	JA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	K	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	KA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	L	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	LA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	M	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	MA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	N	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	NA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	O	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	OA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	P	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	PA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	Q	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	QA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	R	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	RA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	S	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	SA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	T	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	TA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	UA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	V	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	VA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	W	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	WA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	X	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	XA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	Y	226/647 (35%)	222 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	YA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	Z	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	ZA	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
1	a	226/647 (35%)	222 (98%)	4 (2%)	0	100	100
All	All	13560/38820 (35%)	13320 (98%)	240 (2%)	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	A	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	AA	195/526 (37%)	192 (98%)	3 (2%)	60	81
1	AB	195/526 (37%)	194 (100%)	1 (0%)	86	93
1	B	195/526 (37%)	194 (100%)	1 (0%)	86	93
1	BA	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	BB	195/526 (37%)	194 (100%)	1 (0%)	86	93
1	C	195/526 (37%)	194 (100%)	1 (0%)	86	93
1	CA	195/526 (37%)	194 (100%)	1 (0%)	86	93
1	CB	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	D	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	DA	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	DB	195/526 (37%)	191 (98%)	4 (2%)	48	74
1	E	195/526 (37%)	191 (98%)	4 (2%)	48	74
1	EA	195/526 (37%)	191 (98%)	4 (2%)	48	74
1	EB	195/526 (37%)	192 (98%)	3 (2%)	60	81
1	F	195/526 (37%)	192 (98%)	3 (2%)	60	81
1	FA	195/526 (37%)	193 (99%)	2 (1%)	73	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FB	195/526 (37%)	194 (100%)	1 (0%)	86	93
1	G	195/526 (37%)	194 (100%)	1 (0%)	86	93
1	GA	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	GB	195/526 (37%)	194 (100%)	1 (0%)	86	93
1	H	195/526 (37%)	194 (100%)	1 (0%)	86	93
1	HA	195/526 (37%)	194 (100%)	1 (0%)	86	93
1	HB	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	I	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	IA	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	J	195/526 (37%)	191 (98%)	4 (2%)	48	74
1	JA	195/526 (37%)	191 (98%)	4 (2%)	48	74
1	K	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	KA	195/526 (37%)	192 (98%)	3 (2%)	60	81
1	L	195/526 (37%)	194 (100%)	1 (0%)	86	93
1	LA	195/526 (37%)	194 (100%)	1 (0%)	86	93
1	M	195/526 (37%)	194 (100%)	1 (0%)	86	93
1	MA	195/526 (37%)	194 (100%)	1 (0%)	86	93
1	N	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	NA	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	O	195/526 (37%)	191 (98%)	4 (2%)	48	74
1	OA	195/526 (37%)	191 (98%)	4 (2%)	48	74
1	P	195/526 (37%)	192 (98%)	3 (2%)	60	81
1	PA	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	Q	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	QA	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	R	195/526 (37%)	194 (100%)	1 (0%)	86	93
1	RA	195/526 (37%)	194 (100%)	1 (0%)	86	93
1	S	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	SA	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	T	195/526 (37%)	191 (98%)	4 (2%)	48	74
1	TA	195/526 (37%)	191 (98%)	4 (2%)	48	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	UA	195/526 (37%)	192 (98%)	3 (2%)	60	81
1	V	195/526 (37%)	192 (98%)	3 (2%)	60	81
1	VA	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	W	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	WA	195/526 (37%)	194 (100%)	1 (0%)	86	93
1	X	195/526 (37%)	194 (100%)	1 (0%)	86	93
1	XA	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	Y	195/526 (37%)	193 (99%)	2 (1%)	73	87
1	YA	195/526 (37%)	191 (98%)	4 (2%)	48	74
1	Z	195/526 (37%)	191 (98%)	4 (2%)	48	74
1	ZA	195/526 (37%)	192 (98%)	3 (2%)	60	81
1	a	195/526 (37%)	191 (98%)	4 (2%)	48	74
All	All	11700/31560 (37%)	11566 (99%)	134 (1%)	69	86

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	XA	151	MET
1	YA	102	LEU
1	a	102	LEU
1	I	188	ASP
1	I	151	MET

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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

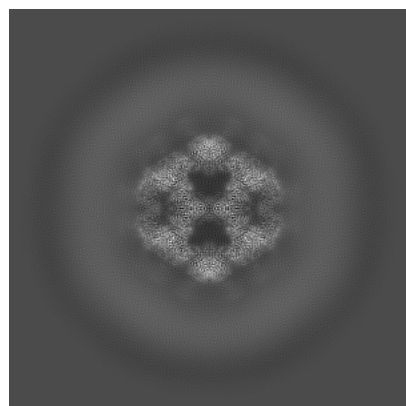
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61080. These allow visual inspection of the internal detail of the map and identification of artifacts.

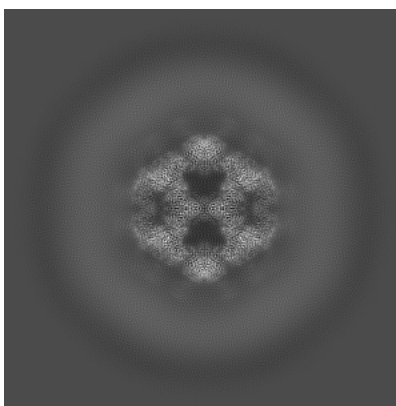
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

