



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:21 AM UTC

PDB ID : 8X03 / pdb_00008x03
EMDB ID : EMD-37969
Title : Structure of mitochondrial soluble protein
Authors : Zhang, S.S.; Chen, M.F.
Deposited on : 2023-11-03
Resolution : 3.66 Å (reported)

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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

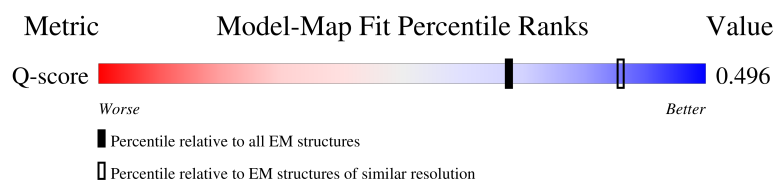
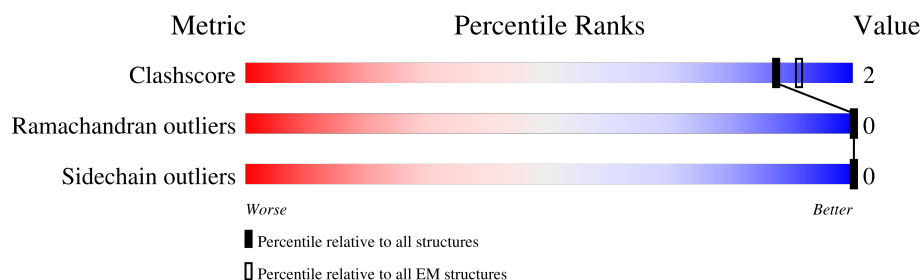
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.66 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.



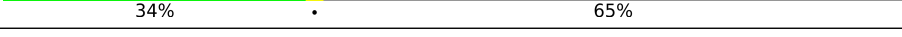
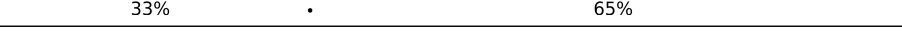
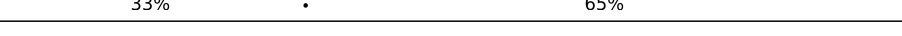
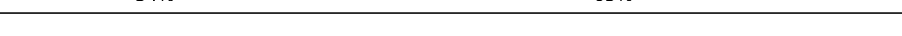
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11491 (3.16 - 4.16)

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 $\leq 5\%$. 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	0	647	
1	1	647	
1	2	647	
1	3	647	

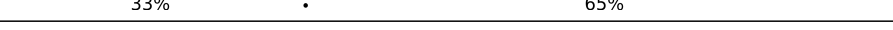
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Mol	Chain	Length	Quality of chain
1	4	647	
1	5	647	
1	6	647	
1	7	647	
1	A	647	
1	B	647	
1	C	647	
1	D	647	
1	E	647	
1	F	647	
1	G	647	
1	H	647	
1	I	647	
1	J	647	
1	K	647	
1	L	647	
1	M	647	
1	N	647	
1	O	647	
1	P	647	
1	Q	647	
1	R	647	
1	S	647	
1	T	647	
1	U	647	

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Mol	Chain	Length	Quality of chain
1	V	647	
1	W	647	
1	X	647	
1	Y	647	
1	Z	647	
1	a	647	
1	b	647	
1	c	647	
1	d	647	
1	e	647	
1	f	647	
1	g	647	
1	h	647	
1	i	647	
1	j	647	
1	k	647	
1	l	647	
1	m	647	
1	n	647	
1	o	647	
1	p	647	
1	q	647	
1	r	647	
1	s	647	
1	t	647	

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Mol	Chain	Length	Quality of chain
1	u	647	33% 65%
1	v	647	33% 65%
1	w	647	33% 65%
1	x	647	33% 65%
1	y	647	33% 65%
1	z	647	33% 65%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 105540 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	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	B	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	C	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	D	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	E	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	F	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	G	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	H	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	I	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	J	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	K	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	L	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	M	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	N	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	O	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	P	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	R	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	S	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	T	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	U	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	V	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	W	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	X	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	Y	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	Z	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	a	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	b	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	c	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	d	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	e	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	f	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	g	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	h	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	i	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	j	229	Total 1759	C 1121	N 304	O 324	S 10	0	0
1	k	229	Total 1759	C 1121	N 304	O 324	S 10	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	l	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	m	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	n	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	o	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	p	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	q	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	r	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	s	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	t	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	u	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	v	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	w	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	x	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	y	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	z	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	0	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	1	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	2	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	3	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	4	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	5	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		

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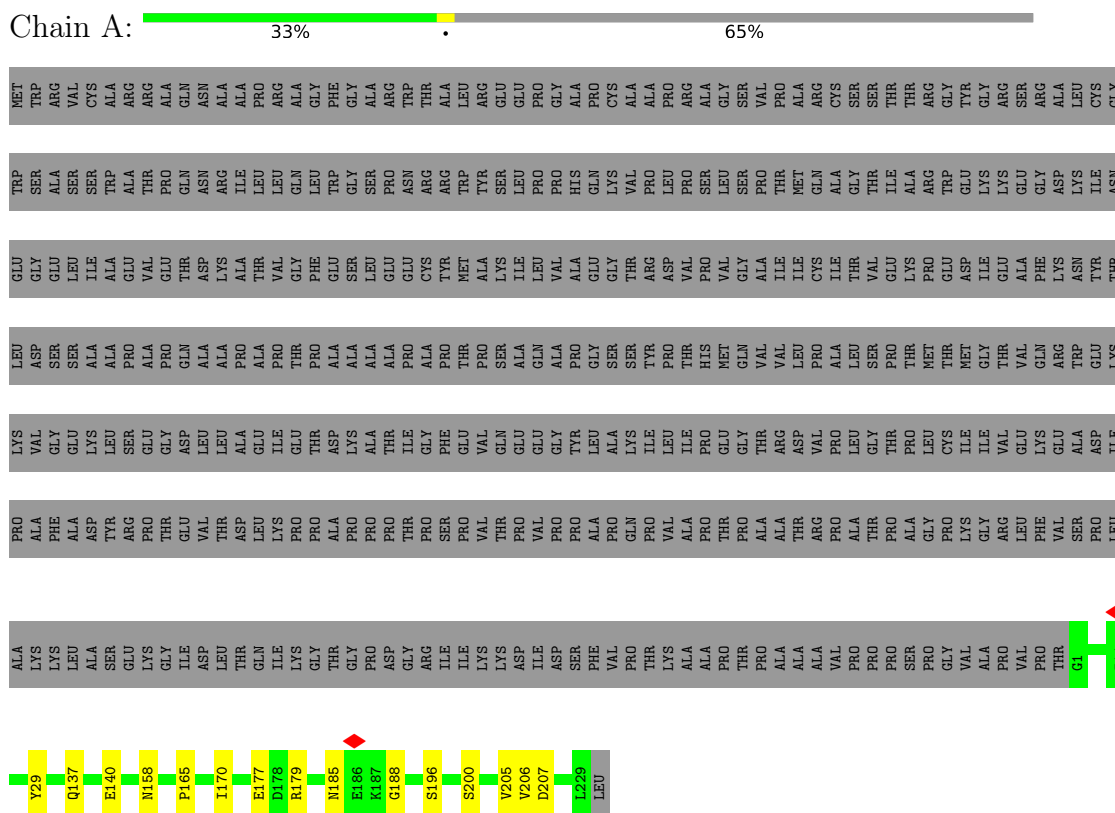
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	6	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		
1	7	229	Total	C	N	O	S	0	0
			1759	1121	304	324	10		

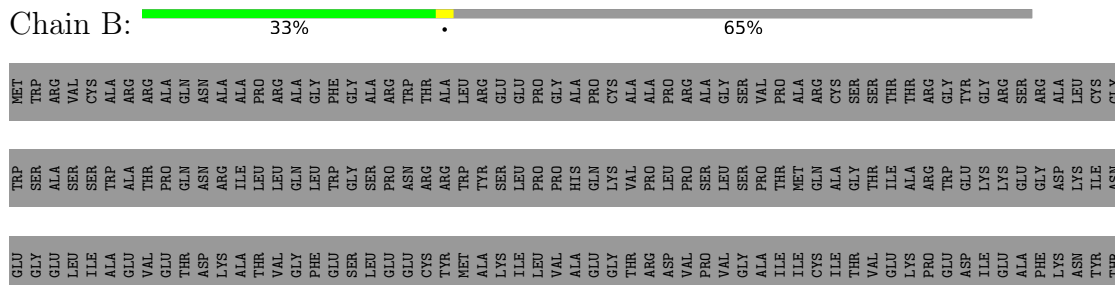
3 Residue-property plots

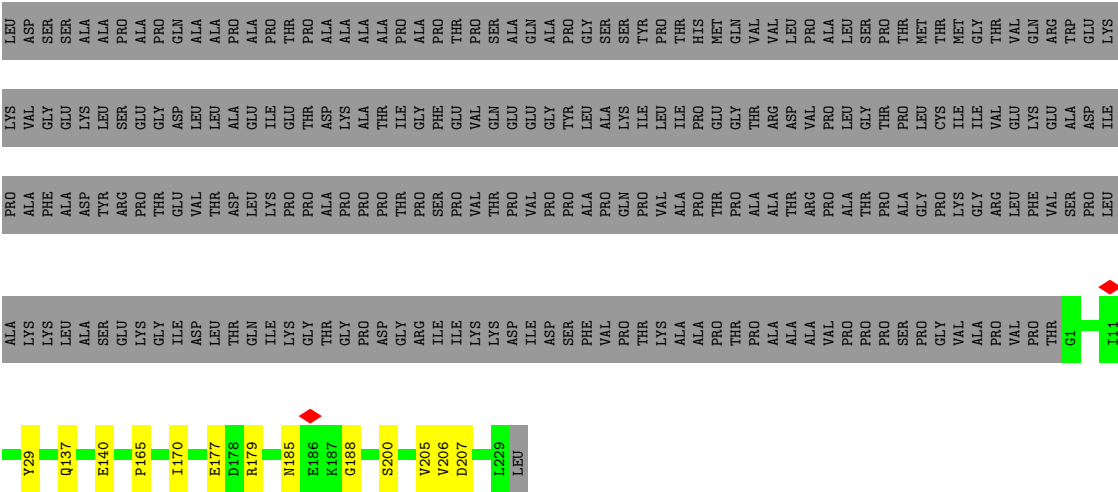
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Acetyltransferase component of pyruvate dehydrogenase complex

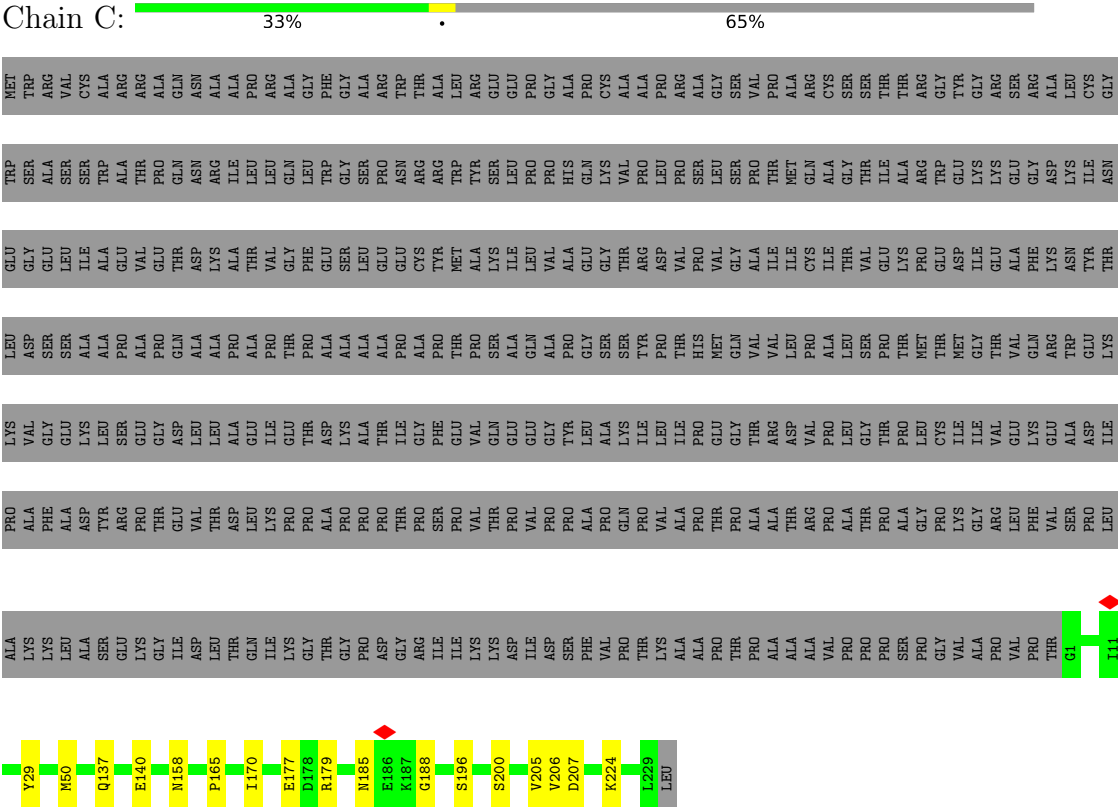


- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

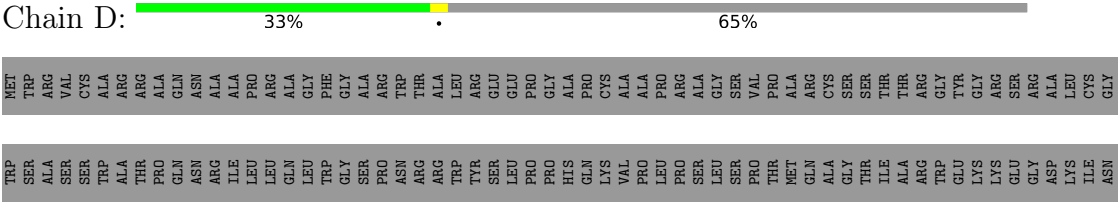




• Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

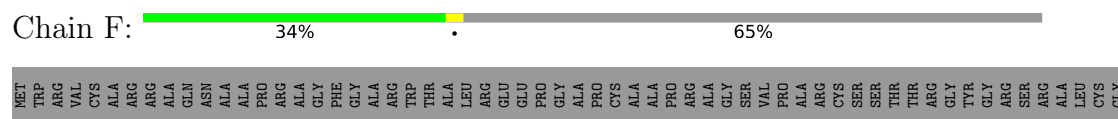


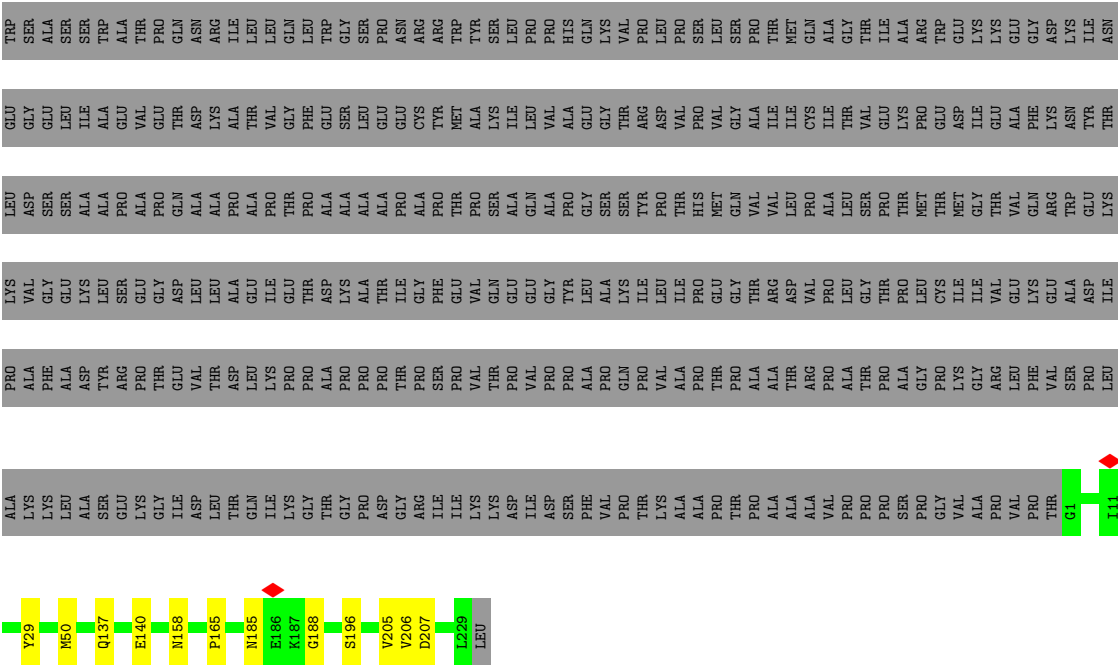
• Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



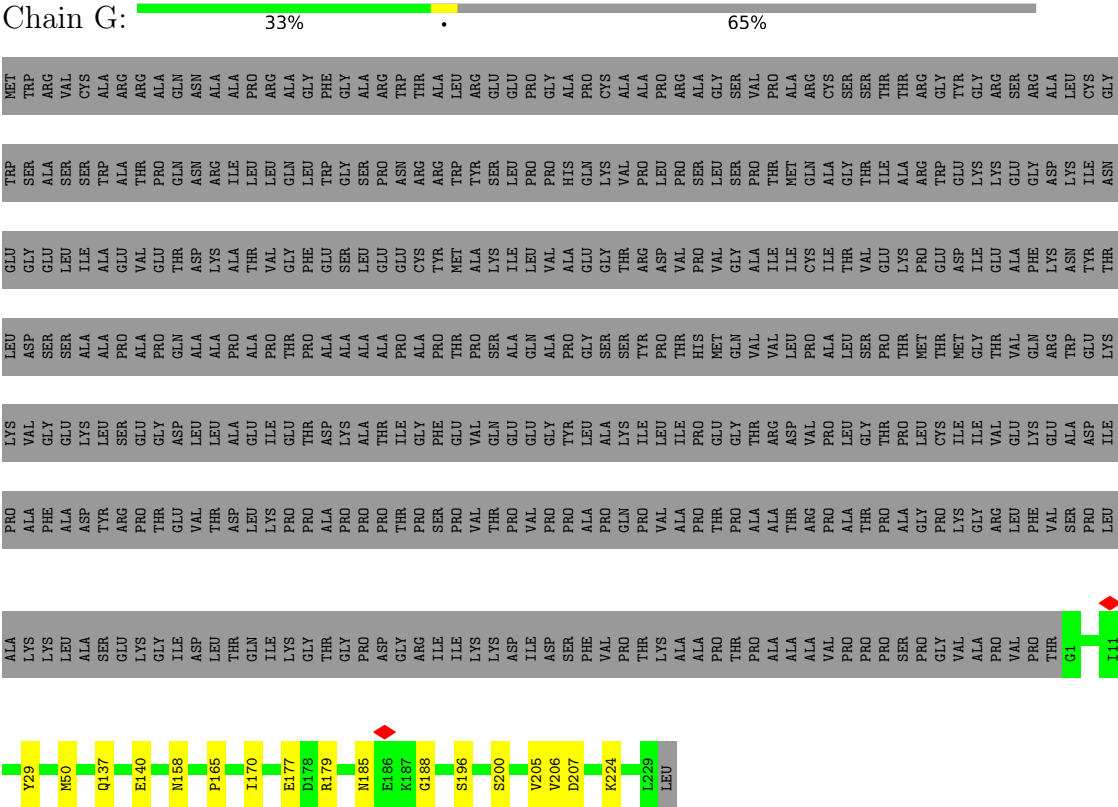
- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex





● Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

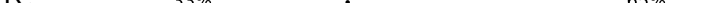


● Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



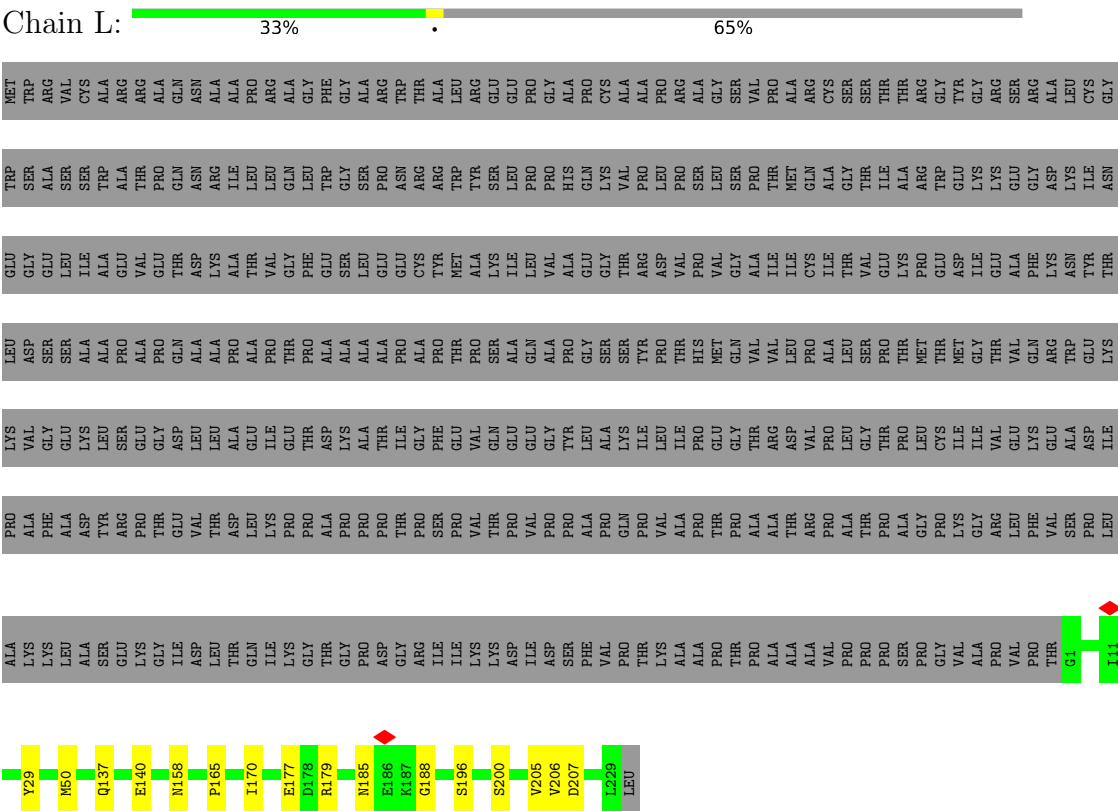
- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