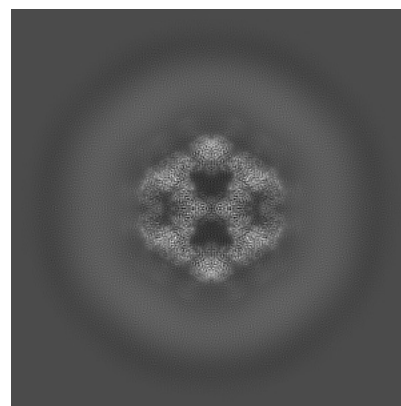
#### 6.1.1 Primary map



X

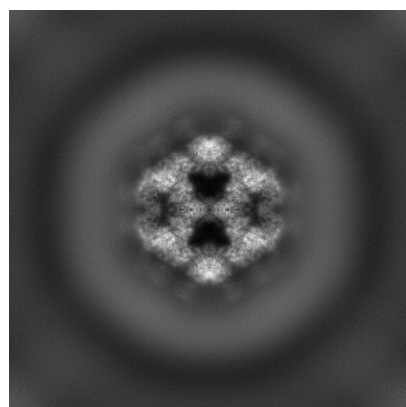


Y

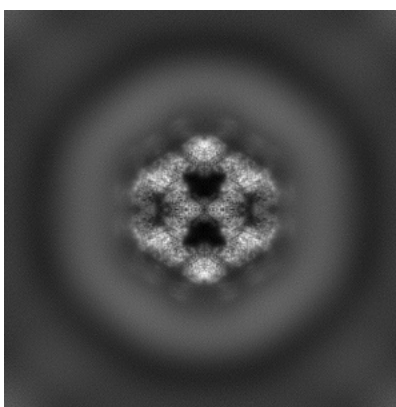


Z

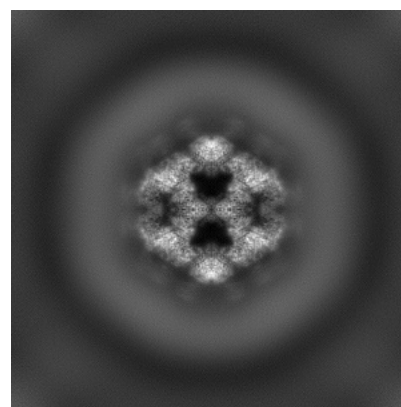
#### 6.1.2 Raw map



X



Y

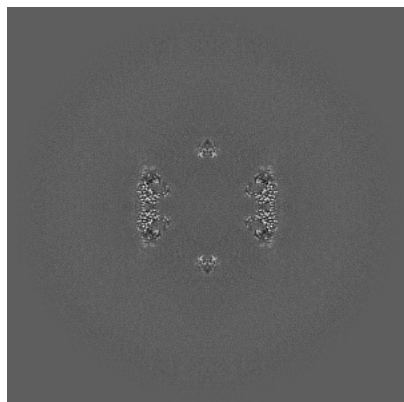


Z

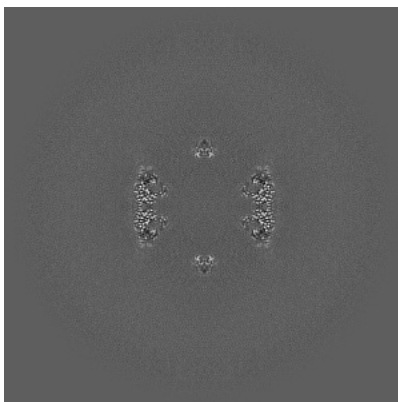
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

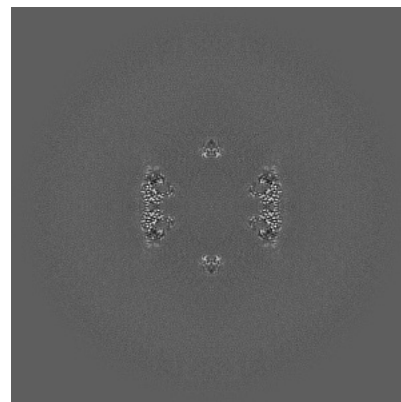
### 6.2.1 Primary map



X Index: 256

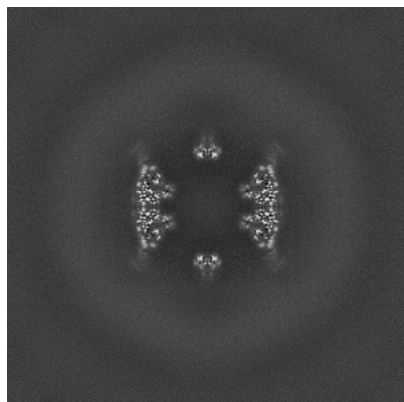


Y Index: 256

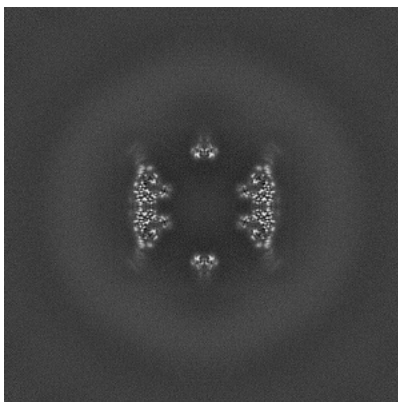


Z Index: 256

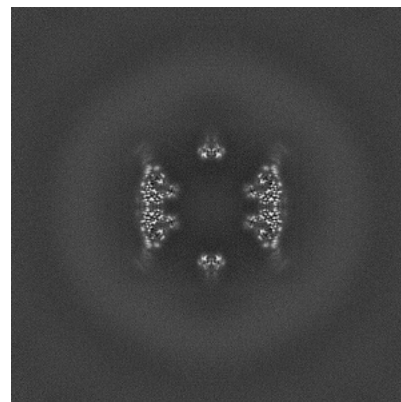
### 6.2.2 Raw map



X Index: 256



Y Index: 256

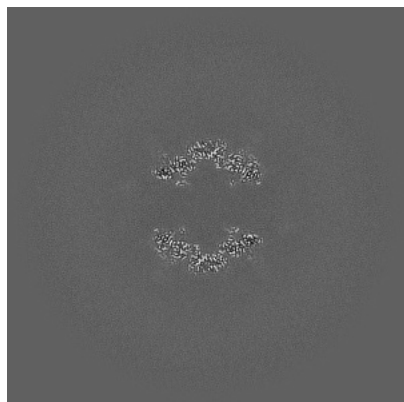


Z Index: 256

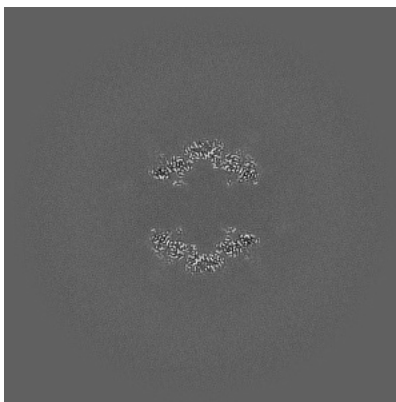
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

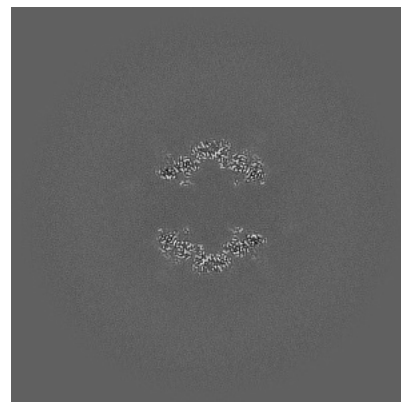
### 6.3.1 Primary map



X Index: 294

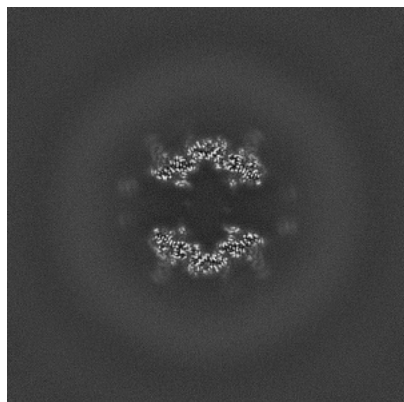


Y Index: 294

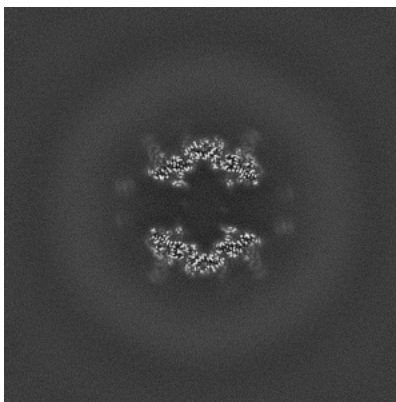


Z Index: 294

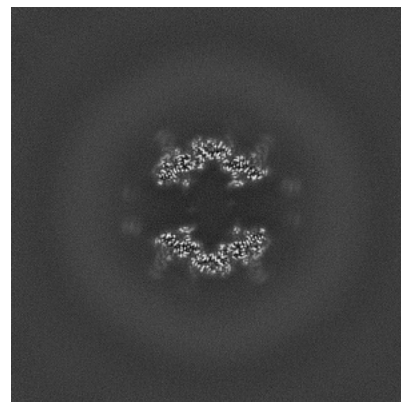
### 6.3.2 Raw map



X Index: 294



Y Index: 294

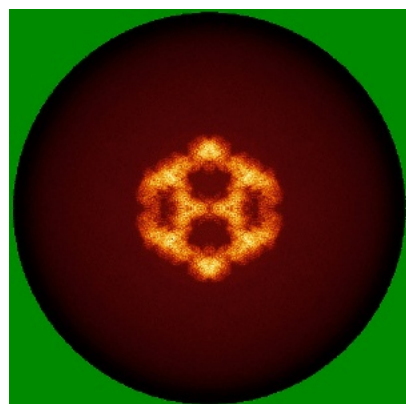


Z Index: 218

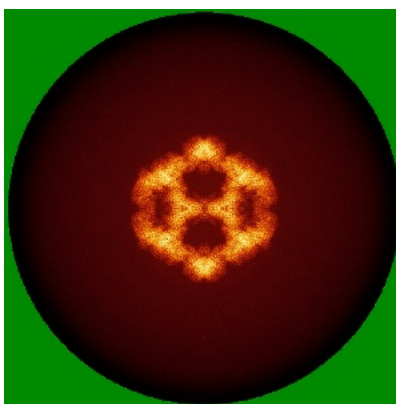
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

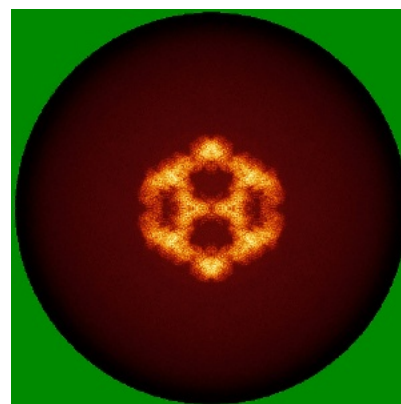
### 6.4.1 Primary map



X

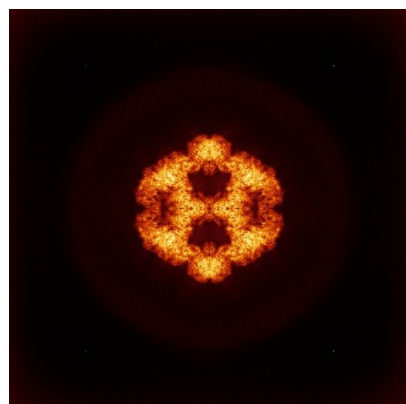


Y

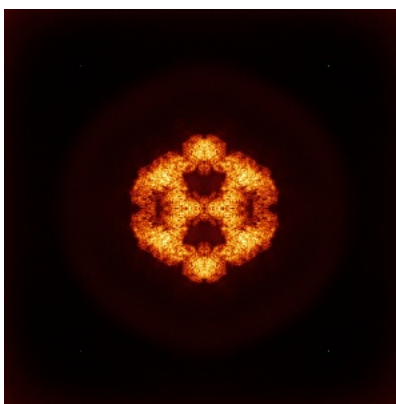


Z

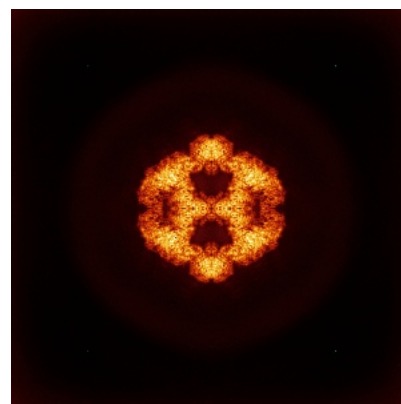
### 6.4.2 Raw map



X



Y

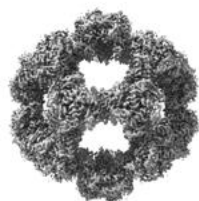


Z

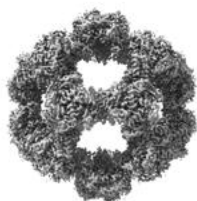
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