		ALA	PRO	LYS	LEU	TRP	GLY	ASP	LEU	TRP	MET
	Y29	LYS	ALA	VAL	ASP	SER	GLY	SER	ASP	SER	TRP
	Q137	LEU	PHE	GLY	SER	GLY	GLY	LEU	SER	ALA	ARG
	E140	ALA	ASP	LYS	ALA	LEU	LYS	ALA	ILE	SER	CYS
	T147	SER	TYR	SER	PRO	GLU	SER	PRO	ALA	TRP	ALA
	N158	GLY	PRO	GLY	ALA	VAL	GLY	PRO	VAL	THR	ARG
	P165	ILE	GLU	ASP	GLN	THR	GLU	GLN	THR	GLN	ALA
	I170	ASP	VAL	LEU	ALA	ASP	ASP	ASN	ASN	ASN	ASN
	E177	LEU	THR	LEU	ALA	LYS	LEU	LYS	ARG	ARG	ALA
	D178	THR	LEU	ALA	ASP	THR	THR	THR	THR	THR	ALA
	R179	GLY	ALA	ASP	ALA	GLY	GLY	PHE	GLY	GLY	GLY
	N185	THR	PRO	LYS	ALA	LEU	LYS	SER	GLY	GLY	PHE
	E186	ILE	PRO	ALA	ALA	LEU	ALA	ALA	LEU	SER	ALA
	K187	ASP	PRO	THR	ALA	GLU	PRO	GLU	PRO	ARG	TRP
	G188	ARG	PRO	ILE	ALA	PRO	GLY	ALA	ASN	ARG	THR
	S196	ILE	SER	PHE	PRO	THR	PHE	PRO	CYS	ARG	ALA
	S200	ILE	PRO	GLU	ALA	THR	GLU	LEU	LEU	LEU	LEU
	V205	ASP	VAL	GLY	GLN	VAL	GLY	GLN	PRO	PRO	PRO
	V206	ILE	VAL	GLY	ALA	VAL	ILE	ALA	ALA	ALA	GLY
	D207	SER	PRO	TYR	PRO	PRO	PRO	THR	VAL	THR	ARG
	L209	PHE	ALA	LEU	ALA	ALA	LEU	GLY	PRO	SER	GLY
	L209	VAL	PRO	GLU	GLY	THR	GLU	VAL	VAL	SER	GLY
	LEU	THR	PRO	THR	GLY	ALA	THR	GLN	ALA	VAL	VAL
		ALA	ALA	ARG	VAL	VAL	ASP	VAL	ILE	THR	PRO
		ALA	THR	ASP	LEU	ILE	ILE	LEU	ILE	MET	ALA
		VAL	PRO	PRO	PRO	ILE	PRO	ALA	THR	CYS	ARG
		PRO	ALA	LEU	LEU	ALA	LEU	LEU	GLY	ALA	CYS
		PRO	THR	GLY	SER	THR	SER	VAL	THR	SER	SER
		PRO	PRO	THR	PRO	GLY	THR	PRO	ILE	THR	THR
		SER	ALA	PRO	THR	ALA	PRO	THR	LYS	ALA	THR
		PRO	GLY	LEU	MET	GLY	PRO	GLY	ARG	GLY	GLY
		GLY	PRO	CYS	THR	THR	THR	GLU	TYR	THR	THR
		VAL	LYS	ILE	MET	ILE	ASP	ILE	LYS	GLY	GLY
		ALA	GLY	ILE	GLY	THR	THR	THR	GLY	LYS	ARG
		PRO	ARG	VAL	THR	VAL	VAL	ALA	GLY	LYS	ARG
		VAL	LEU	GLY	VAL	ALA	PHE	ALA	ALA	GLY	SER
		PRO	PHE	LYS	GLN	THR	GLN	GLN	SER	GLY	ARG
		THR	VAL	GLU	ARG	VAL	ALA	ASP	LYS	ASP	ALA
	G1	ALA	SER	ALA	THR	GLU	THR	ASN	LYS	LEU	LEU
			PRO	ASP	GLY	TYR	THR	TYR	LYS	ILE	CYS
			LEU	THR	LYS	THR	THR	THR	ASN	THR	CYS

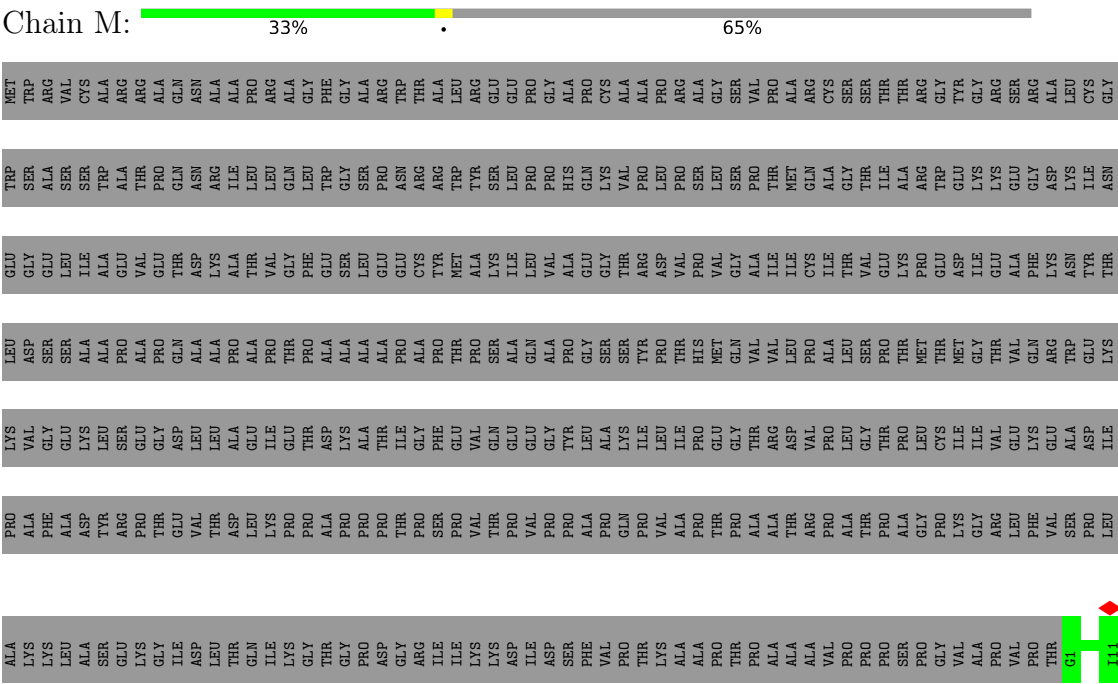
- Chain K:  33% • 65%

I11	ALA	LYS	LYS	LYS	ASP	LEU	LEU	VAL	LYS	LEU	ASP	GLY	TRP	GLY	TRP	MET
	LYS	LYS	PHE	ALA	ASP	ASP	GLY	GLY	GLY	ASP	SER	GLY	SER	GLY	ALA	ARG
	LEU	ALA	ALA	ASP	TYR	TYR	LEU	LEU	LYS	ALA	ALA	ILE	SER	LEU	VAL	VAL
	ALA	SER	ASP	TYR	TYR	ASP	LEU	LEU	LEU	ALA	ALA	ALA	SER	CYS	CYS	ARG
	SER	SER	ASP	TYR	TYR	ASP	LEU	LEU	LEU	ALA	ALA	ALA	TRP	ALA	ALA	ALA
	GLY	GLY	ASP	VAL	VAL	GLY	GLY	ASP	GLY	PRO	PRO	VAL	THR	ALA	ARG	ARG
	LYS	LYS	PRO	PRO	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR
	ILE	ILE	GLY	VAL	VAL	GLY	GLY	ASP	ASP	GLN	GLN	THR	GLN	GLN	ALA	ALA
	ASP	ASP	LEU	THR	THR	LEU	LEU	LEU	LEU	ALA	ALA	ASP	ASN	ASN	ASN	ASN
	LEU	LEU	THR	THR	THR	LEU	LEU	LEU	LEU	ALA	ALA	LYS	ASP	ARG	ALA	ALA
P165	THR	THR	GLN	GLN	ASP	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
	ILE	ILE	LYS	LYS	PRO	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	ILE	ILE	LYS	LYS	PRO	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	LYS	LYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	ASP	ASP	PRO	PRO	PRO	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	GLY	GLY	PRO	PRO	ASP	ASP	ASP	ALA	ALA	GLY	GLY	GLY	GLY	GLY
	GLY	GLY	THR	THR	PRO	PRO	ALA	ALA	ASP	ALA	ALA	ALA	THR	THR	THR	THR
	GLY	GLY	THR	THR	PRO	PRO	ALA	ALA	ASP	ALA	ALA	ALA	THR	THR	THR	THR
	THR	THR	GLY	GLY	PRO	PRO	ALA	ALA	ASP	ALA	ALA	ALA	THR	THR	THR	THR
I170	THR	THR	GLN	GLN	ASP	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
	ILE	ILE	LYS	LYS	PRO	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	ILE	ILE	LYS	LYS	PRO	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	LYS	LYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	ASP	ASP	PRO	PRO	PRO	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	ILE	ILE	LYS	LYS	PRO	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	ILE	ILE	LYS	LYS	PRO	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	ASP	ASP	PRO	PRO	PRO	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	GLY	GLY	PRO	PRO	ALA	ALA	ASP	ALA	ALA	ALA	THR	THR	THR	THR
	THR	THR	GLY	GLY	PRO	PRO	ALA	ALA	ASP	ALA	ALA	ALA	THR	THR	THR	THR
I185	THR	THR	GLY	GLY	PRO	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	ILE	ILE	LYS	LYS	PRO	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	ILE	ILE	LYS	LYS	PRO	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	ASP	ASP	PRO	PRO	PRO	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	GLY	GLY	PRO	PRO	ALA	ALA	ASP	ALA	ALA	ALA	THR	THR	THR	THR
	THR	THR	GLY	GLY	PRO	PRO	ALA	ALA	ASP	ALA	ALA	ALA	THR	THR	THR	THR
	GLY	GLY	THR	THR	PRO	PRO	ALA	ALA	ASP	ALA	ALA	ALA	THR	THR	THR	THR
	GLY	GLY	THR	THR	PRO	PRO	ALA	ALA	ASP	ALA	ALA	ALA	THR	THR	THR	THR
	THR	THR	GLY	GLY	PRO	PRO	ALA	ALA	ASP	ALA	ALA	ALA	THR	THR	THR	THR

- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

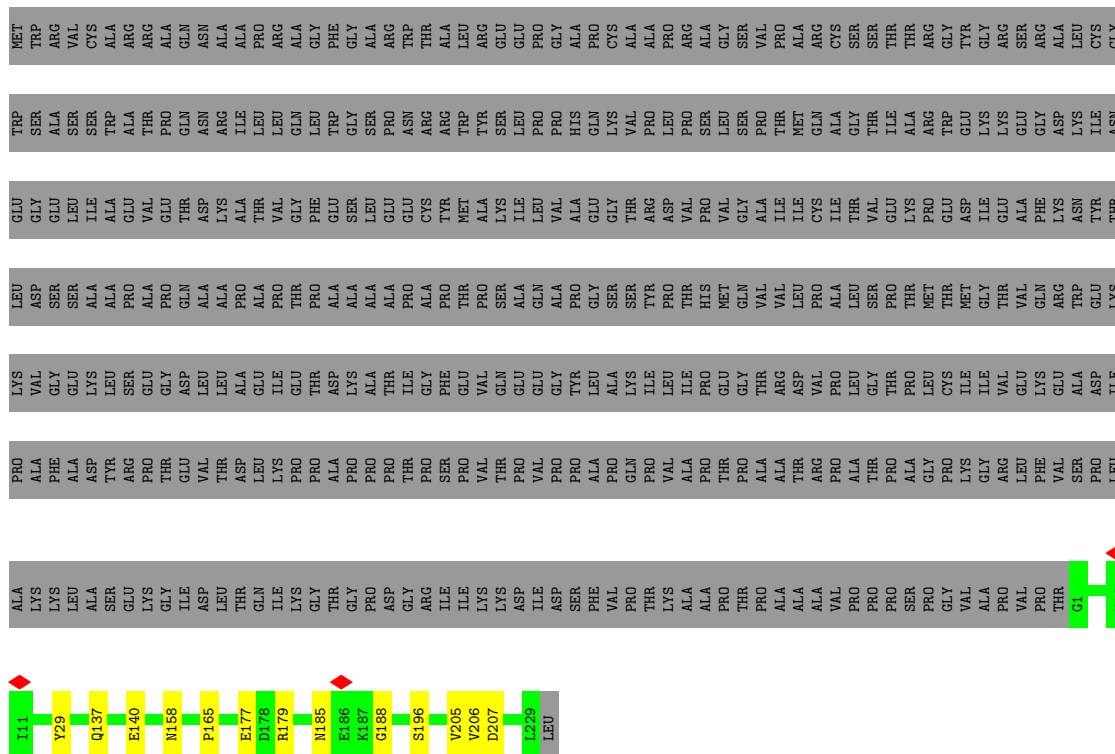


- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

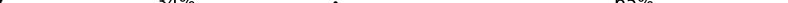


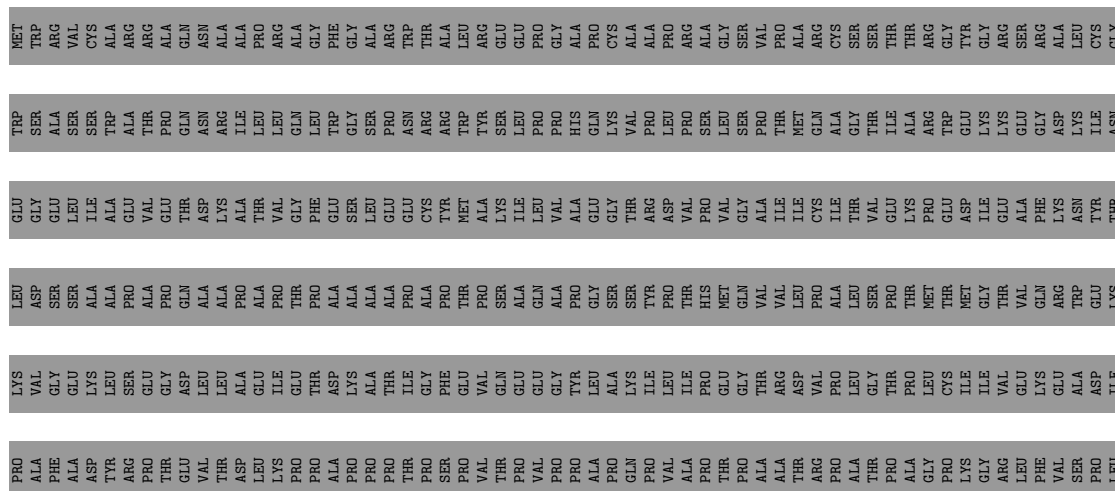
- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

Chain N: 33% . 65%

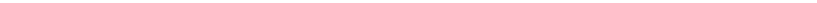


- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

Chain O:  34% . 65%

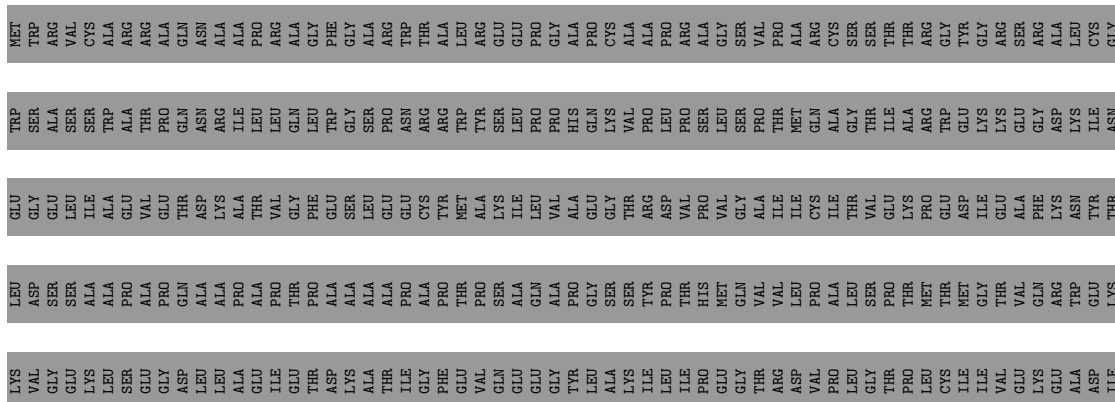


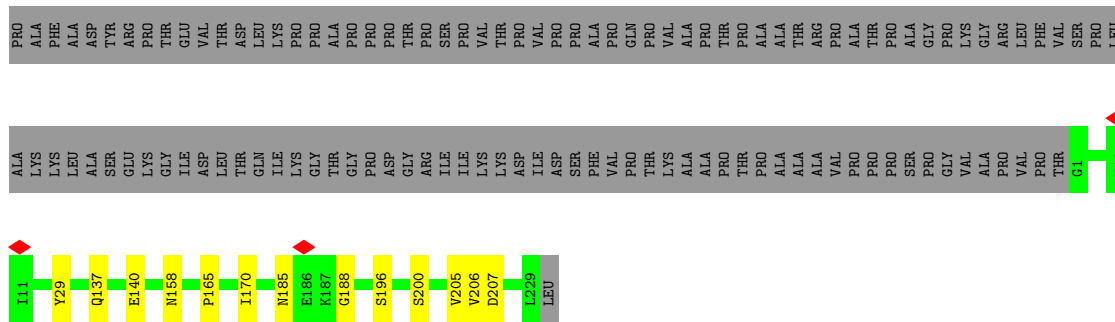
- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

Chain P:  33% . 65%

- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

Chain Q: 33% . 65%

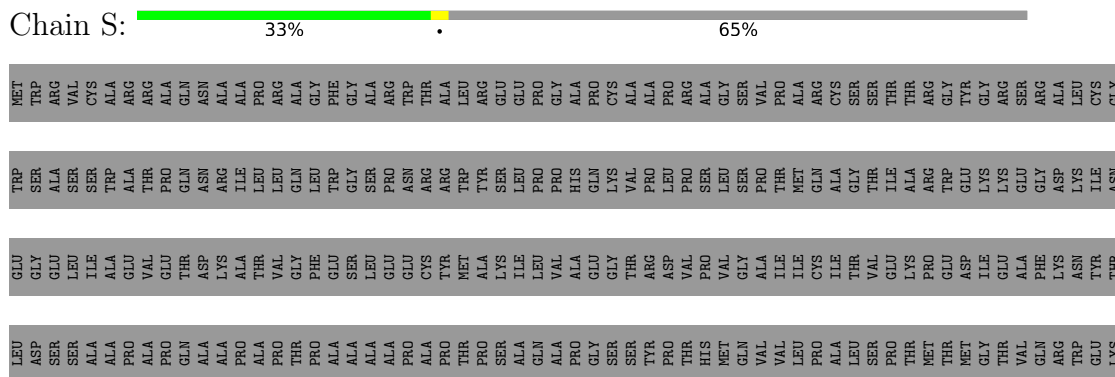




- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

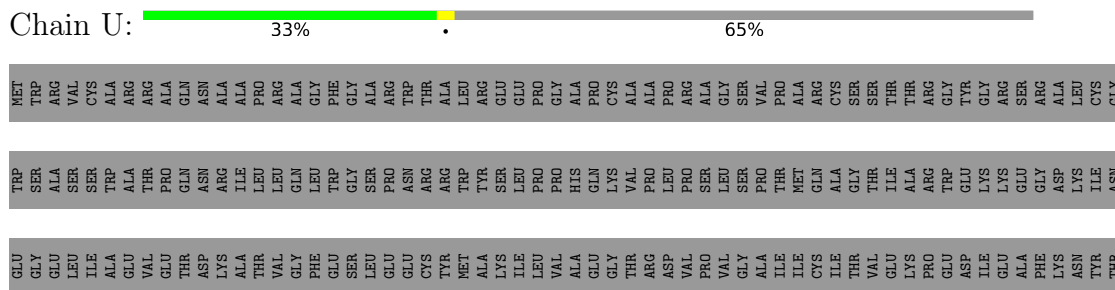


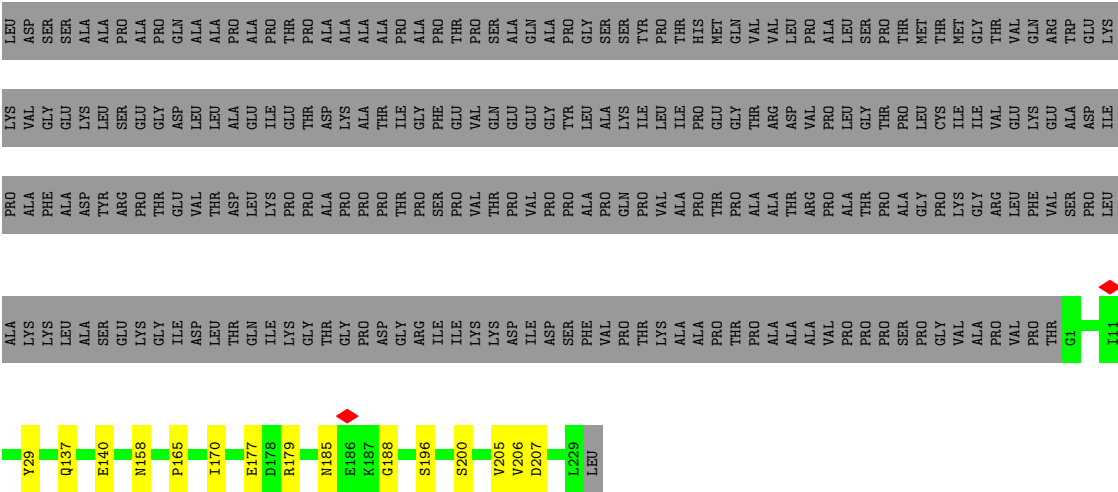
- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