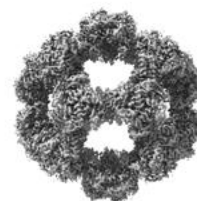
### 6.5.1 Primary map



X



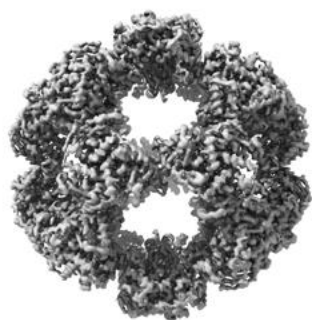
Y



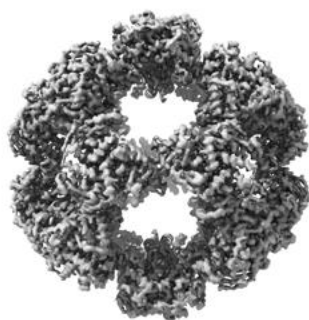
Z

The images above show the 3D surface view of the map at the recommended contour level 0.34. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

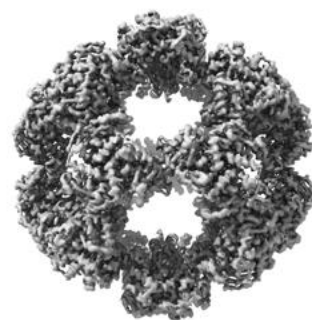
### 6.5.2 Raw map



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.

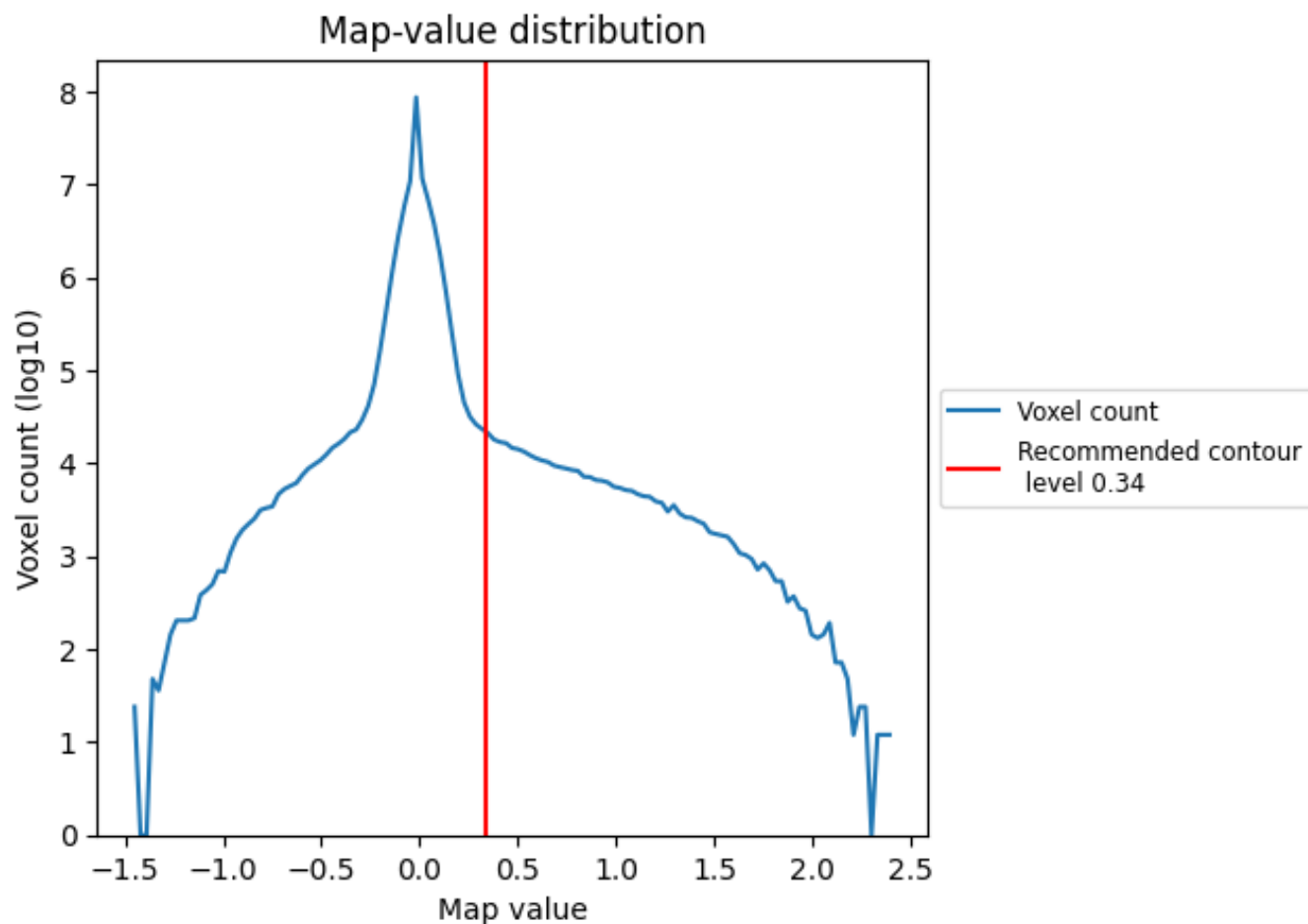
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

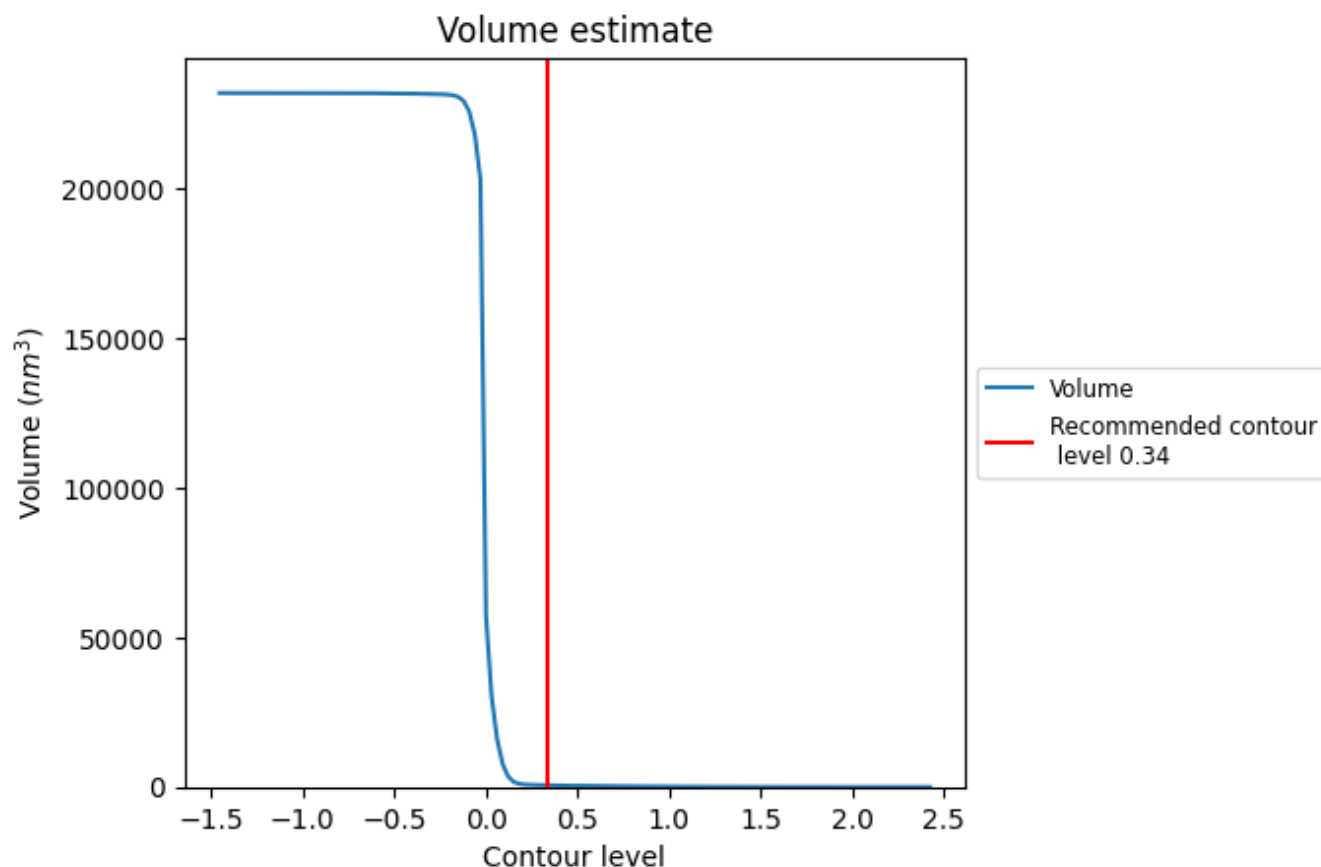
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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 [i](#)