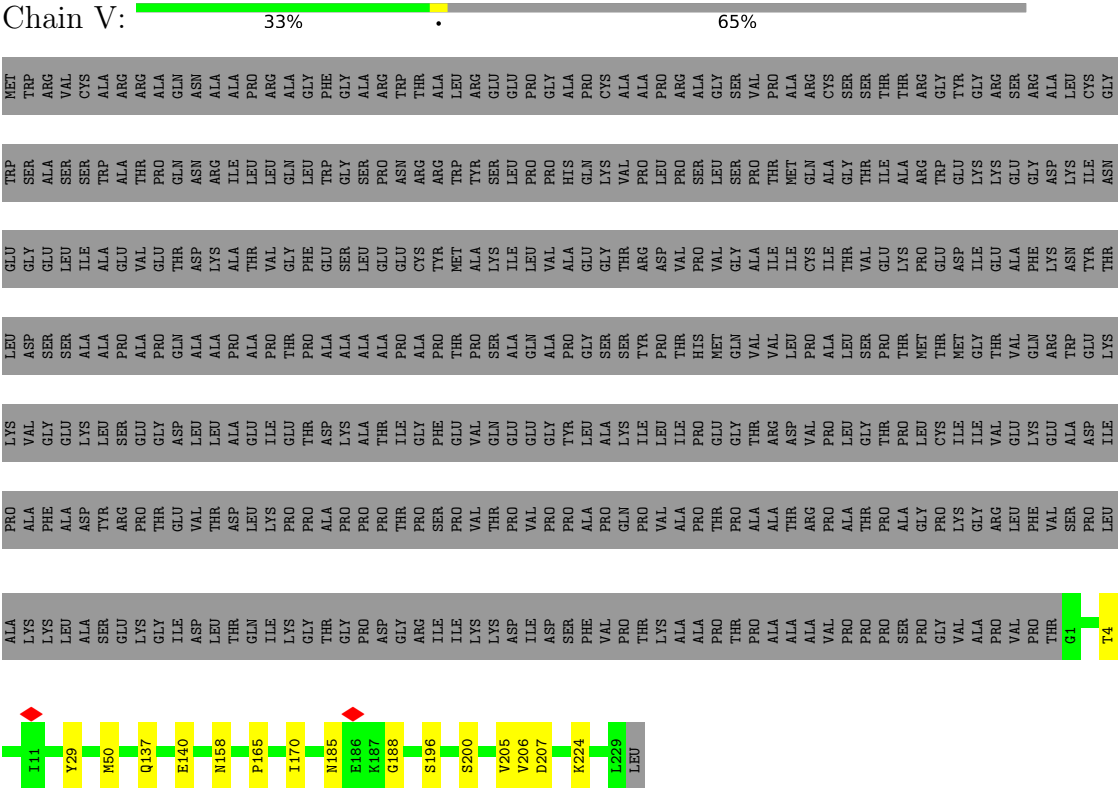
- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

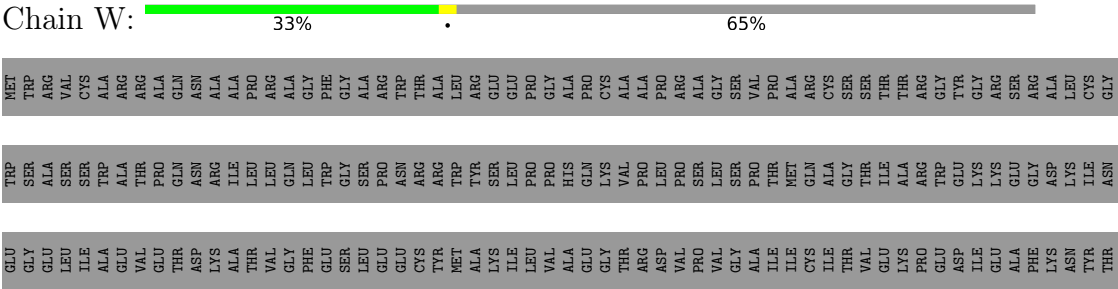


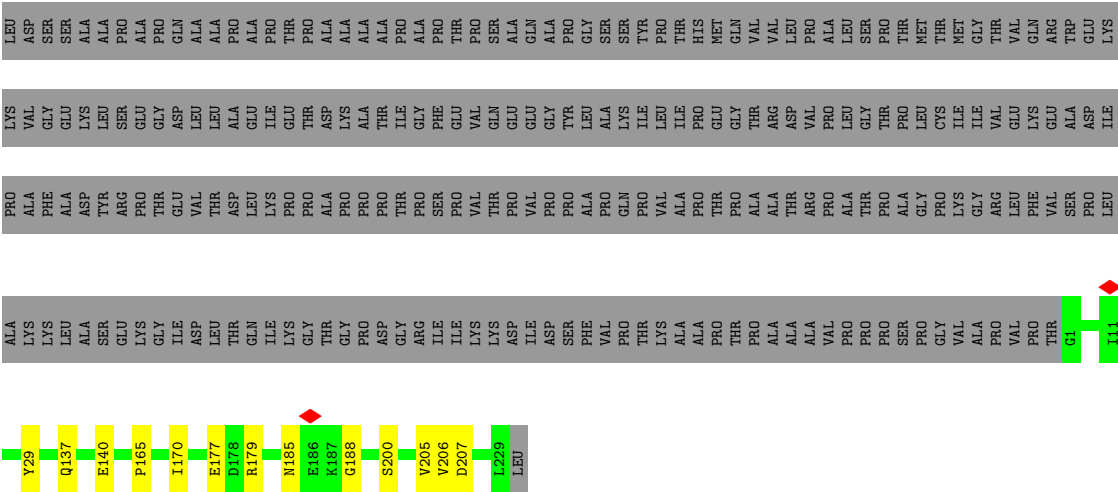


• Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



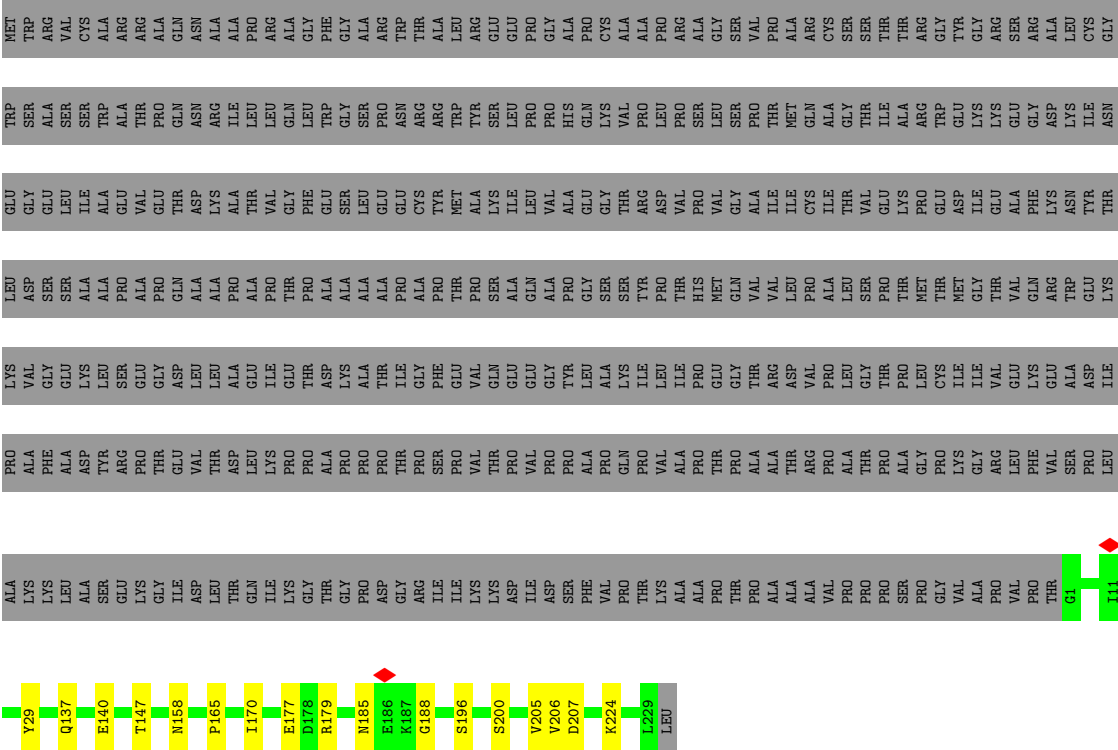
• Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex





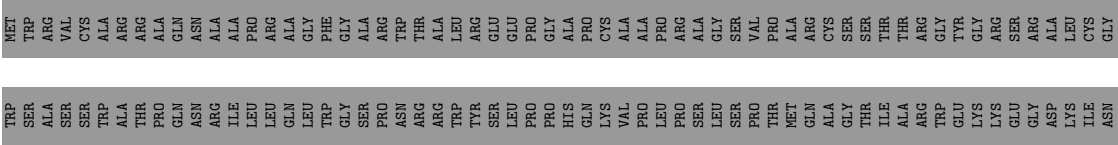
• Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

Chain X: 33% 65%



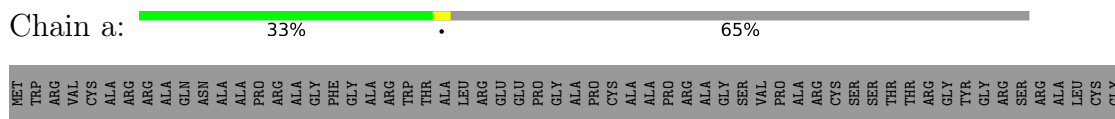
• Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

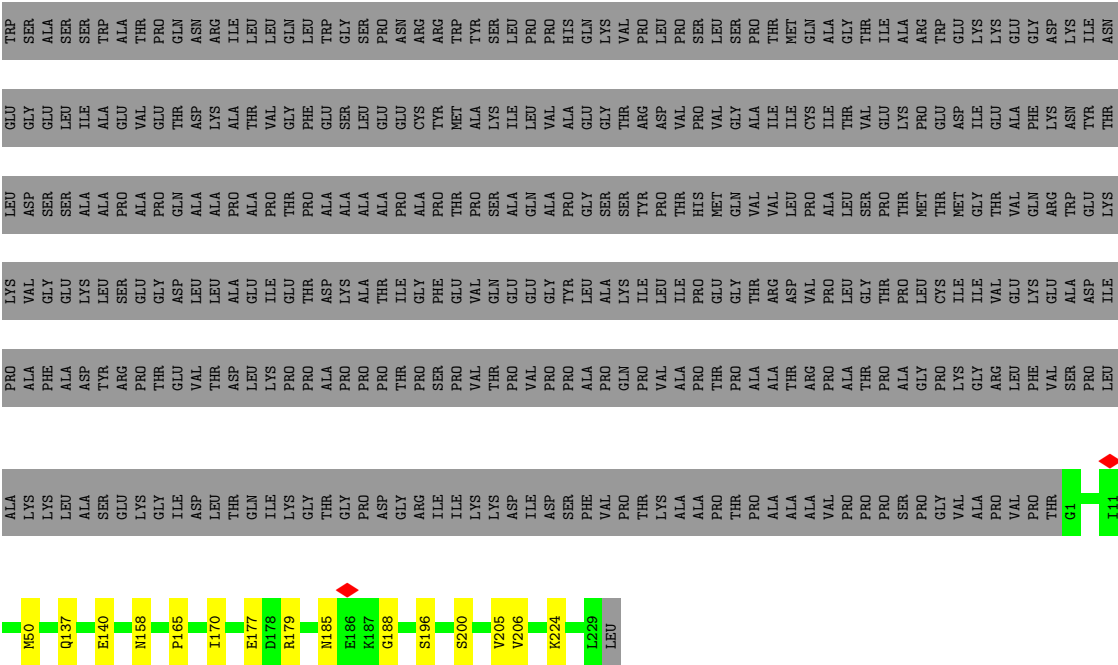
Chain Y: 33% 65%



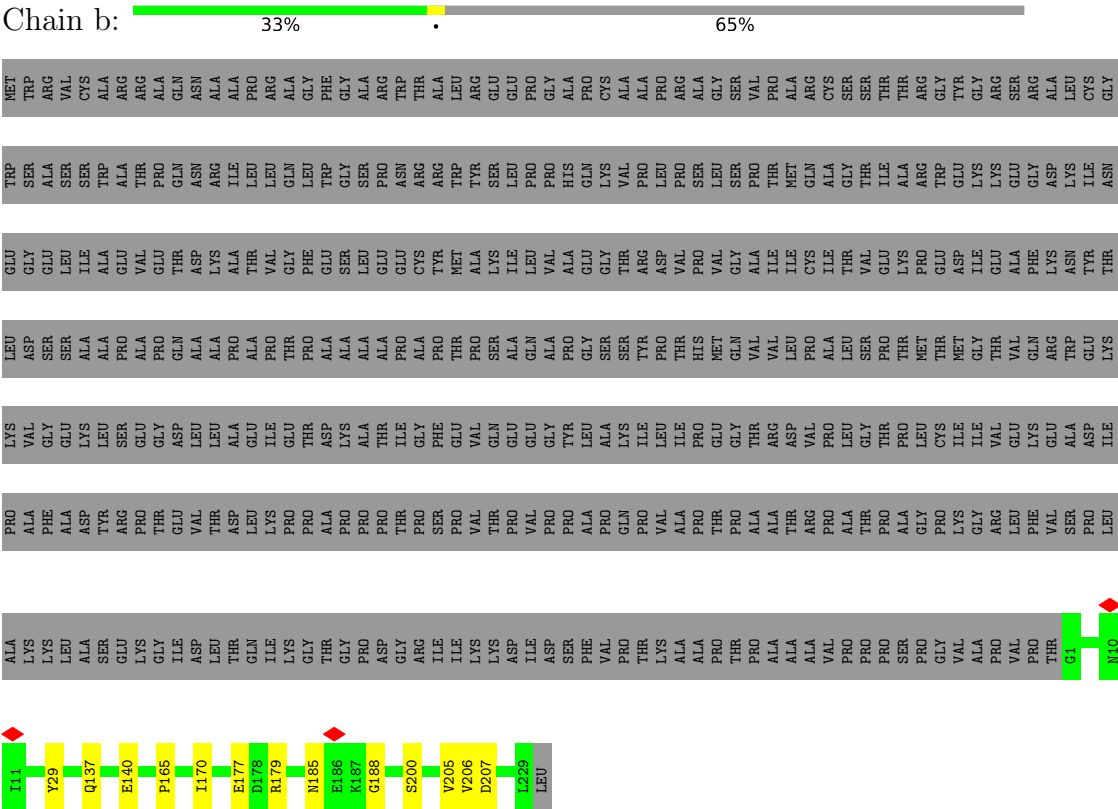
- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



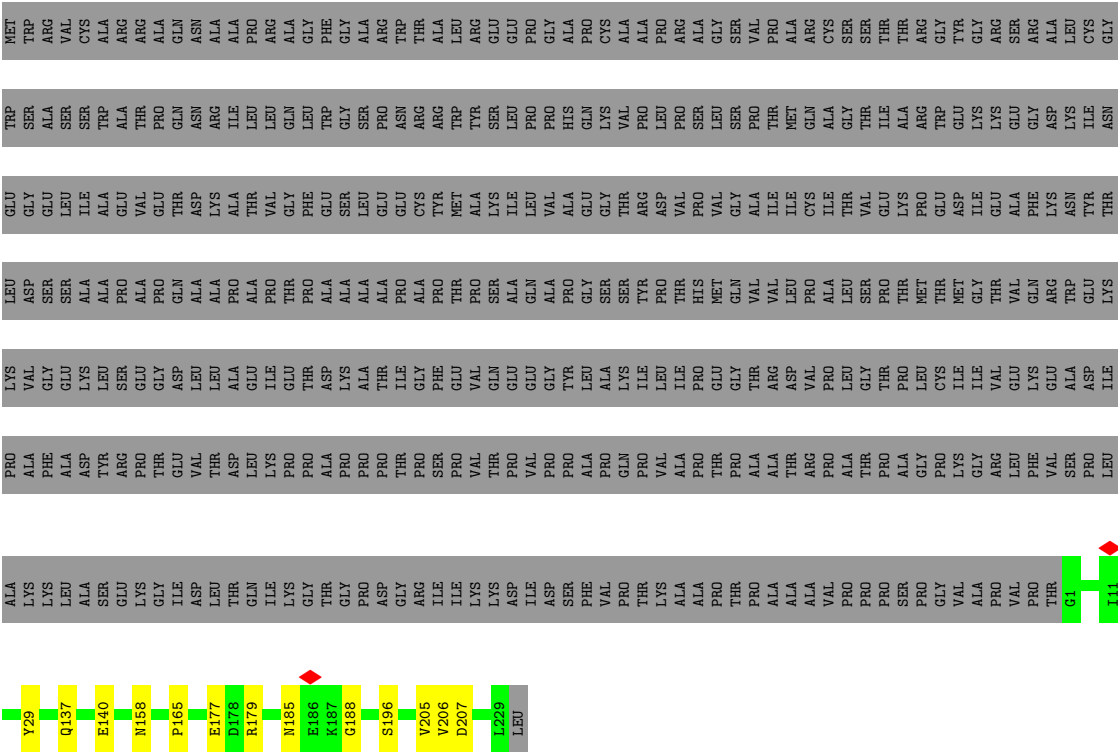


● Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



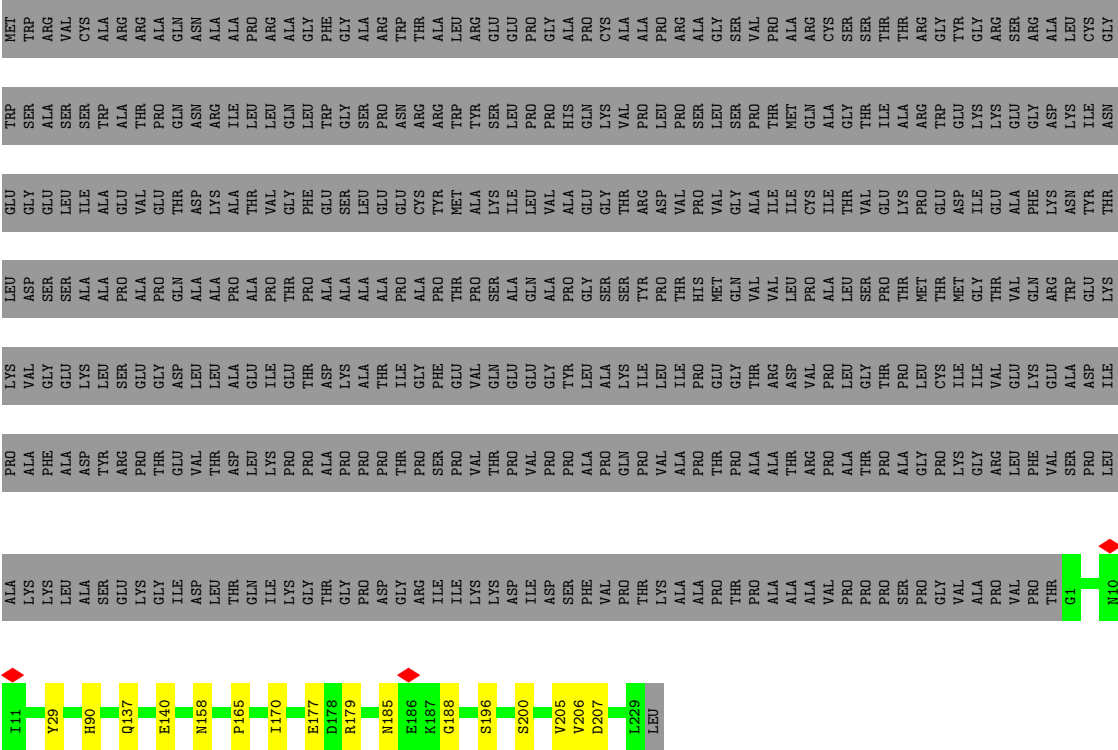
● Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



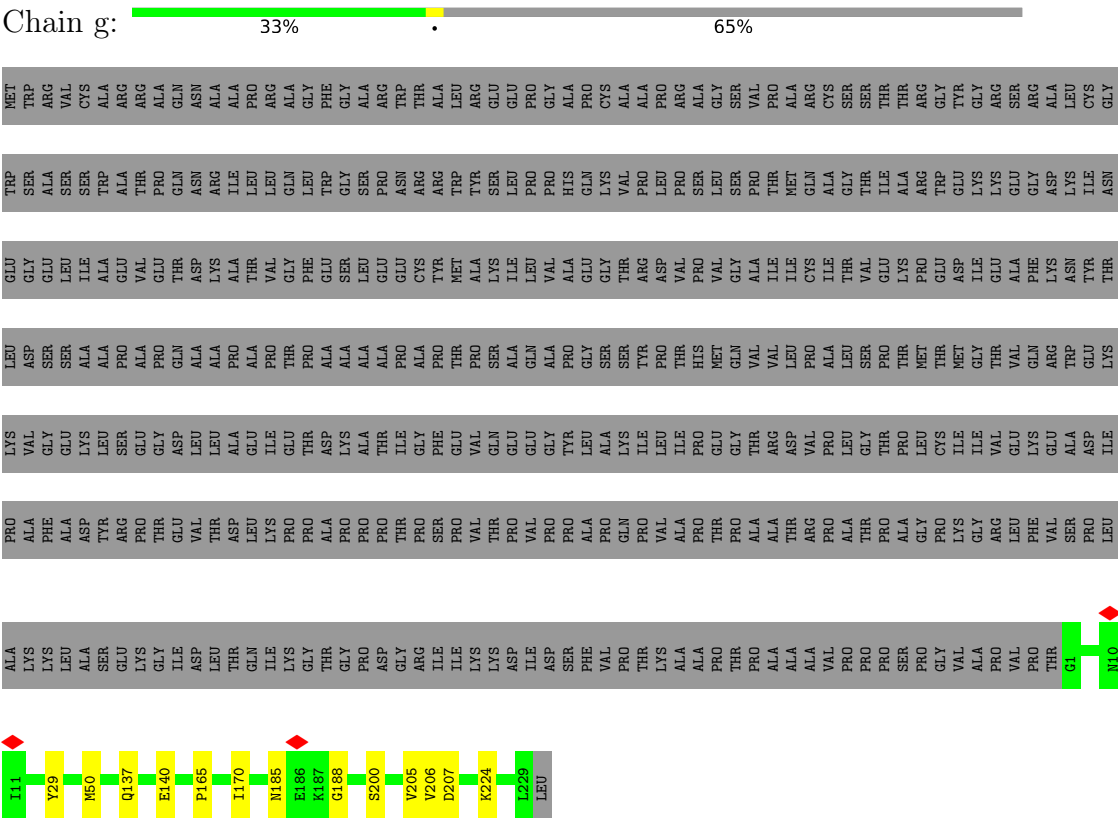


● Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

Chain f: 33% 65%



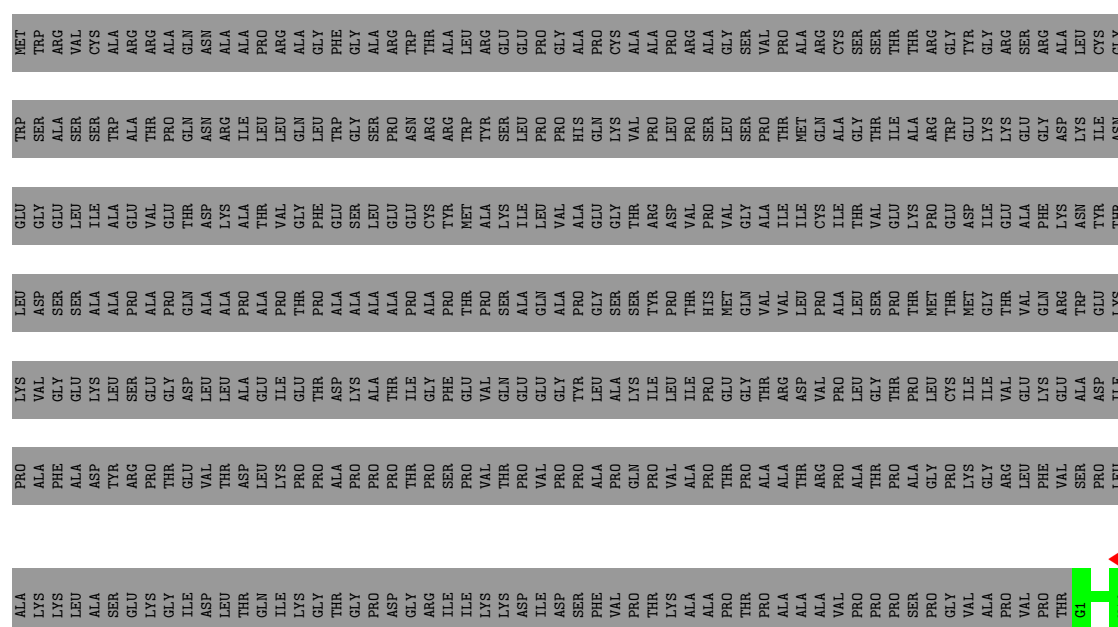
● Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



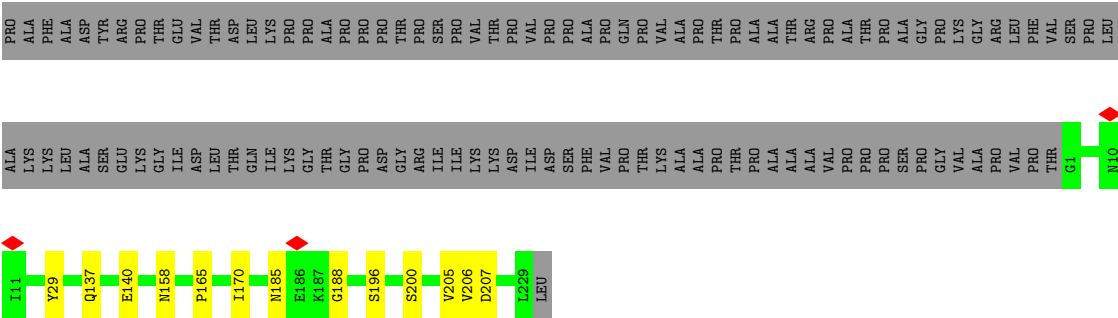
● Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



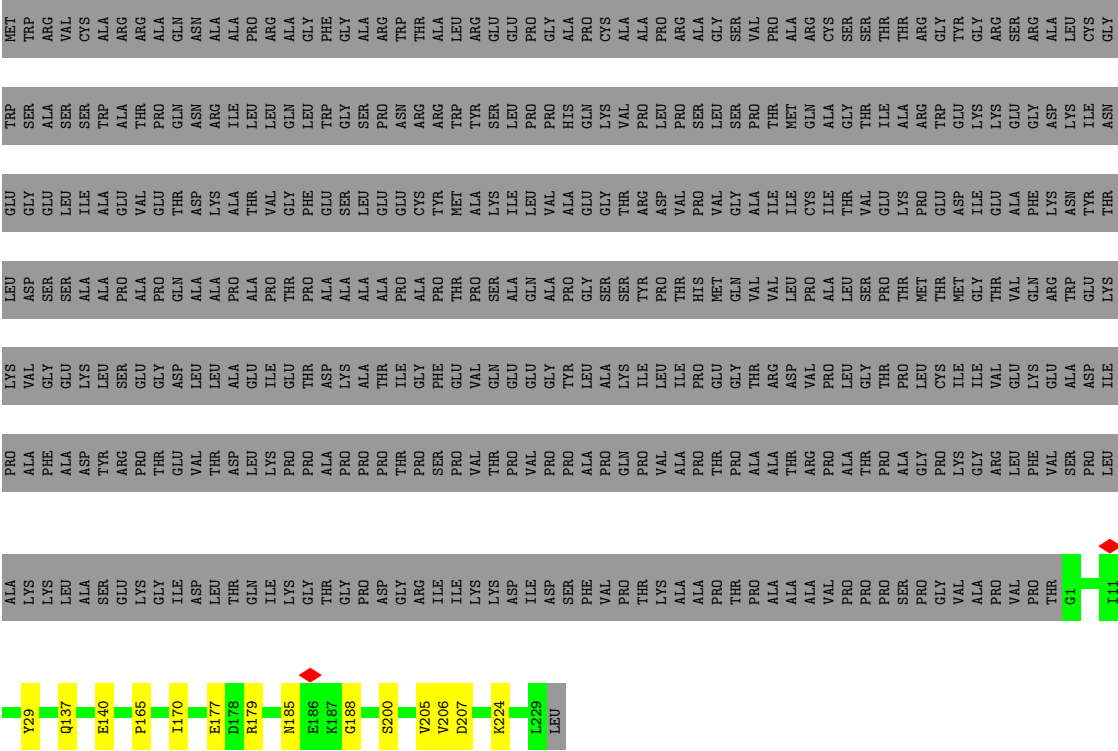
- Chain i: 33% . 65%



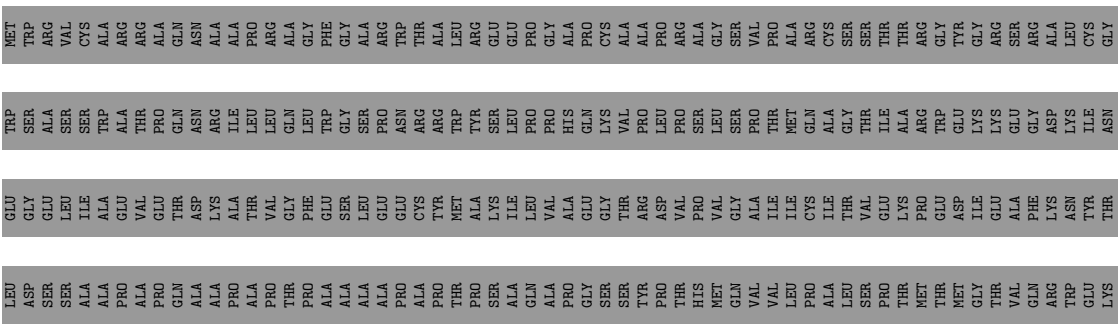




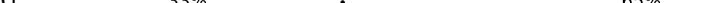
● Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

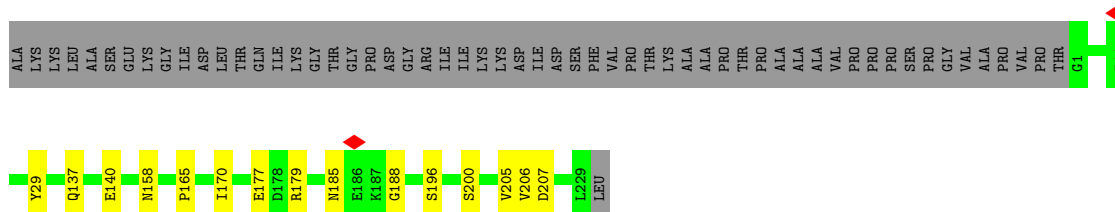


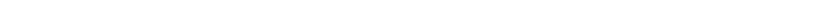
● Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

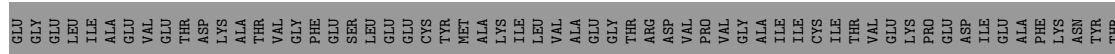




- Chain q:  33% • 65%

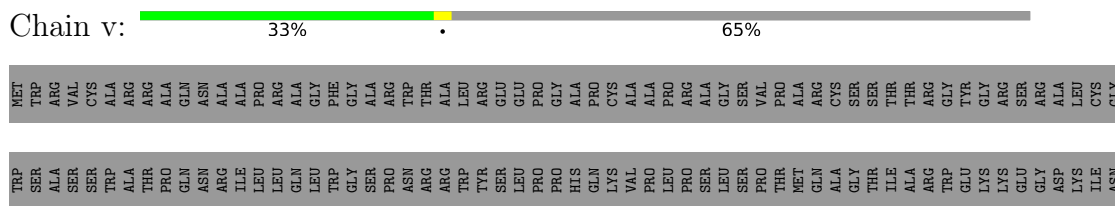


- Chain r:  32% . 65%

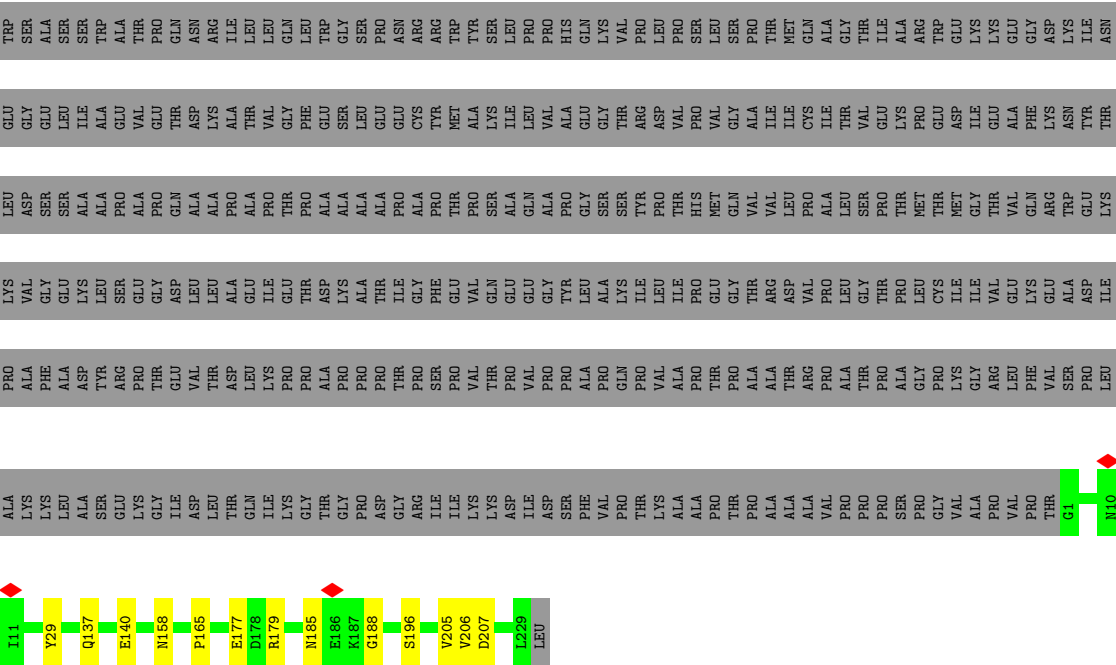


- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

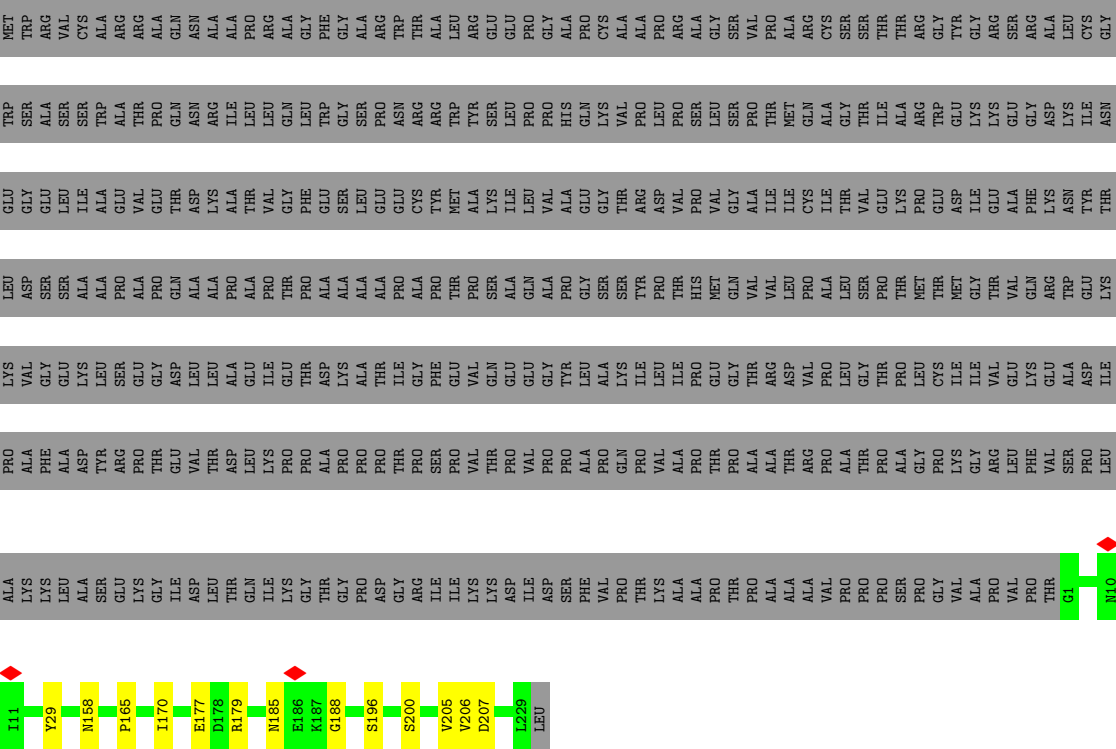
- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex







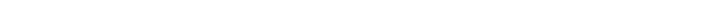
● Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



● Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



Amino Acid	Count
I11	20
Y29	10
Q137	10
E140	10
T147	10
N158	10
P165	10
I170	10
N185	10
E186	20
K187	10
G188	10
S196	10
S200	10
V205	10
V206	10
D207	10
L229	10
LEU	10

- Chain 0:  33% . 65%

Country	Publications
I11	111
Y29	29
Q137	137
E140	140
T147	147
N158	158
P165	165
I170	170
E177	177
D178	178
R179	179
N185	185
E186	186
A187	187
P188	188
S196	196
S200	200
V205	205
V206	206
D207	207
L229	229
LEU	229

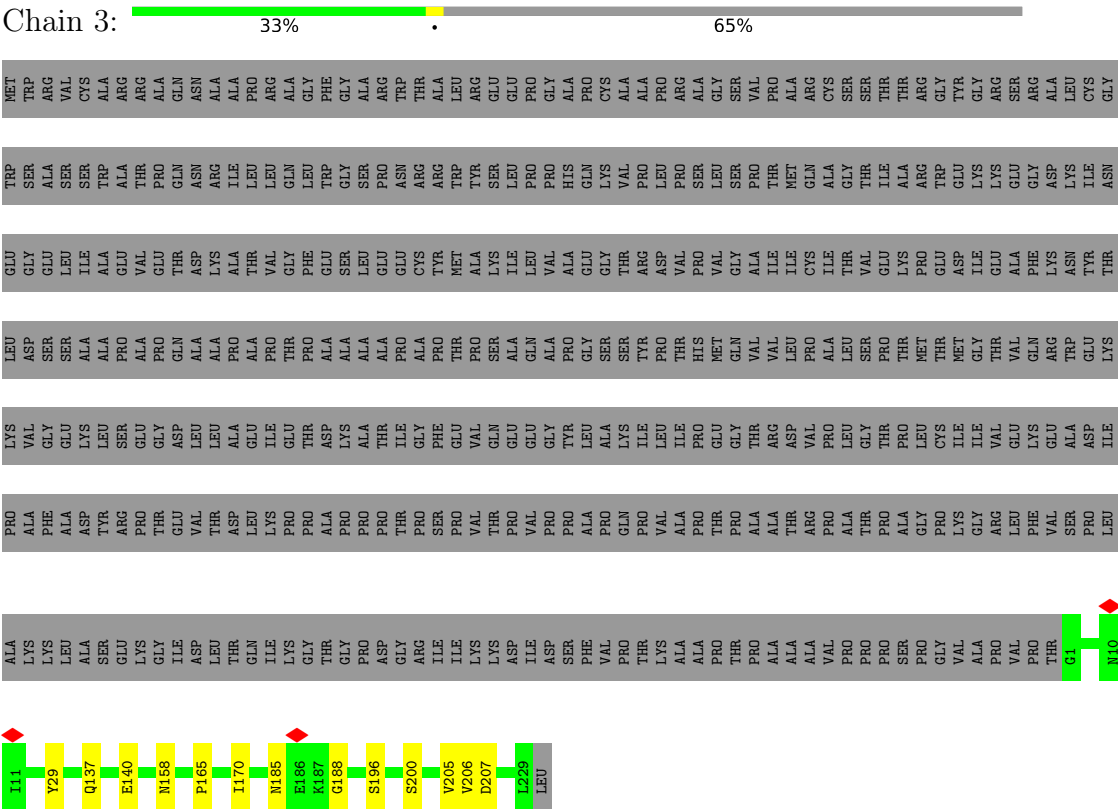
- 

I11	ALA	PRO	LYS	LEU	ASP	LEU	ASP	LEU	TRP	MET
Y29	LYS	ALA	VAL	GLY	ASP	LEU	GLY	GLY	ALA	ARG
Q137	LEU	PHE	GLY	GLY	SER	LEU	GLY	GLY	SER	ARG
E140	ALA	ASP	LYS	LYS	ALA	ALA	ALA	ILE	SER	CYS
T147	SER	TYR	LEU	LEU	ALA	ALA	PRO	ALA	TRP	ALA
N188	GLY	ARG	SER	SER	PRO	GLY	GLY	GLY	ALA	ARG
P165	LYS	THR	GLY	GLY	ALA	GLY	ALA	VAL	PRO	ALA
I170	ILE	LYS	ILE	ILE	PRO	THR	PRO	VAL	ARG	ARG
E177	LYS	PRO	GLY	THR	PRO	ALA	PHE	PHE	GLY	ALA
D178	THR	ALA	ASP	ALA	ALA	ALA	GLY	GLY	TRP	THR
R179	GLY	PRO	LYS	LYS	PRO	PRO	LYS	SER	ALA	ALA
N185	GLN	ASP	THR	THR	THR	THR	ILE	GLY	ARG	ARG
E186	GLY	PRO	ILE	GLY	PRO	PRO	GLY	CYS	THR	THR
K187	ILE	SER	PHE	THR	ALA	ALA	ALA	TYR	ARG	ALA
G188	ILE	PRO	VAL	VAL	THR	THR	VAL	GLY	GLY	GLY
S196	LYS	THR	LYS	ASP	THR	THR	GLN	ILE	SER	GLY
S200	ILE	VAL	GLY	GLY	PRO	PRO	ALA	LEU	PRO	PRO
V205	ASP	PRO	GLY	GLY	PRO	PRO	ALA	VAL	PRO	GLY
V206	SER	PRO	TYR	THR	ALA	ALA	GLY	ALA	HIS	ALA
D207	PHE	ALA	LEU	LEU	PRO	PRO	PRO	SER	GLN	PRO
L229	VAL	PRO	ALA	LYS	GLY	GLY	SER	THR	VAL	CYS
LEU	THR	PRO	ALA	ILE	PRO	VAL	ARG	ARG	ALA	ALA