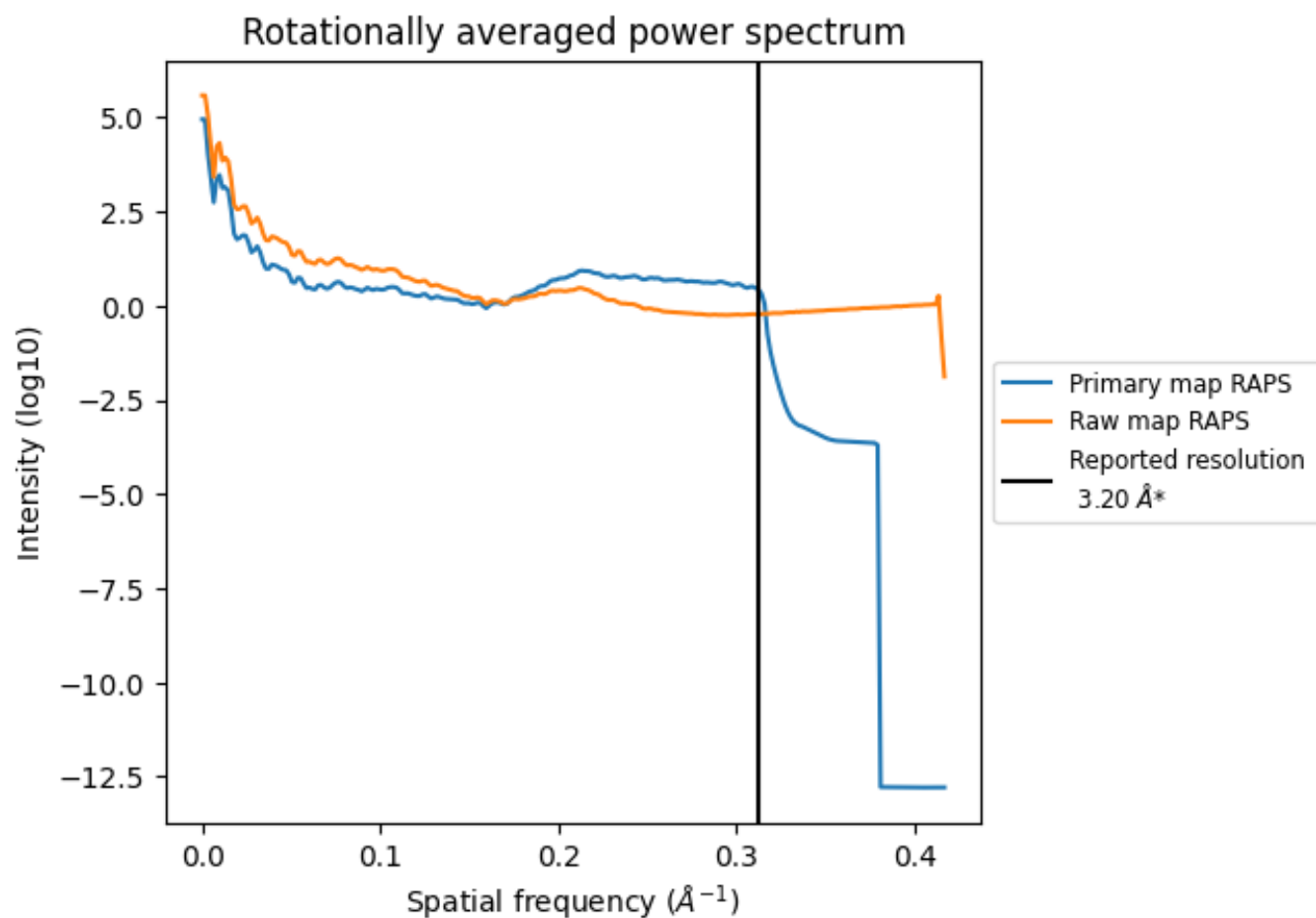


The volume at the recommended contour level is 558 nm<sup>3</sup>; this corresponds to an approximate mass of 504 kDa.

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 ⓘ

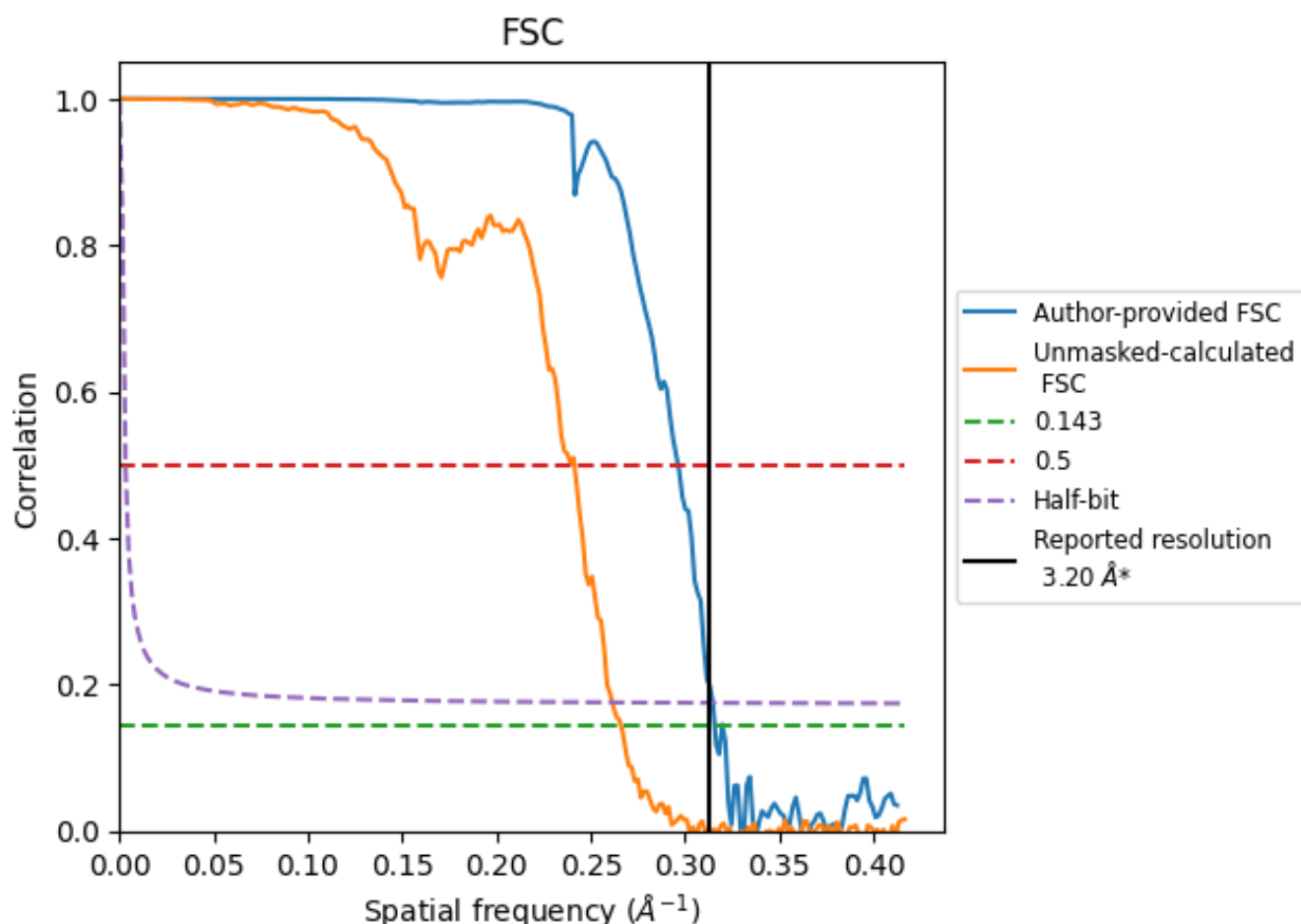


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.312 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