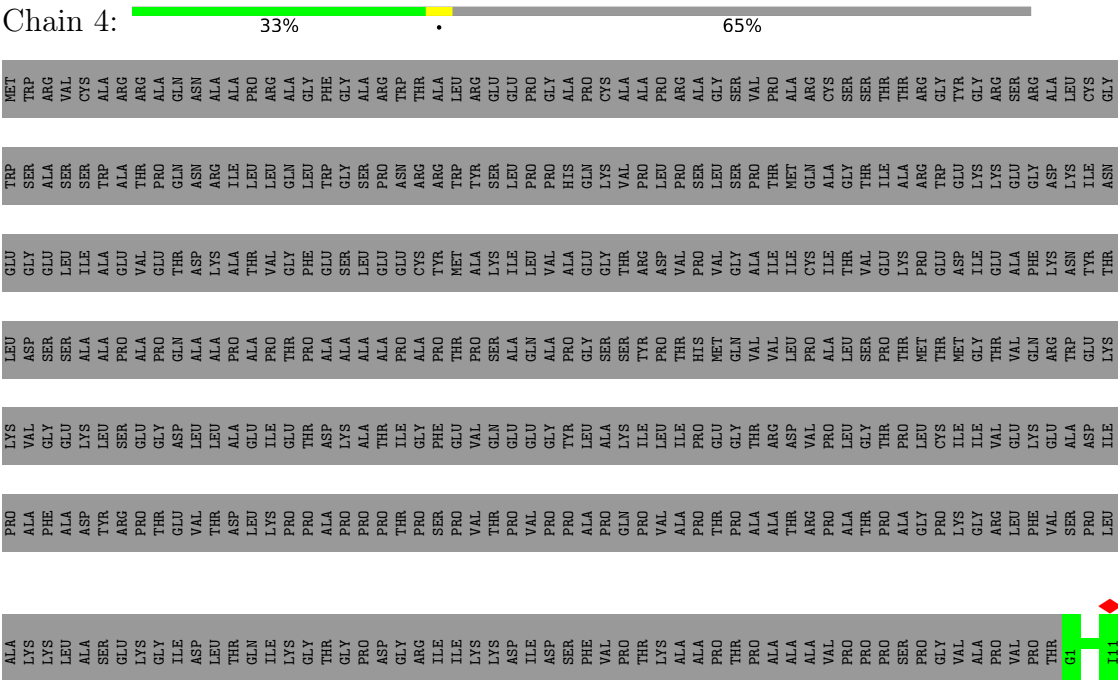
- Chain 2: 

[illegible]

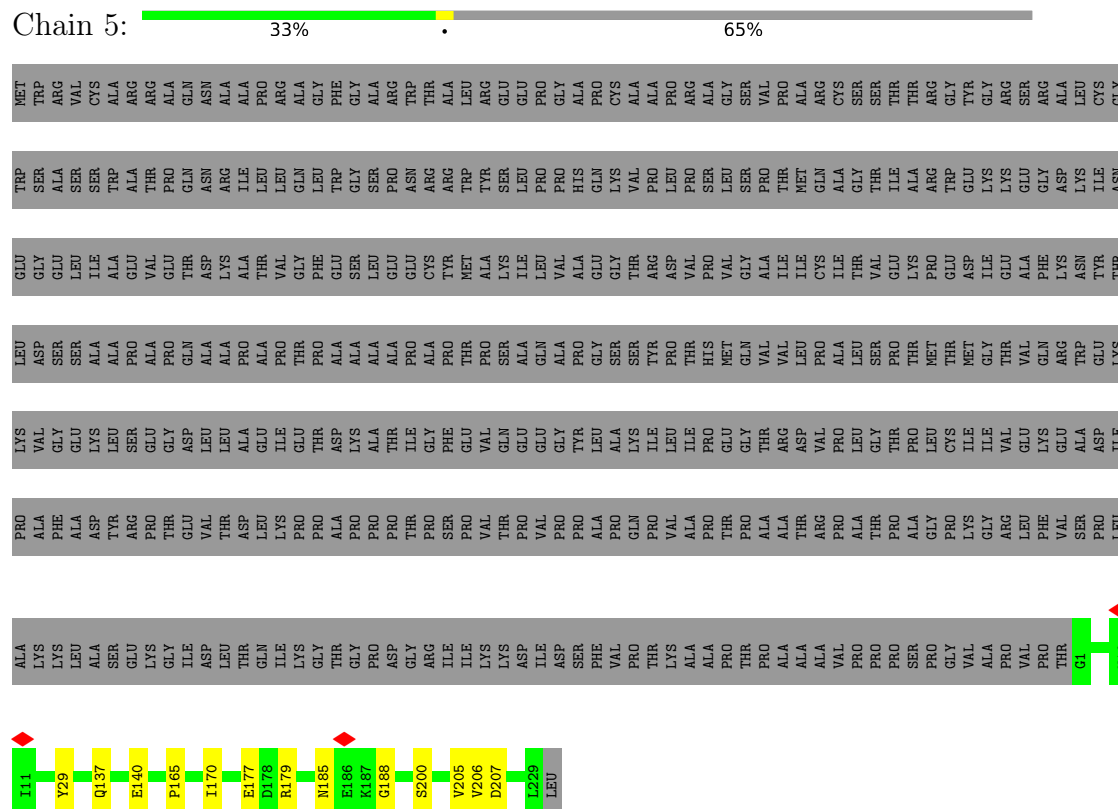
- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



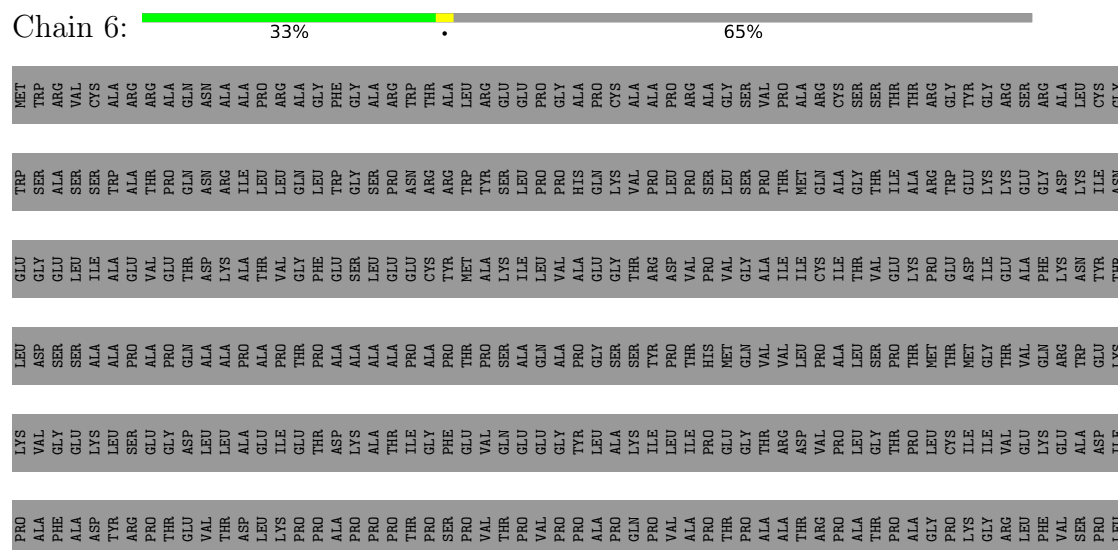
- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

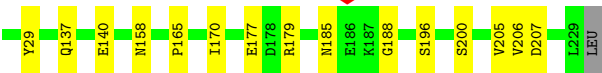
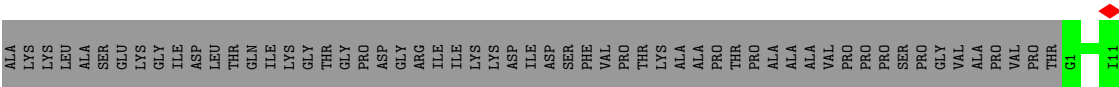


- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex

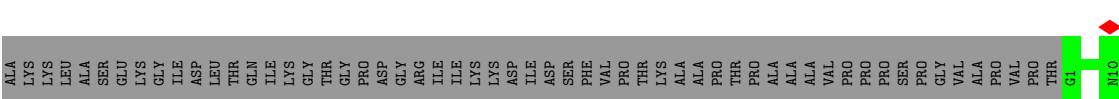
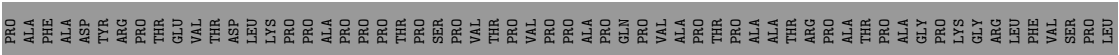
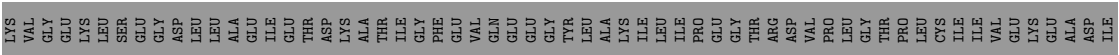
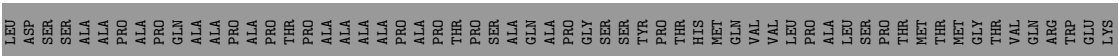
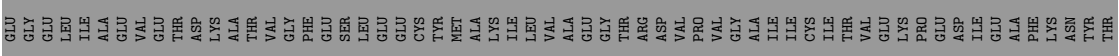
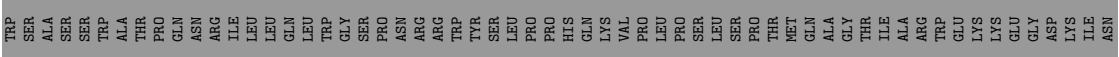
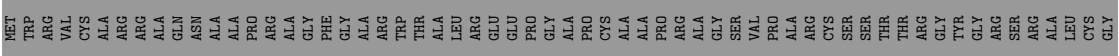


- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex





- Molecule 1: Acetyltransferase component of pyruvate dehydrogenase complex



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35220	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.129	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	395.09998, 395.09998, 395.09998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0975, 1.0975, 1.0975	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	0.25	0/1790	0.59	3/2426 (0.1%)
1	1	0.25	0/1790	0.59	3/2426 (0.1%)
1	2	0.25	0/1790	0.59	3/2426 (0.1%)
1	3	0.25	0/1790	0.59	3/2426 (0.1%)
1	4	0.25	0/1790	0.59	3/2426 (0.1%)
1	5	0.25	0/1790	0.59	3/2426 (0.1%)
1	6	0.25	0/1790	0.59	3/2426 (0.1%)
1	7	0.25	0/1790	0.59	3/2426 (0.1%)
1	A	0.24	0/1790	0.59	3/2426 (0.1%)
1	B	0.25	0/1790	0.59	3/2426 (0.1%)
1	C	0.25	0/1790	0.59	3/2426 (0.1%)
1	D	0.25	0/1790	0.59	3/2426 (0.1%)
1	E	0.25	0/1790	0.59	3/2426 (0.1%)
1	F	0.25	0/1790	0.59	3/2426 (0.1%)
1	G	0.25	0/1790	0.59	3/2426 (0.1%)
1	H	0.25	0/1790	0.59	3/2426 (0.1%)
1	I	0.25	0/1790	0.59	3/2426 (0.1%)
1	J	0.25	0/1790	0.59	3/2426 (0.1%)
1	K	0.25	0/1790	0.59	3/2426 (0.1%)
1	L	0.25	0/1790	0.59	3/2426 (0.1%)
1	M	0.25	0/1790	0.59	3/2426 (0.1%)
1	N	0.25	0/1790	0.59	3/2426 (0.1%)
1	O	0.25	0/1790	0.59	3/2426 (0.1%)
1	P	0.25	0/1790	0.59	3/2426 (0.1%)
1	Q	0.25	0/1790	0.59	3/2426 (0.1%)
1	R	0.25	0/1790	0.59	3/2426 (0.1%)
1	S	0.25	0/1790	0.59	3/2426 (0.1%)
1	T	0.25	0/1790	0.59	3/2426 (0.1%)
1	U	0.25	0/1790	0.59	3/2426 (0.1%)
1	V	0.25	0/1790	0.59	3/2426 (0.1%)
1	W	0.25	0/1790	0.59	3/2426 (0.1%)
1	X	0.25	0/1790	0.59	3/2426 (0.1%)
1	Y	0.25	0/1790	0.59	3/2426 (0.1%)
1	Z	0.25	0/1790	0.59	3/2426 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.25	0/1790	0.59	3/2426 (0.1%)
1	b	0.25	0/1790	0.59	3/2426 (0.1%)
1	c	0.25	0/1790	0.59	3/2426 (0.1%)
1	d	0.25	0/1790	0.59	3/2426 (0.1%)
1	e	0.25	0/1790	0.59	3/2426 (0.1%)
1	f	0.25	0/1790	0.59	3/2426 (0.1%)
1	g	0.25	0/1790	0.59	3/2426 (0.1%)
1	h	0.25	0/1790	0.59	3/2426 (0.1%)
1	i	0.25	0/1790	0.59	3/2426 (0.1%)
1	j	0.25	0/1790	0.59	3/2426 (0.1%)
1	k	0.25	0/1790	0.59	3/2426 (0.1%)
1	l	0.25	0/1790	0.59	3/2426 (0.1%)
1	m	0.25	0/1790	0.59	3/2426 (0.1%)
1	n	0.25	0/1790	0.59	3/2426 (0.1%)
1	o	0.25	0/1790	0.59	3/2426 (0.1%)
1	p	0.25	0/1790	0.59	3/2426 (0.1%)
1	q	0.25	0/1790	0.59	3/2426 (0.1%)
1	r	0.25	0/1790	0.59	3/2426 (0.1%)
1	s	0.25	0/1790	0.59	3/2426 (0.1%)
1	t	0.25	0/1790	0.59	3/2426 (0.1%)
1	u	0.24	0/1790	0.59	3/2426 (0.1%)
1	v	0.25	0/1790	0.59	3/2426 (0.1%)
1	w	0.25	0/1790	0.59	3/2426 (0.1%)
1	x	0.25	0/1790	0.59	3/2426 (0.1%)
1	y	0.25	0/1790	0.59	3/2426 (0.1%)
1	z	0.25	0/1790	0.59	3/2426 (0.1%)
All	All	0.25	0/107400	0.59	180/145560 (0.1%)

There are no bond length outliers.