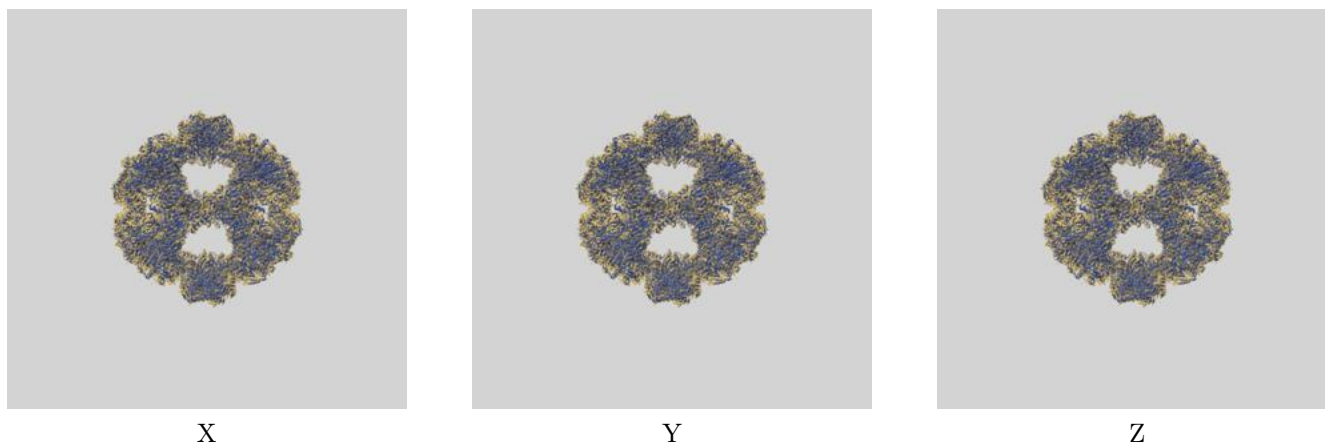
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.17	3.37	3.18
Unmasked-calculated*	3.76	4.14	3.82

\*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 3.76 differs from the reported value 3.2 by more than 10 %

## 9 Map-model fit [i](#)

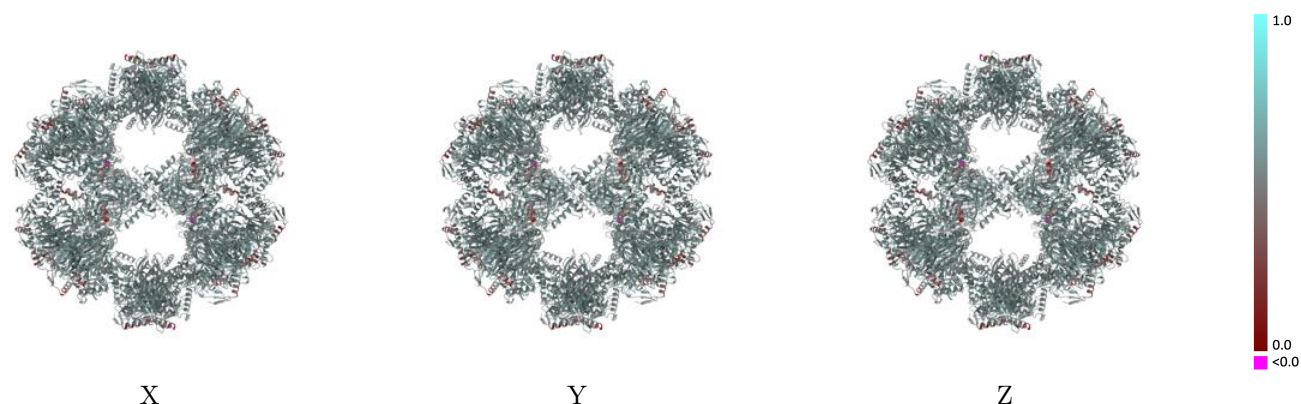
This section contains information regarding the fit between EMDB map EMD-61080 and PDB model 9J1W. Per-residue inclusion information can be found in section [3](#) on page [10](#).

### 9.1 Map-model overlay [i](#)



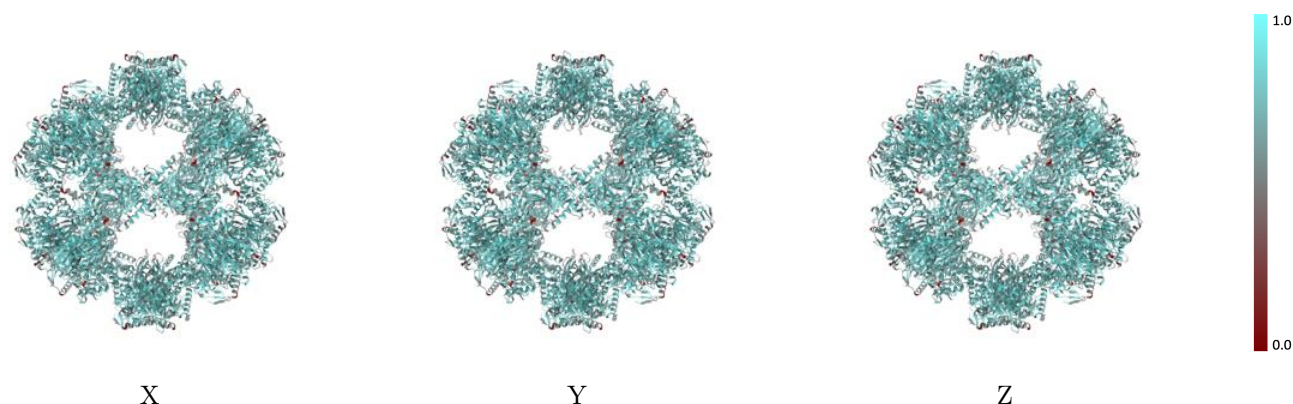
The images above show the 3D surface view of the map at the recommended contour level 0.34 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