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	PRO	CA-C-N	-6.52	111.69	119.84
1	B	165	PRO	C-N-CA	-6.52	111.69	119.84
1	l	165	PRO	CA-C-N	-6.52	111.69	119.84
1	l	165	PRO	C-N-CA	-6.52	111.69	119.84
1	Q	165	PRO	CA-C-N	-6.51	111.70	119.84
1	Q	165	PRO	C-N-CA	-6.51	111.70	119.84
1	y	165	PRO	CA-C-N	-6.51	111.70	119.84
1	y	165	PRO	C-N-CA	-6.51	111.70	119.84
1	L	165	PRO	CA-C-N	-6.51	111.70	119.84
1	L	165	PRO	C-N-CA	-6.51	111.70	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	n	165	PRO	CA-C-N	-6.51	111.70	119.84
1	n	165	PRO	C-N-CA	-6.51	111.70	119.84
1	F	165	PRO	CA-C-N	-6.51	111.70	119.84
1	F	165	PRO	C-N-CA	-6.51	111.70	119.84
1	T	165	PRO	CA-C-N	-6.51	111.70	119.84
1	T	165	PRO	C-N-CA	-6.51	111.70	119.84
1	w	165	PRO	CA-C-N	-6.51	111.71	119.84
1	w	165	PRO	C-N-CA	-6.51	111.71	119.84
1	G	165	PRO	CA-C-N	-6.50	111.71	119.84
1	G	165	PRO	C-N-CA	-6.50	111.71	119.84
1	x	165	PRO	CA-C-N	-6.50	111.71	119.84
1	x	165	PRO	C-N-CA	-6.50	111.71	119.84
1	t	165	PRO	CA-C-N	-6.50	111.72	119.84
1	t	165	PRO	C-N-CA	-6.50	111.72	119.84
1	4	165	PRO	CA-C-N	-6.50	111.72	119.84
1	4	165	PRO	C-N-CA	-6.50	111.72	119.84
1	f	165	PRO	CA-C-N	-6.50	111.72	119.84
1	f	165	PRO	C-N-CA	-6.50	111.72	119.84
1	h	165	PRO	CA-C-N	-6.50	111.72	119.84
1	h	165	PRO	C-N-CA	-6.50	111.72	119.84
1	d	165	PRO	CA-C-N	-6.49	111.72	119.84
1	d	165	PRO	C-N-CA	-6.49	111.72	119.84
1	g	165	PRO	CA-C-N	-6.49	111.72	119.84
1	g	165	PRO	C-N-CA	-6.49	111.72	119.84
1	6	165	PRO	CA-C-N	-6.49	111.72	119.84
1	6	165	PRO	C-N-CA	-6.49	111.72	119.84
1	S	165	PRO	CA-C-N	-6.49	111.73	119.84
1	S	165	PRO	C-N-CA	-6.49	111.73	119.84
1	Y	165	PRO	CA-C-N	-6.49	111.73	119.84
1	Y	165	PRO	C-N-CA	-6.49	111.73	119.84
1	A	165	PRO	CA-C-N	-6.49	111.73	119.84
1	A	165	PRO	C-N-CA	-6.49	111.73	119.84
1	M	165	PRO	CA-C-N	-6.49	111.73	119.84
1	M	165	PRO	C-N-CA	-6.49	111.73	119.84
1	O	165	PRO	CA-C-N	-6.49	111.73	119.84
1	O	165	PRO	C-N-CA	-6.49	111.73	119.84
1	i	165	PRO	CA-C-N	-6.49	111.73	119.84
1	i	165	PRO	C-N-CA	-6.49	111.73	119.84
1	q	165	PRO	CA-C-N	-6.49	111.73	119.84
1	q	165	PRO	C-N-CA	-6.49	111.73	119.84
1	7	165	PRO	CA-C-N	-6.49	111.73	119.84
1	7	165	PRO	C-N-CA	-6.49	111.73	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	165	PRO	CA-C-N	-6.49	111.73	119.84
1	j	165	PRO	C-N-CA	-6.49	111.73	119.84
1	a	165	PRO	CA-C-N	-6.48	111.73	119.84
1	a	165	PRO	C-N-CA	-6.48	111.73	119.84
1	k	165	PRO	CA-C-N	-6.48	111.74	119.84
1	k	165	PRO	C-N-CA	-6.48	111.74	119.84
1	5	165	PRO	CA-C-N	-6.48	111.74	119.84
1	5	165	PRO	C-N-CA	-6.48	111.74	119.84
1	I	165	PRO	CA-C-N	-6.48	111.74	119.84
1	I	165	PRO	C-N-CA	-6.48	111.74	119.84
1	W	165	PRO	CA-C-N	-6.48	111.74	119.84
1	W	165	PRO	C-N-CA	-6.48	111.74	119.84
1	H	165	PRO	CA-C-N	-6.48	111.74	119.84
1	H	165	PRO	C-N-CA	-6.48	111.74	119.84
1	p	165	PRO	CA-C-N	-6.48	111.74	119.84
1	p	165	PRO	C-N-CA	-6.48	111.74	119.84
1	m	165	PRO	CA-C-N	-6.48	111.74	119.84
1	m	165	PRO	C-N-CA	-6.48	111.74	119.84
1	b	165	PRO	CA-C-N	-6.47	111.75	119.84
1	b	165	PRO	C-N-CA	-6.47	111.75	119.84
1	N	165	PRO	CA-C-N	-6.47	111.75	119.84
1	N	165	PRO	C-N-CA	-6.47	111.75	119.84
1	X	165	PRO	CA-C-N	-6.47	111.75	119.84
1	X	165	PRO	C-N-CA	-6.47	111.75	119.84
1	u	165	PRO	CA-C-N	-6.47	111.75	119.84
1	u	165	PRO	C-N-CA	-6.47	111.75	119.84
1	J	165	PRO	CA-C-N	-6.47	111.75	119.84
1	J	165	PRO	C-N-CA	-6.47	111.75	119.84
1	c	165	PRO	CA-C-N	-6.47	111.75	119.84
1	c	165	PRO	C-N-CA	-6.47	111.75	119.84
1	o	165	PRO	CA-C-N	-6.47	111.75	119.84
1	o	165	PRO	C-N-CA	-6.47	111.75	119.84
1	0	165	PRO	CA-C-N	-6.47	111.75	119.84
1	0	165	PRO	C-N-CA	-6.47	111.75	119.84
1	D	165	PRO	CA-C-N	-6.47	111.75	119.84
1	D	165	PRO	C-N-CA	-6.47	111.75	119.84
1	E	165	PRO	CA-C-N	-6.47	111.76	119.84
1	E	165	PRO	C-N-CA	-6.47	111.76	119.84
1	z	165	PRO	CA-C-N	-6.47	111.76	119.84
1	z	165	PRO	C-N-CA	-6.47	111.76	119.84
1	Z	165	PRO	CA-C-N	-6.46	111.76	119.84
1	Z	165	PRO	C-N-CA	-6.46	111.76	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	165	PRO	CA-C-N	-6.46	111.76	119.84
1	2	165	PRO	C-N-CA	-6.46	111.76	119.84
1	C	165	PRO	CA-C-N	-6.46	111.76	119.84
1	C	165	PRO	C-N-CA	-6.46	111.76	119.84
1	R	165	PRO	CA-C-N	-6.46	111.76	119.84
1	R	165	PRO	C-N-CA	-6.46	111.76	119.84
1	v	165	PRO	CA-C-N	-6.46	111.76	119.84
1	v	165	PRO	C-N-CA	-6.46	111.76	119.84
1	e	165	PRO	CA-C-N	-6.46	111.76	119.84
1	e	165	PRO	C-N-CA	-6.46	111.76	119.84
1	s	165	PRO	CA-C-N	-6.46	111.76	119.84
1	s	165	PRO	C-N-CA	-6.46	111.76	119.84
1	3	165	PRO	CA-C-N	-6.46	111.77	119.84
1	3	165	PRO	C-N-CA	-6.46	111.77	119.84
1	r	165	PRO	CA-C-N	-6.45	111.77	119.84
1	r	165	PRO	C-N-CA	-6.45	111.77	119.84
1	P	165	PRO	CA-C-N	-6.45	111.78	119.84
1	P	165	PRO	C-N-CA	-6.45	111.78	119.84
1	K	165	PRO	CA-C-N	-6.45	111.78	119.84
1	K	165	PRO	C-N-CA	-6.45	111.78	119.84
1	V	165	PRO	CA-C-N	-6.45	111.78	119.84
1	V	165	PRO	C-N-CA	-6.45	111.78	119.84
1	U	165	PRO	CA-C-N	-6.44	111.79	119.84
1	U	165	PRO	C-N-CA	-6.44	111.79	119.84
1	1	165	PRO	CA-C-N	-6.42	111.81	119.84
1	1	165	PRO	C-N-CA	-6.42	111.81	119.84
1	A	165	PRO	N-CA-C	6.09	118.13	110.70
1	4	165	PRO	N-CA-C	6.07	118.11	110.70
1	P	165	PRO	N-CA-C	6.06	118.10	110.70
1	w	165	PRO	N-CA-C	6.06	118.10	110.70
1	J	165	PRO	N-CA-C	6.06	118.09	110.70
1	K	165	PRO	N-CA-C	6.06	118.09	110.70
1	g	165	PRO	N-CA-C	6.05	118.08	110.70
1	h	165	PRO	N-CA-C	6.05	118.08	110.70
1	t	165	PRO	N-CA-C	6.05	118.08	110.70
1	c	165	PRO	N-CA-C	6.05	118.08	110.70
1	f	165	PRO	N-CA-C	6.05	118.08	110.70
1	7	165	PRO	N-CA-C	6.05	118.08	110.70
1	N	165	PRO	N-CA-C	6.04	118.07	110.70
1	U	165	PRO	N-CA-C	6.04	118.07	110.70
1	M	165	PRO	N-CA-C	6.04	118.07	110.70
1	Y	165	PRO	N-CA-C	6.04	118.07	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	o	165	PRO	N-CA-C	6.04	118.07	110.70
1	v	165	PRO	N-CA-C	6.04	118.07	110.70
1	L	165	PRO	N-CA-C	6.04	118.07	110.70
1	R	165	PRO	N-CA-C	6.04	118.06	110.70
1	O	165	PRO	N-CA-C	6.04	118.06	110.70
1	5	165	PRO	N-CA-C	6.04	118.06	110.70
1	G	165	PRO	N-CA-C	6.03	118.06	110.70
1	k	165	PRO	N-CA-C	6.03	118.06	110.70
1	m	165	PRO	N-CA-C	6.03	118.06	110.70
1	T	165	PRO	N-CA-C	6.03	118.06	110.70
1	l	165	PRO	N-CA-C	6.03	118.06	110.70
1	n	165	PRO	N-CA-C	6.03	118.06	110.70
1	r	165	PRO	N-CA-C	6.03	118.06	110.70
1	u	165	PRO	N-CA-C	6.03	118.06	110.70
1	z	165	PRO	N-CA-C	6.03	118.06	110.70
1	X	165	PRO	N-CA-C	6.03	118.05	110.70
1	b	165	PRO	N-CA-C	6.03	118.05	110.70
1	j	165	PRO	N-CA-C	6.03	118.05	110.70
1	s	165	PRO	N-CA-C	6.03	118.05	110.70
1	F	165	PRO	N-CA-C	6.03	118.05	110.70
1	I	165	PRO	N-CA-C	6.02	118.05	110.70
1	a	165	PRO	N-CA-C	6.02	118.05	110.70
1	e	165	PRO	N-CA-C	6.02	118.05	110.70
1	3	165	PRO	N-CA-C	6.02	118.05	110.70
1	D	165	PRO	N-CA-C	6.02	118.04	110.70
1	V	165	PRO	N-CA-C	6.02	118.04	110.70
1	6	165	PRO	N-CA-C	6.02	118.04	110.70
1	Q	165	PRO	N-CA-C	6.01	118.04	110.70
1	x	165	PRO	N-CA-C	6.01	118.04	110.70
1	1	165	PRO	N-CA-C	6.01	118.04	110.70
1	S	165	PRO	N-CA-C	6.01	118.03	110.70
1	0	165	PRO	N-CA-C	6.01	118.03	110.70
1	B	165	PRO	N-CA-C	6.01	118.03	110.70
1	E	165	PRO	N-CA-C	6.01	118.03	110.70
1	Z	165	PRO	N-CA-C	6.01	118.03	110.70
1	q	165	PRO	N-CA-C	6.01	118.03	110.70
1	i	165	PRO	N-CA-C	6.01	118.03	110.70
1	d	165	PRO	N-CA-C	6.01	118.03	110.70
1	W	165	PRO	N-CA-C	6.00	118.03	110.70
1	2	165	PRO	N-CA-C	6.00	118.02	110.70
1	H	165	PRO	N-CA-C	6.00	118.02	110.70
1	p	165	PRO	N-CA-C	6.00	118.02	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	165	PRO	N-CA-C	5.99	118.01	110.70
1	y	165	PRO	N-CA-C	5.99	118.01	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1759	0	1809	8	0
1	1	1759	0	1809	8	0
1	2	1759	0	1809	10	0
1	3	1759	0	1809	6	0
1	4	1759	0	1809	10	0
1	5	1759	0	1809	6	0
1	6	1759	0	1809	7	0
1	7	1759	0	1809	8	0
1	A	1759	0	1809	7	0
1	B	1759	0	1809	6	0
1	C	1759	0	1809	9	0
1	D	1759	0	1809	8	0
1	E	1759	0	1809	8	0
1	F	1759	0	1809	6	0
1	G	1759	0	1809	9	0
1	H	1759	0	1809	8	0
1	I	1759	0	1809	7	0
1	J	1759	0	1809	8	0
1	K	1759	0	1809	9	0
1	L	1759	0	1809	8	0
1	M	1759	0	1809	7	0
1	N	1759	0	1809	6	0
1	O	1759	0	1809	5	0
1	P	1759	0	1809	8	0
1	Q	1759	0	1809	6	0
1	R	1759	0	1809	7	0
1	S	1759	0	1809	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	1759	0	1809	7	0
1	U	1759	0	1809	7	0
1	V	1759	0	1809	9	0
1	W	1759	0	1809	6	0
1	X	1759	0	1809	9	0
1	Y	1759	0	1809	7	0
1	Z	1759	0	1809	7	0
1	a	1759	0	1809	8	0
1	b	1759	0	1809	6	0
1	c	1759	0	1809	8	0
1	d	1759	0	1809	7	0
1	e	1759	0	1809	6	0
1	f	1759	0	1809	8	0
1	g	1759	0	1809	7	0
1	h	1759	0	1809	8	0
1	i	1759	0	1809	7	0
1	j	1759	0	1809	8	0
1	k	1759	0	1809	6	0
1	l	1759	0	1809	9	0
1	m	1759	0	1809	8	0
1	n	1759	0	1809	6	0
1	o	1759	0	1809	7	0
1	p	1759	0	1809	7	0
1	q	1759	0	1809	7	0
1	r	1759	0	1809	11	0
1	s	1759	0	1809	5	0
1	t	1759	0	1809	6	0
1	u	1759	0	1809	9	0
1	v	1759	0	1809	8	0
1	w	1759	0	1809	8	0
1	x	1759	0	1809	6	0
1	y	1759	0	1809	6	0
1	z	1759	0	1809	7	0
All	All	105540	0	108540	426	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (426) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:VAL:HG23	1:B:206:VAL:HG23	1.88	0.56
1:W:205:VAL:HG23	1:W:206:VAL:HG23	1.88	0.56
1:s:205:VAL:HG23	1:s:206:VAL:HG23	1.88	0.56
1:y:205:VAL:HG23	1:y:206:VAL:HG23	1.88	0.56
1:5:205:VAL:HG23	1:5:206:VAL:HG23	1.88	0.56
1:F:205:VAL:HG23	1:F:206:VAL:HG23	1.88	0.56
1:H:205:VAL:HG23	1:H:206:VAL:HG23	1.88	0.56
1:Y:205:VAL:HG23	1:Y:206:VAL:HG23	1.88	0.56
1:e:205:VAL:HG23	1:e:206:VAL:HG23	1.88	0.56
1:n:205:VAL:HG23	1:n:206:VAL:HG23	1.88	0.56
1:u:205:VAL:HG23	1:u:206:VAL:HG23	1.88	0.56
1:Q:205:VAL:HG23	1:Q:206:VAL:HG23	1.88	0.56
1:w:205:VAL:HG23	1:w:206:VAL:HG23	1.88	0.56
1:3:205:VAL:HG23	1:3:206:VAL:HG23	1.88	0.56
1:6:205:VAL:HG23	1:6:206:VAL:HG23	1.88	0.56
1:m:205:VAL:HG23	1:m:206:VAL:HG23	1.88	0.55
1:J:205:VAL:HG23	1:J:206:VAL:HG23	1.88	0.55
1:c:205:VAL:HG23	1:c:206:VAL:HG23	1.88	0.55
1:j:205:VAL:HG23	1:j:206:VAL:HG23	1.88	0.55
1:l:205:VAL:HG23	1:l:206:VAL:HG23	1.88	0.55
1:4:205:VAL:HG23	1:4:206:VAL:HG23	1.88	0.55
1:K:205:VAL:HG23	1:K:206:VAL:HG23	1.88	0.55
1:L:205:VAL:HG23	1:L:206:VAL:HG23	1.88	0.55
1:U:205:VAL:HG23	1:U:206:VAL:HG23	1.88	0.55
1:X:205:VAL:HG23	1:X:206:VAL:HG23	1.88	0.55
1:2:205:VAL:HG23	1:2:206:VAL:HG23	1.88	0.55
1:A:205:VAL:HG23	1:A:206:VAL:HG23	1.88	0.55
1:R:205:VAL:HG23	1:R:206:VAL:HG23	1.88	0.55
1:C:205:VAL:HG23	1:C:206:VAL:HG23	1.88	0.55
1:D:205:VAL:HG23	1:D:206:VAL:HG23	1.88	0.55
1:E:205:VAL:HG23	1:E:206:VAL:HG23	1.88	0.55
1:G:205:VAL:HG23	1:G:206:VAL:HG23	1.88	0.55
1:q:205:VAL:HG23	1:q:206:VAL:HG23	1.88	0.55
1:I:205:VAL:HG23	1:I:206:VAL:HG23	1.88	0.55
1:S:205:VAL:HG23	1:S:206:VAL:HG23	1.88	0.55
1:Z:205:VAL:HG23	1:Z:206:VAL:HG23	1.88	0.55
1:t:205:VAL:HG23	1:t:206:VAL:HG23	1.88	0.55
1:v:205:VAL:HG23	1:v:206:VAL:HG23	1.88	0.55
1:O:205:VAL:HG23	1:O:206:VAL:HG23	1.88	0.55
1:V:205:VAL:HG23	1:V:206:VAL:HG23	1.88	0.55
1:b:205:VAL:HG23	1:b:206:VAL:HG23	1.88	0.55
1:o:205:VAL:HG23	1:o:206:VAL:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:205:VAL:HG23	1:g:206:VAL:HG23	1.88	0.55
1:k:205:VAL:HG23	1:k:206:VAL:HG23	1.88	0.55
1:z:205:VAL:HG23	1:z:206:VAL:HG23	1.88	0.55
1:N:205:VAL:HG23	1:N:206:VAL:HG23	1.88	0.54
1:a:205:VAL:HG23	1:a:206:VAL:HG23	1.88	0.54
1:d:205:VAL:HG23	1:d:206:VAL:HG23	1.88	0.54
1:i:205:VAL:HG23	1:i:206:VAL:HG23	1.88	0.54
1:x:205:VAL:HG23	1:x:206:VAL:HG23	1.88	0.54
1:T:205:VAL:HG23	1:T:206:VAL:HG23	1.88	0.54
1:p:205:VAL:HG23	1:p:206:VAL:HG23	1.88	0.54
1:O:205:VAL:HG23	1:O:206:VAL:HG23	1.88	0.54
1:r:205:VAL:HG23	1:r:206:VAL:HG23	1.88	0.54
1:P:205:VAL:HG23	1:P:206:VAL:HG23	1.88	0.54
1:f:205:VAL:HG23	1:f:206:VAL:HG23	1.88	0.54
1:7:205:VAL:HG23	1:7:206:VAL:HG23	1.88	0.54
1:M:205:VAL:HG23	1:M:206:VAL:HG23	1.88	0.53
1:h:205:VAL:HG23	1:h:206:VAL:HG23	1.88	0.53
1:l:205:VAL:HG23	1:l:206:VAL:HG23	1.88	0.53
1:Y:177:GLU:OE2	1:Y:179:ARG:NE	2.42	0.48
1:p:177:GLU:OE2	1:p:179:ARG:NE	2.42	0.48
1:6:177:GLU:OE2	1:6:179:ARG:NE	2.42	0.48
1:N:177:GLU:OE2	1:N:179:ARG:NE	2.42	0.48
1:O:177:GLU:OE2	1:O:179:ARG:NE	2.42	0.47
1:G:50:MET:HE3	1:u:224:LYS:HE3	1.96	0.47
1:P:177:GLU:OE2	1:P:179:ARG:NE	2.42	0.47
1:m:177:GLU:OE2	1:m:179:ARG:NE	2.42	0.47
1:w:177:GLU:OE2	1:w:179:ARG:NE	2.42	0.47
1:e:177:GLU:OE2	1:e:179:ARG:NE	2.42	0.47
1:x:177:GLU:OE2	1:x:179:ARG:NE	2.42	0.47
1:a:224:LYS:HE3	1:2:50:MET:HE3	1.97	0.47
1:h:177:GLU:OE2	1:h:179:ARG:NE	2.42	0.47
1:u:177:GLU:OE2	1:u:179:ARG:NE	2.42	0.47
1:l:177:GLU:OE2	1:l:179:ARG:NE	2.42	0.47
1:r:177:GLU:OE2	1:r:179:ARG:NE	2.42	0.45
1:5:177:GLU:OE2	1:5:179:ARG:NE	2.42	0.45
1:B:177:GLU:OE2	1:B:179:ARG:NE	2.42	0.45
1:C:224:LYS:HE3	1:r:50:MET:HE3	1.99	0.45
1:a:177:GLU:OE2	1:a:179:ARG:NE	2.42	0.45
1:7:177:GLU:OE2	1:7:179:ARG:NE	2.42	0.45
1:D:177:GLU:OE2	1:D:179:ARG:NE	2.42	0.45
1:F:50:MET:HE3	1:4:224:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:177:GLU:OE2	1:J:179:ARG:NE	2.42	0.45
1:M:177:GLU:OE2	1:M:179:ARG:NE	2.42	0.45
1:f:177:GLU:OE2	1:f:179:ARG:NE	2.42	0.45
1:k:177:GLU:OE2	1:k:179:ARG:NE	2.42	0.45
1:G:224:LYS:HE3	1:u:50:MET:HE3	1.99	0.45
1:a:50:MET:HE3	1:2:224:LYS:HE3	1.98	0.45
1:4:177:GLU:OE2	1:4:179:ARG:NE	2.42	0.45
1:E:177:GLU:OE2	1:E:179:ARG:NE	2.42	0.45
1:r:4:THR:OG1	1:v:90:HIS:NE2	2.38	0.45
1:G:177:GLU:OE2	1:G:179:ARG:NE	2.42	0.44
1:q:177:GLU:OE2	1:q:179:ARG:NE	2.42	0.44
1:c:177:GLU:OE2	1:c:179:ARG:NE	2.42	0.44
1:Z:177:GLU:OE2	1:Z:179:ARG:NE	2.42	0.44
1:v:177:GLU:OE2	1:v:179:ARG:NE	2.42	0.44
1:C:50:MET:HE3	1:r:224:LYS:HE3	2.00	0.43
1:N:185:ASN:HB3	1:N:188:GLY:H	1.83	0.43
1:2:177:GLU:OE2	1:2:179:ARG:NE	2.42	0.43
1:3:185:ASN:HB3	1:3:188:GLY:H	1.84	0.43
1:F:185:ASN:HB3	1:F:188:GLY:H	1.84	0.43
1:H:185:ASN:HB3	1:H:188:GLY:H	1.84	0.43
1:S:177:GLU:OE2	1:S:179:ARG:NE	2.42	0.43
1:Z:185:ASN:HB3	1:Z:188:GLY:H	1.84	0.43
1:v:185:ASN:HB3	1:v:188:GLY:H	1.84	0.43
1:x:185:ASN:HB3	1:x:188:GLY:H	1.84	0.43
1:y:185:ASN:HB3	1:y:188:GLY:H	1.83	0.43
1:5:185:ASN:HB3	1:5:188:GLY:H	1.83	0.43
1:B:185:ASN:HB3	1:B:188:GLY:H	1.84	0.43
1:P:185:ASN:HB3	1:P:188:GLY:H	1.84	0.43
1:R:50:MET:HE3	1:X:224:LYS:HE3	2.00	0.43
1:V:4:THR:OG1	1:4:90:HIS:NE2	2.41	0.43
1:k:185:ASN:HB3	1:k:188:GLY:H	1.83	0.43
1:t:177:GLU:OE2	1:t:179:ARG:NE	2.42	0.43
1:0:185:ASN:HB3	1:0:188:GLY:H	1.84	0.43
1:A:185:ASN:HB3	1:A:188:GLY:H	1.84	0.43
1:Q:185:ASN:HB3	1:Q:188:GLY:H	1.83	0.43
1:a:185:ASN:HB3	1:a:188:GLY:H	1.84	0.43
1:G:185:ASN:HB3	1:G:188:GLY:H	1.83	0.43
1:L:185:ASN:HB3	1:L:188:GLY:H	1.84	0.43
1:R:185:ASN:HB3	1:R:188:GLY:H	1.83	0.43
1:S:185:ASN:HB3	1:S:188:GLY:H	1.83	0.43
1:e:185:ASN:HB3	1:e:188:GLY:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:185:ASN:HB3	1:g:188:GLY:H	1.84	0.43
1:l:177:GLU:OE2	1:l:179:ARG:NE	2.42	0.43
1:n:185:ASN:HB3	1:n:188:GLY:H	1.84	0.43
1:y:177:GLU:OE2	1:y:179:ARG:NE	2.42	0.43
1:U:185:ASN:HB3	1:U:188:GLY:H	1.83	0.43
1:t:185:ASN:HB3	1:t:188:GLY:H	1.84	0.43
1:u:185:ASN:HB3	1:u:188:GLY:H	1.84	0.43
1:I:177:GLU:OE2	1:I:179:ARG:NE	2.42	0.43
1:J:185:ASN:HB3	1:J:188:GLY:H	1.83	0.43
1:M:185:ASN:HB3	1:M:188:GLY:H	1.84	0.43
1:O:185:ASN:HB3	1:O:188:GLY:H	1.84	0.43
1:o:185:ASN:HB3	1:o:188:GLY:H	1.83	0.43
1:U:177:GLU:OE2	1:U:179:ARG:NE	2.42	0.43
1:q:185:ASN:HB3	1:q:188:GLY:H	1.84	0.43
1:4:185:ASN:HB3	1:4:188:GLY:H	1.84	0.43
1:W:177:GLU:OE2	1:W:179:ARG:NE	2.42	0.43
1:f:185:ASN:HB3	1:f:188:GLY:H	1.83	0.43
1:j:185:ASN:HB3	1:j:188:GLY:H	1.84	0.43
1:H:177:GLU:OE2	1:H:179:ARG:NE	2.42	0.42
1:V:185:ASN:HB3	1:V:188:GLY:H	1.83	0.42
1:X:185:ASN:HB3	1:X:188:GLY:H	1.83	0.42
1:b:185:ASN:HB3	1:b:188:GLY:H	1.84	0.42
1:D:185:ASN:HB3	1:D:188:GLY:H	1.84	0.42
1:K:177:GLU:OE2	1:K:179:ARG:NE	2.42	0.42
1:V:50:MET:HE3	1:g:224:LYS:HE3	2.00	0.42
1:z:185:ASN:HB3	1:z:188:GLY:H	1.83	0.42
1:6:185:ASN:HB3	1:6:188:GLY:H	1.83	0.42
1:R:177:GLU:OE2	1:R:179:ARG:NE	2.42	0.42
1:T:177:GLU:OE2	1:T:179:ARG:NE	2.42	0.42
1:c:185:ASN:HB3	1:c:188:GLY:H	1.84	0.42
1:i:177:GLU:OE2	1:i:179:ARG:NE	2.42	0.42
1:L:177:GLU:OE2	1:L:179:ARG:NE	2.42	0.42
1:N:29:TYR:OH	1:N:207:ASP:O	2.38	0.42
1:P:29:TYR:OH	1:P:207:ASP:O	2.38	0.42
1:T:185:ASN:HB3	1:T:188:GLY:H	1.83	0.42
1:i:185:ASN:HB3	1:i:188:GLY:H	1.83	0.42
1:v:29:TYR:OH	1:v:207:ASP:O	2.38	0.42
1:w:185:ASN:HB3	1:w:188:GLY:H	1.84	0.42
1:0:29:TYR:OH	1:0:207:ASP:O	2.38	0.42
1:C:177:GLU:OE2	1:C:179:ARG:NE	2.42	0.42
1:E:185:ASN:HB3	1:E:188:GLY:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:29:TYR:OH	1:Z:207:ASP:O	2.38	0.42
1:d:185:ASN:HB3	1:d:188:GLY:H	1.84	0.42
1:m:185:ASN:HB3	1:m:188:GLY:H	1.84	0.42
1:p:185:ASN:HB3	1:p:188:GLY:H	1.84	0.42
1:s:177:GLU:OE2	1:s:179:ARG:NE	2.42	0.42
1:x:29:TYR:OH	1:x:207:ASP:O	2.38	0.42
1:X:177:GLU:OE2	1:X:179:ARG:NE	2.42	0.42
1:Y:185:ASN:HB3	1:Y:188:GLY:H	1.84	0.42
1:s:29:TYR:OH	1:s:207:ASP:O	2.38	0.42
1:2:185:ASN:HB3	1:2:188:GLY:H	1.83	0.42
1:D:29:TYR:OH	1:D:207:ASP:O	2.38	0.42
1:K:29:TYR:OH	1:K:207:ASP:O	2.38	0.42
1:l:29:TYR:OH	1:l:207:ASP:O	2.38	0.42
1:E:29:TYR:OH	1:E:207:ASP:O	2.38	0.42
1:F:137:GLN:HB2	1:F:140:GLU:HG3	2.02	0.42
1:J:137:GLN:HB2	1:J:140:GLU:HG3	2.02	0.42
1:K:185:ASN:HB3	1:K:188:GLY:H	1.84	0.42
1:V:224:LYS:HE3	1:g:50:MET:HE3	2.02	0.42
1:Y:137:GLN:HB2	1:Y:140:GLU:HG3	2.02	0.42
1:m:137:GLN:HB2	1:m:140:GLU:HG3	2.02	0.42
1:w:29:TYR:OH	1:w:207:ASP:O	2.38	0.42
1:A:177:GLU:OE2	1:A:179:ARG:NE	2.42	0.42
1:c:29:TYR:OH	1:c:207:ASP:O	2.38	0.42
1:d:4:THR:OG1	1:f:90:HIS:NE2	2.42	0.42
1:h:137:GLN:HB2	1:h:140:GLU:HG3	2.02	0.42
1:l:185:ASN:HB3	1:l:188:GLY:H	1.84	0.42
1:m:29:TYR:OH	1:m:207:ASP:O	2.38	0.42
1:2:29:TYR:OH	1:2:207:ASP:O	2.38	0.42
1:3:137:GLN:HB2	1:3:140:GLU:HG3	2.02	0.42
1:4:137:GLN:HB2	1:4:140:GLU:HG3	2.02	0.42
1:6:137:GLN:HB2	1:6:140:GLU:HG3	2.02	0.42
1:P:137:GLN:HB2	1:P:140:GLU:HG3	2.02	0.42
1:W:29:TYR:OH	1:W:207:ASP:O	2.38	0.42
1:e:137:GLN:HB2	1:e:140:GLU:HG3	2.02	0.42
1:k:137:GLN:HB2	1:k:140:GLU:HG3	2.02	0.42
1:m:170:ILE:HG22	1:m:200:SER:HB2	2.02	0.42
1:7:185:ASN:HB3	1:7:188:GLY:H	1.84	0.42
1:A:137:GLN:HB2	1:A:140:GLU:HG3	2.02	0.41
1:H:158:ASN:HD21	1:H:196:SER:HB3	1.85	0.41
1:I:137:GLN:HB2	1:I:140:GLU:HG3	2.02	0.41
1:O:137:GLN:HB2	1:O:140:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:185:ASN:HB3	1:W:188:GLY:H	1.84	0.41
1:a:137:GLN:HB2	1:a:140:GLU:HG3	2.02	0.41
1:d:29:TYR:OH	1:d:207:ASP:O	2.38	0.41
1:f:137:GLN:HB2	1:f:140:GLU:HG3	2.02	0.41
1:g:137:GLN:HB2	1:g:140:GLU:HG3	2.02	0.41
1:j:177:GLU:OE2	1:j:179:ARG:NE	2.42	0.41
1:p:29:TYR:OH	1:p:207:ASP:O	2.38	0.41
1:r:185:ASN:HB3	1:r:188:GLY:H	1.84	0.41
1:w:137:GLN:HB2	1:w:140:GLU:HG3	2.02	0.41
1:y:29:TYR:OH	1:y:207:ASP:O	2.38	0.41
1:y:158:ASN:HD21	1:y:196:SER:HB3	1.85	0.41
1:0:137:GLN:HB2	1:0:140:GLU:HG3	2.02	0.41
1:C:137:GLN:HB2	1:C:140:GLU:HG3	2.02	0.41
1:G:158:ASN:HD21	1:G:196:SER:HB3	1.86	0.41
1:L:137:GLN:HB2	1:L:140:GLU:HG3	2.02	0.41
1:M:29:TYR:OH	1:M:207:ASP:O	2.38	0.41
1:M:137:GLN:HB2	1:M:140:GLU:HG3	2.02	0.41
1:Y:29:TYR:OH	1:Y:207:ASP:O	2.38	0.41
1:Y:170:ILE:HG22	1:Y:200:SER:HB2	2.03	0.41
1:e:29:TYR:OH	1:e:207:ASP:O	2.38	0.41
1:q:158:ASN:HD21	1:q:196:SER:HB3	1.85	0.41
1:q:170:ILE:HG22	1:q:200:SER:HB2	2.03	0.41
1:s:185:ASN:HB3	1:s:188:GLY:H	1.83	0.41
1:u:137:GLN:HB2	1:u:140:GLU:HG3	2.02	0.41
1:w:158:ASN:HD21	1:w:196:SER:HB3	1.86	0.41
1:1:137:GLN:HB2	1:1:140:GLU:HG3	2.02	0.41
1:6:29:TYR:OH	1:6:207:ASP:O	2.38	0.41
1:6:170:ILE:HG22	1:6:200:SER:HB2	2.03	0.41
1:G:170:ILE:HG22	1:G:200:SER:HB2	2.03	0.41
1:H:29:TYR:OH	1:H:207:ASP:O	2.38	0.41
1:N:158:ASN:HD21	1:N:196:SER:HB3	1.86	0.41
1:O:170:ILE:HG22	1:O:200:SER:HB2	2.03	0.41
1:P:158:ASN:HD21	1:P:196:SER:HB3	1.86	0.41
1:Q:170:ILE:HG22	1:Q:200:SER:HB2	2.03	0.41
1:R:137:GLN:HB2	1:R:140:GLU:HG3	2.02	0.41
1:R:158:ASN:HD21	1:R:196:SER:HB3	1.86	0.41
1:S:158:ASN:HD21	1:S:196:SER:HB3	1.86	0.41
1:T:29:TYR:OH	1:T:207:ASP:O	2.38	0.41
1:U:158:ASN:HD21	1:U:196:SER:HB3	1.86	0.41
1:V:137:GLN:HB2	1:V:140:GLU:HG3	2.02	0.41
1:f:29:TYR:OH	1:f:207:ASP:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:137:GLN:HB2	1:l:140:GLU:HG3	2.02	0.41
1:m:158:ASN:HD21	1:m:196:SER:HB3	1.86	0.41
1:n:170:ILE:HG22	1:n:200:SER:HB2	2.03	0.41
1:t:158:ASN:HD21	1:t:196:SER:HB3	1.86	0.41
1:u:29:TYR:OH	1:u:207:ASP:O	2.38	0.41
1:w:170:ILE:HG22	1:w:200:SER:HB2	2.03	0.41
1:z:137:GLN:HB2	1:z:140:GLU:HG3	2.02	0.41
1:1:158:ASN:HD21	1:1:196:SER:HB3	1.86	0.41
1:1:170:ILE:HG22	1:1:200:SER:HB2	2.03	0.41
1:T:137:GLN:HB2	1:T:140:GLU:HG3	2.02	0.41
1:U:137:GLN:HB2	1:U:140:GLU:HG3	2.02	0.41
1:V:158:ASN:HD21	1:V:196:SER:HB3	1.85	0.41
1:b:177:GLU:OE2	1:b:179:ARG:NE	2.42	0.41
1:d:137:GLN:HB2	1:d:140:GLU:HG3	2.02	0.41
1:h:158:ASN:HD21	1:h:196:SER:HB3	1.85	0.41
1:i:29:TYR:OH	1:i:207:ASP:O	2.38	0.41
1:o:137:GLN:HB2	1:o:140:GLU:HG3	2.02	0.41
1:p:137:GLN:HB2	1:p:140:GLU:HG3	2.02	0.41
1:x:158:ASN:HD21	1:x:196:SER:HB3	1.86	0.41
1:1:185:ASN:HB3	1:1:188:GLY:H	1.84	0.41
1:B:29:TYR:OH	1:B:207:ASP:O	2.38	0.41
1:B:170:ILE:HG22	1:B:200:SER:HB2	2.02	0.41
1:C:170:ILE:HG22	1:C:200:SER:HB2	2.02	0.41
1:I:170:ILE:HG22	1:I:200:SER:HB2	2.02	0.41
1:Q:158:ASN:HD21	1:Q:196:SER:HB3	1.85	0.41
1:W:137:GLN:HB2	1:W:140:GLU:HG3	2.02	0.41
1:X:158:ASN:HD21	1:X:196:SER:HB3	1.85	0.41
1:g:170:ILE:HG22	1:g:200:SER:HB2	2.03	0.41
1:h:170:ILE:HG22	1:h:200:SER:HB2	2.03	0.41
1:h:185:ASN:HB3	1:h:188:GLY:H	1.84	0.41
1:n:158:ASN:HD21	1:n:196:SER:HB3	1.86	0.41
1:p:170:ILE:HG22	1:p:200:SER:HB2	2.02	0.41
1:v:158:ASN:HD21	1:v:196:SER:HB3	1.85	0.41
1:z:158:ASN:HD21	1:z:196:SER:HB3	1.86	0.41
1:z:170:ILE:HG22	1:z:200:SER:HB2	2.02	0.41
1:O:158:ASN:HD21	1:O:196:SER:HB3	1.86	0.41
1:3:29:TYR:OH	1:3:207:ASP:O	2.38	0.41
1:5:29:TYR:OH	1:5:207:ASP:O	2.38	0.41
1:5:137:GLN:HB2	1:5:140:GLU:HG3	2.02	0.41
1:B:137:GLN:HB2	1:B:140:GLU:HG3	2.02	0.41
1:C:185:ASN:HB3	1:C:188:GLY:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:TYR:OH	1:F:207:ASP:O	2.38	0.41
1:G:29:TYR:OH	1:G:207:ASP:O	2.38	0.41
1:J:158:ASN:HD21	1:J:196:SER:HB3	1.85	0.41
1:S:29:TYR:OH	1:S:207:ASP:O	2.38	0.41
1:V:170:ILE:HG22	1:V:200:SER:HB2	2.03	0.41
1:Y:158:ASN:HD21	1:Y:196:SER:HB3	1.86	0.41
1:Z:158:ASN:HD21	1:Z:196:SER:HB3	1.85	0.41
1:b:137:GLN:HB2	1:b:140:GLU:HG3	2.02	0.41
1:d:170:ILE:HG22	1:d:200:SER:HB2	2.02	0.41
1:f:170:ILE:HG22	1:f:200:SER:HB2	2.02	0.41
1:i:137:GLN:HB2	1:i:140:GLU:HG3	2.02	0.41
1:s:137:GLN:HB2	1:s:140:GLU:HG3	2.02	0.41
1:6:158:ASN:HD21	1:6:196:SER:HB3	1.86	0.41
1:I:185:ASN:HB3	1:I:188:GLY:H	1.84	0.41
1:K:224:LYS:HE3	1:l:50:MET:HE3	2.03	0.41
1:L:50:MET:HE3	1:o:224:LYS:HE3	2.03	0.41
1:M:170:ILE:HG22	1:M:200:SER:HB2	2.03	0.41
1:R:170:ILE:HG22	1:R:200:SER:HB2	2.03	0.41
1:U:170:ILE:HG22	1:U:200:SER:HB2	2.03	0.41
1:e:158:ASN:HD21	1:e:196:SER:HB3	1.86	0.41
1:g:29:TYR:OH	1:g:207:ASP:O	2.38	0.41
1:j:158:ASN:HD21	1:j:196:SER:HB3	1.86	0.41
1:n:137:GLN:HB2	1:n:140:GLU:HG3	2.02	0.41
1:q:29:TYR:OH	1:q:207:ASP:O	2.38	0.41
1:v:170:ILE:HG22	1:v:200:SER:HB2	2.03	0.41
1:5:170:ILE:HG22	1:5:200:SER:HB2	2.03	0.41
1:A:29:TYR:OH	1:A:207:ASP:O	2.38	0.41
1:K:137:GLN:HB2	1:K:140:GLU:HG3	2.02	0.41
1:L:158:ASN:HD21	1:L:196:SER:HB3	1.85	0.41
1:M:158:ASN:HD21	1:M:196:SER:HB3	1.86	0.41
1:O:29:TYR:OH	1:O:207:ASP:O	2.38	0.41
1:Q:137:GLN:HB2	1:Q:140:GLU:HG3	2.02	0.41
1:X:170:ILE:HG22	1:X:200:SER:HB2	2.03	0.41
1:Z:170:ILE:HG22	1:Z:200:SER:HB2	2.03	0.41
1:a:170:ILE:HG22	1:a:200:SER:HB2	2.03	0.41
1:b:29:TYR:OH	1:b:207:ASP:O	2.38	0.41
1:c:170:ILE:HG22	1:c:200:SER:HB2	2.03	0.41
1:d:158:ASN:HD21	1:d:196:SER:HB3	1.86	0.41
1:j:29:TYR:OH	1:j:207:ASP:O	2.38	0.41
1:j:170:ILE:HG22	1:j:200:SER:HB2	2.03	0.41
1:k:170:ILE:HG22	1:k:200:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:29:TYR:OH	1:o:207:ASP:O	2.38	0.41
1:o:177:GLU:OE2	1:o:179:ARG:NE	2.42	0.41
1:p:158:ASN:HD21	1:p:196:SER:HB3	1.86	0.41
1:t:29:TYR:OH	1:t:207:ASP:O	2.38	0.41
1:v:137:GLN:HB2	1:v:140:GLU:HG3	2.02	0.41
1:4:158:ASN:HD21	1:4:196:SER:HB3	1.86	0.41
1:A:158:ASN:HD21	1:A:196:SER:HB3	1.86	0.41
1:A:170:ILE:HG22	1:A:200:SER:HB2	2.03	0.41
1:C:158:ASN:HD21	1:C:196:SER:HB3	1.85	0.41
1:D:147:THR:HB	1:D:170:ILE:HG13	2.03	0.41
1:D:158:ASN:HD21	1:D:196:SER:HB3	1.85	0.41
1:E:158:ASN:HD21	1:E:196:SER:HB3	1.86	0.41
1:F:158:ASN:HD21	1:F:196:SER:HB3	1.85	0.41
1:I:158:ASN:HD21	1:I:196:SER:HB3	1.86	0.41
1:L:29:TYR:OH	1:L:207:ASP:O	2.38	0.41
1:L:170:ILE:HG22	1:L:200:SER:HB2	2.03	0.41
1:P:170:ILE:HG22	1:P:200:SER:HB2	2.03	0.41
1:V:29:TYR:OH	1:V:207:ASP:O	2.38	0.41
1:X:29:TYR:OH	1:X:207:ASP:O	2.38	0.41
1:X:137:GLN:HB2	1:X:140:GLU:HG3	2.02	0.41
1:Z:137:GLN:HB2	1:Z:140:GLU:HG3	2.02	0.41
1:f:158:ASN:HD21	1:f:196:SER:HB3	1.86	0.41
1:h:29:TYR:OH	1:h:207:ASP:O	2.38	0.41
1:m:147:THR:HB	1:m:170:ILE:HG13	2.03	0.41
1:r:137:GLN:HB2	1:r:140:GLU:HG3	2.02	0.41
1:u:158:ASN:HD21	1:u:196:SER:HB3	1.86	0.41
1:0:170:ILE:HG22	1:0:200:SER:HB2	2.03	0.41
1:1:29:TYR:OH	1:1:207:ASP:O	2.38	0.41
1:2:137:GLN:HB2	1:2:140:GLU:HG3	2.02	0.41
1:2:170:ILE:HG22	1:2:200:SER:HB2	2.03	0.41
1:3:158:ASN:HD21	1:3:196:SER:HB3	1.86	0.41
1:4:147:THR:HB	1:4:170:ILE:HG13	2.03	0.41
1:7:137:GLN:HB2	1:7:140:GLU:HG3	2.02	0.41
1:7:170:ILE:HG22	1:7:200:SER:HB2	2.02	0.41
1:C:29:TYR:OH	1:C:207:ASP:O	2.38	0.41
1:E:147:THR:HB	1:E:170:ILE:HG13	2.03	0.41
1:G:137:GLN:HB2	1:G:140:GLU:HG3	2.02	0.41
1:H:170:ILE:HG22	1:H:200:SER:HB2	2.03	0.41
1:J:147:THR:HB	1:J:170:ILE:HG13	2.03	0.41
1:X:147:THR:HB	1:X:170:ILE:HG13	2.04	0.41
1:a:158:ASN:HD21	1:a:196:SER:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:170:ILE:HG22	1:b:200:SER:HB2	2.03	0.41
1:c:137:GLN:HB2	1:c:140:GLU:HG3	2.02	0.41
1:j:137:GLN:HB2	1:j:140:GLU:HG3	2.02	0.41
1:j:147:THR:HB	1:j:170:ILE:HG13	2.03	0.41
1:r:170:ILE:HG22	1:r:200:SER:HB2	2.03	0.41
1:t:137:GLN:HB2	1:t:140:GLU:HG3	2.02	0.41
1:w:147:THR:HB	1:w:170:ILE:HG13	2.03	0.41
1:y:170:ILE:HG22	1:y:200:SER:HB2	2.03	0.41
1:D:137:GLN:HB2	1:D:140:GLU:HG3	2.02	0.40
1:K:50:MET:HE3	1:l:224:LYS:HE3	2.03	0.40
1:S:137:GLN:HB2	1:S:140:GLU:HG3	2.02	0.40
1:T:147:THR:HB	1:T:170:ILE:HG13	2.03	0.40
1:c:158:ASN:HD21	1:c:196:SER:HB3	1.86	0.40
1:n:29:TYR:OH	1:n:207:ASP:O	2.38	0.40
1:o:170:ILE:HG22	1:o:200:SER:HB2	2.02	0.40
1:z:29:TYR:OH	1:z:207:ASP:O	2.38	0.40
1:4:29:TYR:OH	1:4:207:ASP:O	2.38	0.40
1:4:170:ILE:HG22	1:4:200:SER:HB2	2.02	0.40
1:E:170:ILE:HG22	1:E:200:SER:HB2	2.02	0.40
1:P:147:THR:HB	1:P:170:ILE:HG13	2.03	0.40
1:Q:29:TYR:OH	1:Q:207:ASP:O	2.38	0.40
1:c:147:THR:HB	1:c:170:ILE:HG13	2.03	0.40
1:i:147:THR:HB	1:i:170:ILE:HG13	2.03	0.40
1:i:158:ASN:HD21	1:i:196:SER:HB3	1.85	0.40
1:q:137:GLN:HB2	1:q:140:GLU:HG3	2.02	0.40
1:0:147:THR:HB	1:0:170:ILE:HG13	2.03	0.40
1:2:147:THR:HB	1:2:170:ILE:HG13	2.04	0.40
1:2:158:ASN:HD21	1:2:196:SER:HB3	1.86	0.40
1:D:170:ILE:HG22	1:D:200:SER:HB2	2.02	0.40
1:H:137:GLN:HB2	1:H:140:GLU:HG3	2.02	0.40
1:I:29:TYR:OH	1:I:207:ASP:O	2.38	0.40
1:J:29:TYR:OH	1:J:207:ASP:O	2.38	0.40
1:J:170:ILE:HG22	1:J:200:SER:HB2	2.03	0.40
1:K:147:THR:HB	1:K:170:ILE:HG13	2.03	0.40
1:W:170:ILE:HG22	1:W:200:SER:HB2	2.03	0.40
1:k:158:ASN:HD21	1:k:196:SER:HB3	1.86	0.40
1:r:29:TYR:OH	1:r:207:ASP:O	2.38	0.40
1:7:158:ASN:HD21	1:7:196:SER:HB3	1.86	0.40
1:K:170:ILE:HG22	1:K:200:SER:HB2	2.03	0.40
1:N:137:GLN:HB2	1:N:140:GLU:HG3	2.02	0.40
1:T:158:ASN:HD21	1:T:196:SER:HB3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:147:THR:HB	1:h:170:ILE:HG13	2.03	0.40
1:l:147:THR:HB	1:l:170:ILE:HG13	2.03	0.40
1:l:170:ILE:HG22	1:l:200:SER:HB2	2.03	0.40
1:x:137:GLN:HB2	1:x:140:GLU:HG3	2.02	0.40
1:1:147:THR:HB	1:1:170:ILE:HG13	2.03	0.40
1:7:29:TYR:OH	1:7:207:ASP:O	2.38	0.40
1:7:147:THR:HB	1:7:170:ILE:HG13	2.03	0.40
1:E:137:GLN:HB2	1:E:140:GLU:HG3	2.02	0.40
1:H:147:THR:HB	1:H:170:ILE:HG13	2.03	0.40
1:U:29:TYR:OH	1:U:207:ASP:O	2.38	0.40
1:r:147:THR:HB	1:r:170:ILE:HG13	2.03	0.40
1:r:158:ASN:HD21	1:r:196:SER:HB3	1.86	0.40
1:u:170:ILE:HG22	1:u:200:SER:HB2	2.02	0.40
1:z:147:THR:HB	1:z:170:ILE:HG13	2.03	0.40
1:3:170:ILE:HG22	1:3:200:SER:HB2	2.02	0.40