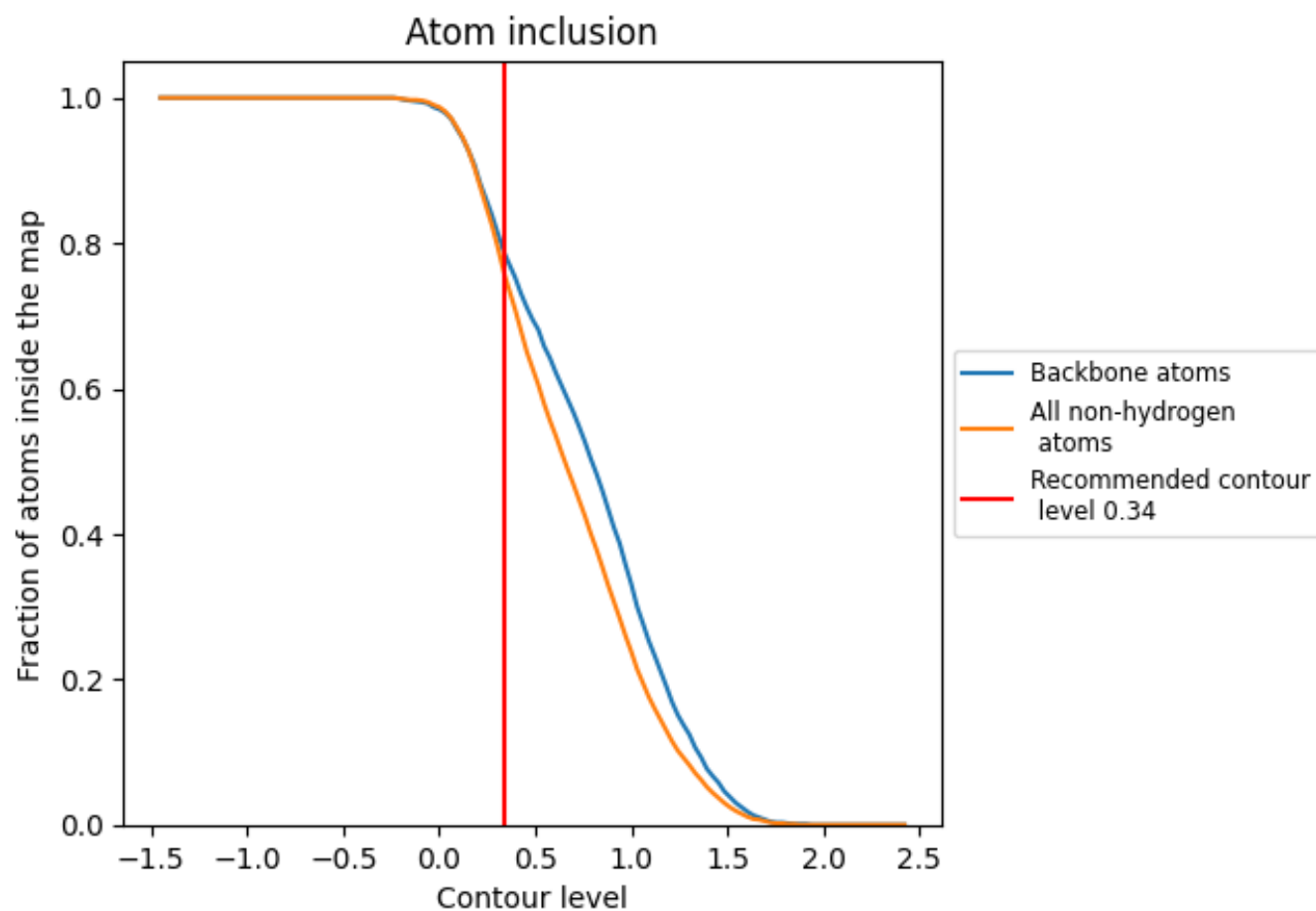
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [i](#)



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 (0.34).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 76% 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 (0.34) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7570	 0.5430
A	 0.7550	 0.5400
AA	 0.7590	 0.5420
AB	 0.7600	 0.5430
B	 0.7600	 0.5460
BA	 0.7590	 0.5450
BB	 0.7570	 0.5420
C	 0.7580	 0.5430
CA	 0.7590	 0.5410
CB	 0.7510	 0.5460
D	 0.7520	 0.5440
DA	 0.7540	 0.5440
DB	 0.7610	 0.5410
E	 0.7610	 0.5420
EA	 0.7610	 0.5410
EB	 0.7560	 0.5420
F	 0.7570	 0.5440
FA	 0.7570	 0.5420
FB	 0.7570	 0.5470
G	 0.7590	 0.5440
GA	 0.7570	 0.5460
GB	 0.7580	 0.5410
H	 0.7560	 0.5410
HA	 0.7570	 0.5420
HB	 0.7520	 0.5450
I	 0.7510	 0.5440
IA	 0.7500	 0.5430
J	 0.7600	 0.5420
JA	 0.7610	 0.5410
K	 0.7590	 0.5420
KA	 0.7570	 0.5420
L	 0.7610	 0.5450
LA	 0.7600	 0.5450
M	 0.7570	 0.5420
MA	 0.7580	 0.5410



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Chain	Atom inclusion	Q-score
N	 0.7530	 0.5440
NA	 0.7510	 0.5420
O	 0.7610	 0.5430
OA	 0.7610	 0.5400
P	 0.7590	 0.5420
PA	 0.7570	 0.5430
Q	 0.7600	 0.5450
QA	 0.7570	 0.5440
R	 0.7580	 0.5440
RA	 0.7570	 0.5410
S	 0.7510	 0.5450
SA	 0.7530	 0.5430
T	 0.7610	 0.5430
TA	 0.7610	 0.5410
UA	 0.7580	 0.5410
V	 0.7570	 0.5410
VA	 0.7600	 0.5450
W	 0.7600	 0.5440
WA	 0.7580	 0.5420
X	 0.7580	 0.5400
XA	 0.7520	 0.5470
Y	 0.7510	 0.5440
YA	 0.7610	 0.5400
Z	 0.7600	 0.5440
ZA	 0.7570	 0.5410
a	 0.7610	 0.5440