There are no symmetry-related clashes.

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	0	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	1	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	2	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	3	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	4	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	5	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	6	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	7	227/647 (35%)	220 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	B	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	C	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	D	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	E	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	F	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	G	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	H	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	I	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	J	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	K	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	L	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	M	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	N	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	O	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	P	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	Q	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	R	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	S	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	T	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	U	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	V	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	W	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	X	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	Y	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	Z	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	a	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	b	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	c	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	d	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	e	227/647 (35%)	220 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	f	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	g	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	h	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	i	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	j	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	k	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	l	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	m	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	n	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	o	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	p	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	q	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	r	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	s	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	t	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	u	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	v	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	w	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	x	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	y	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
1	z	227/647 (35%)	220 (97%)	7 (3%)	0	100	100
All	All	13620/38820 (35%)	13200 (97%)	420 (3%)	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	195/526 (37%)	195 (100%)	0	100	100
1	1	195/526 (37%)	195 (100%)	0	100	100
1	2	195/526 (37%)	195 (100%)	0	100	100
1	3	195/526 (37%)	195 (100%)	0	100	100
1	4	195/526 (37%)	195 (100%)	0	100	100
1	5	195/526 (37%)	195 (100%)	0	100	100
1	6	195/526 (37%)	195 (100%)	0	100	100
1	7	195/526 (37%)	195 (100%)	0	100	100
1	A	195/526 (37%)	195 (100%)	0	100	100
1	B	195/526 (37%)	195 (100%)	0	100	100
1	C	195/526 (37%)	195 (100%)	0	100	100
1	D	195/526 (37%)	195 (100%)	0	100	100
1	E	195/526 (37%)	195 (100%)	0	100	100
1	F	195/526 (37%)	195 (100%)	0	100	100
1	G	195/526 (37%)	195 (100%)	0	100	100
1	H	195/526 (37%)	195 (100%)	0	100	100
1	I	195/526 (37%)	195 (100%)	0	100	100
1	J	195/526 (37%)	195 (100%)	0	100	100
1	K	195/526 (37%)	195 (100%)	0	100	100
1	L	195/526 (37%)	195 (100%)	0	100	100
1	M	195/526 (37%)	195 (100%)	0	100	100
1	N	195/526 (37%)	195 (100%)	0	100	100
1	O	195/526 (37%)	195 (100%)	0	100	100
1	P	195/526 (37%)	195 (100%)	0	100	100
1	Q	195/526 (37%)	195 (100%)	0	100	100
1	R	195/526 (37%)	195 (100%)	0	100	100
1	S	195/526 (37%)	195 (100%)	0	100	100
1	T	195/526 (37%)	195 (100%)	0	100	100
1	U	195/526 (37%)	195 (100%)	0	100	100
1	V	195/526 (37%)	195 (100%)	0	100	100
1	W	195/526 (37%)	195 (100%)	0	100	100
1	X	195/526 (37%)	195 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	195/526 (37%)	195 (100%)	0	100	100
1	Z	195/526 (37%)	195 (100%)	0	100	100
1	a	195/526 (37%)	195 (100%)	0	100	100
1	b	195/526 (37%)	195 (100%)	0	100	100
1	c	195/526 (37%)	195 (100%)	0	100	100
1	d	195/526 (37%)	195 (100%)	0	100	100
1	e	195/526 (37%)	195 (100%)	0	100	100
1	f	195/526 (37%)	195 (100%)	0	100	100
1	g	195/526 (37%)	195 (100%)	0	100	100
1	h	195/526 (37%)	195 (100%)	0	100	100
1	i	195/526 (37%)	195 (100%)	0	100	100
1	j	195/526 (37%)	195 (100%)	0	100	100
1	k	195/526 (37%)	195 (100%)	0	100	100
1	l	195/526 (37%)	195 (100%)	0	100	100
1	m	195/526 (37%)	195 (100%)	0	100	100
1	n	195/526 (37%)	195 (100%)	0	100	100
1	o	195/526 (37%)	195 (100%)	0	100	100
1	p	195/526 (37%)	195 (100%)	0	100	100
1	q	195/526 (37%)	195 (100%)	0	100	100
1	r	195/526 (37%)	195 (100%)	0	100	100
1	s	195/526 (37%)	195 (100%)	0	100	100
1	t	195/526 (37%)	195 (100%)	0	100	100
1	u	195/526 (37%)	195 (100%)	0	100	100
1	v	195/526 (37%)	195 (100%)	0	100	100
1	w	195/526 (37%)	195 (100%)	0	100	100
1	x	195/526 (37%)	195 (100%)	0	100	100
1	y	195/526 (37%)	195 (100%)	0	100	100
1	z	195/526 (37%)	195 (100%)	0	100	100
All	All	11700/31560 (37%)	11700 (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. All (145)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	158	ASN
1	B	17	GLN
1	B	88	GLN
1	B	158	ASN
1	C	88	GLN
1	C	158	ASN
1	D	88	GLN
1	D	158	ASN
1	E	17	GLN
1	E	88	GLN
1	E	158	ASN
1	F	88	GLN
1	F	158	ASN
1	G	17	GLN
1	G	88	GLN
1	G	158	ASN
1	H	88	GLN
1	H	158	ASN
1	I	88	GLN
1	I	158	ASN
1	J	88	GLN
1	J	158	ASN
1	K	17	GLN
1	K	88	GLN
1	K	158	ASN
1	L	88	GLN
1	L	158	ASN
1	M	17	GLN
1	M	88	GLN
1	M	158	ASN
1	N	88	GLN
1	N	158	ASN
1	O	17	GLN
1	O	88	GLN
1	O	158	ASN
1	P	17	GLN
1	P	88	GLN
1	P	158	ASN
1	Q	88	GLN
1	Q	158	ASN
1	R	88	GLN

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Mol	Chain	Res	Type
1	R	158	ASN
1	S	88	GLN
1	S	158	ASN
1	T	17	GLN
1	T	88	GLN
1	T	158	ASN
1	U	88	GLN
1	U	158	ASN
1	V	17	GLN
1	V	88	GLN
1	V	158	ASN
1	W	88	GLN
1	W	158	ASN
1	X	17	GLN
1	X	88	GLN
1	X	158	ASN
1	Y	17	GLN
1	Y	88	GLN
1	Y	158	ASN
1	Z	88	GLN
1	Z	158	ASN
1	a	88	GLN
1	a	158	ASN
1	b	17	GLN
1	b	88	GLN
1	b	158	ASN
1	c	88	GLN
1	c	158	ASN
1	d	88	GLN
1	d	158	ASN
1	e	17	GLN
1	e	88	GLN
1	e	158	ASN
1	f	17	GLN
1	f	88	GLN
1	f	158	ASN
1	g	17	GLN
1	g	88	GLN
1	g	158	ASN
1	h	88	GLN
1	h	158	ASN
1	i	17	GLN

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Mol	Chain	Res	Type
1	i	88	GLN
1	i	158	ASN
1	j	17	GLN
1	j	88	GLN
1	j	158	ASN
1	k	88	GLN
1	k	158	ASN
1	l	17	GLN
1	l	88	GLN
1	l	158	ASN
1	m	88	GLN
1	m	158	ASN
1	n	88	GLN
1	n	158	ASN
1	o	88	GLN
1	o	158	ASN
1	p	88	GLN
1	p	158	ASN
1	q	17	GLN
1	q	88	GLN
1	q	158	ASN
1	r	88	GLN
1	r	158	ASN
1	s	17	GLN
1	s	88	GLN
1	s	158	ASN
1	t	88	GLN
1	t	158	ASN
1	u	88	GLN
1	u	158	ASN
1	v	88	GLN
1	v	158	ASN
1	w	88	GLN
1	w	158	ASN
1	x	17	GLN
1	x	88	GLN
1	x	158	ASN
1	y	88	GLN
1	y	158	ASN
1	z	17	GLN
1	z	88	GLN
1	z	158	ASN

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Mol	Chain	Res	Type
1	0	17	GLN
1	0	88	GLN
1	0	158	ASN
1	1	88	GLN
1	1	158	ASN
1	2	88	GLN
1	2	158	ASN
1	3	88	GLN
1	3	158	ASN
1	4	88	GLN
1	4	158	ASN
1	5	17	GLN
1	5	88	GLN
1	5	158	ASN
1	6	17	GLN
1	6	88	GLN
1	6	158	ASN
1	7	88	GLN
1	7	158	ASN

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

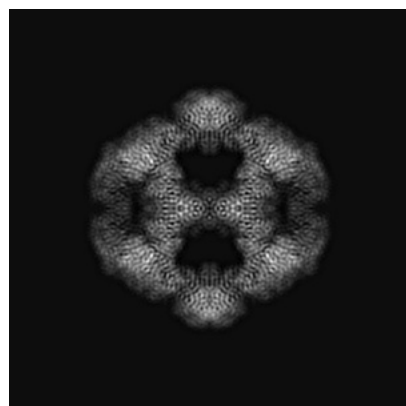
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37969. These allow visual inspection of the internal detail of the map and identification of artifacts.

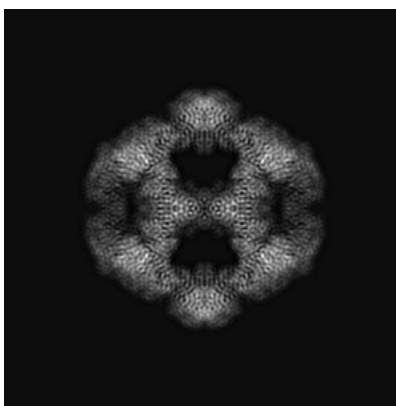
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

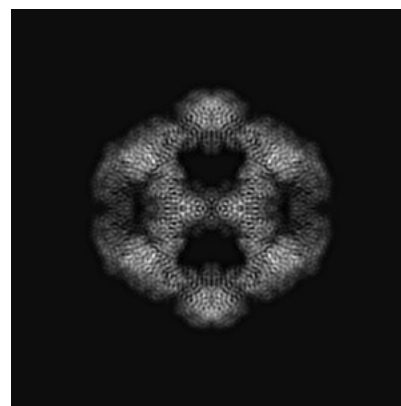
6.1.1 Primary map



X

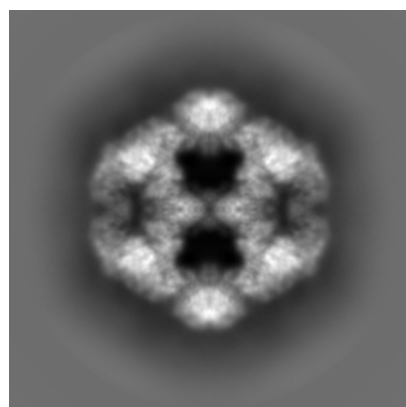


Y

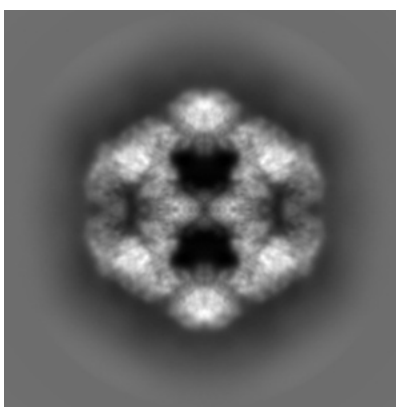


Z

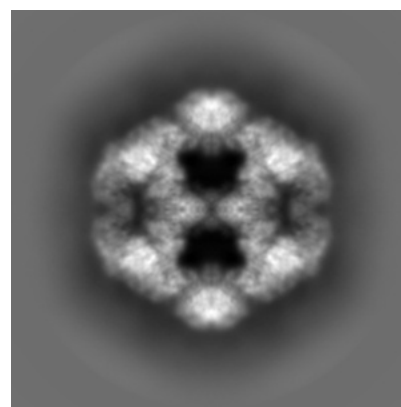
6.1.2 Raw map



X



Y

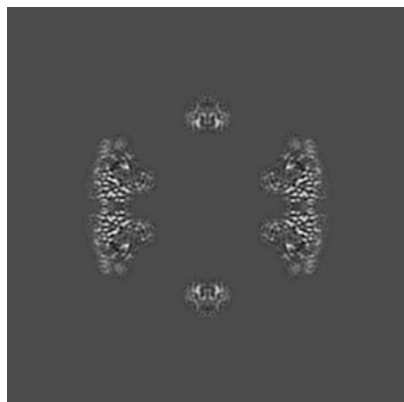


Z

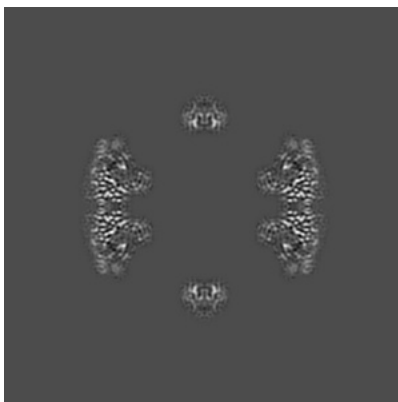
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

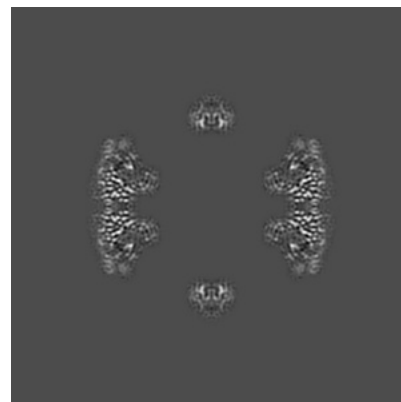
6.2.1 Primary map



X Index: 180

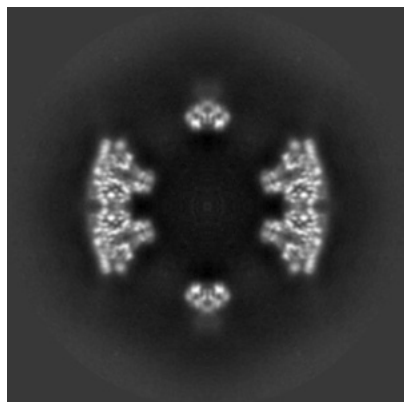


Y Index: 180

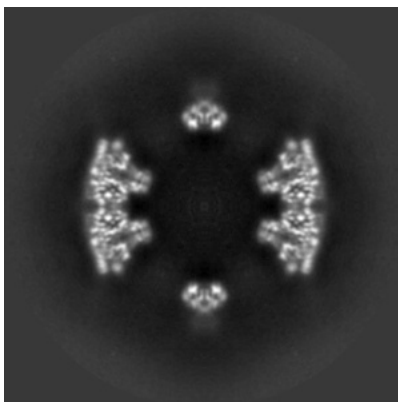


Z Index: 180

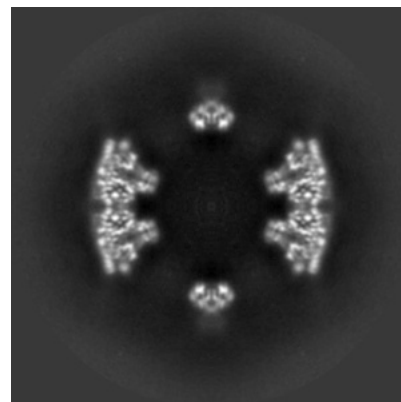
6.2.2 Raw map



X Index: 180



Y Index: 180

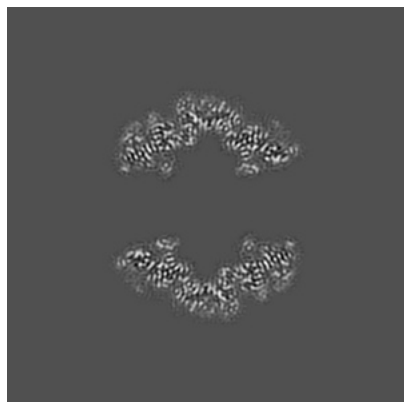


Z Index: 180

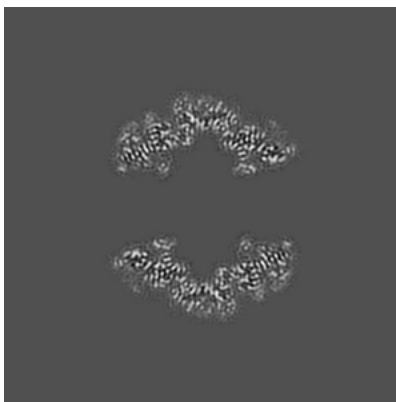
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

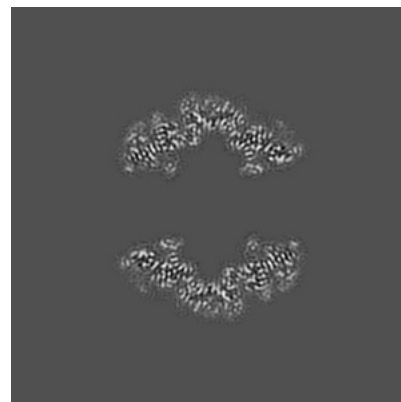
6.3.1 Primary map



X Index: 137

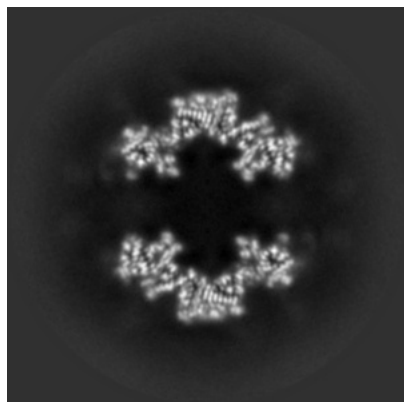


Y Index: 137

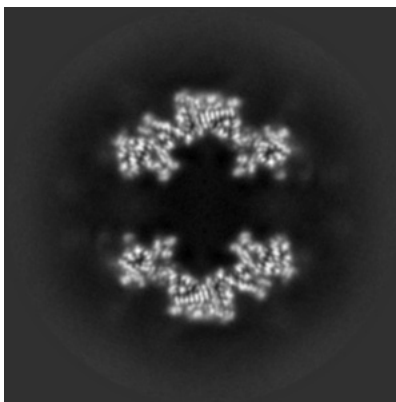


Z Index: 137

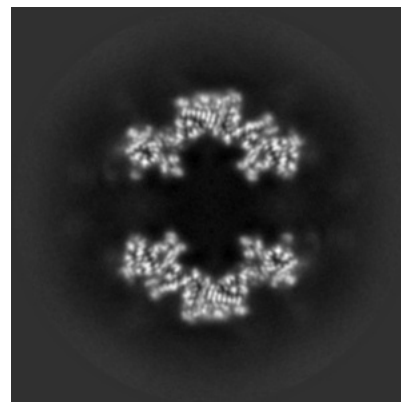
6.3.2 Raw map



X Index: 217



Y Index: 143

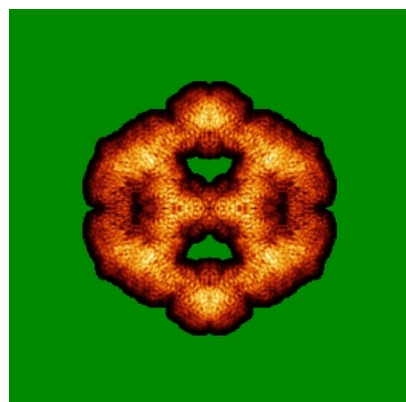


Z Index: 217

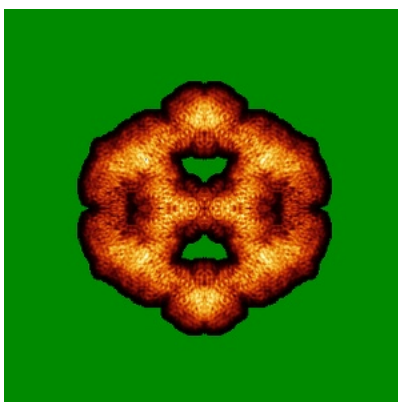
The images above show the largest variance slices of the map in three orthogonal directions.

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

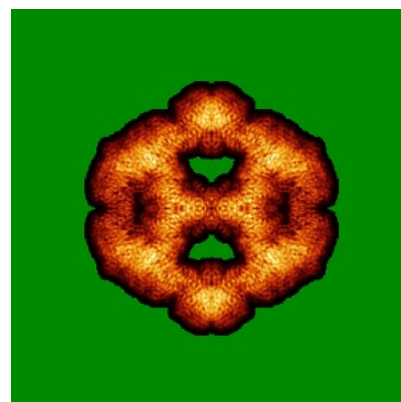
6.4.1 Primary map



X

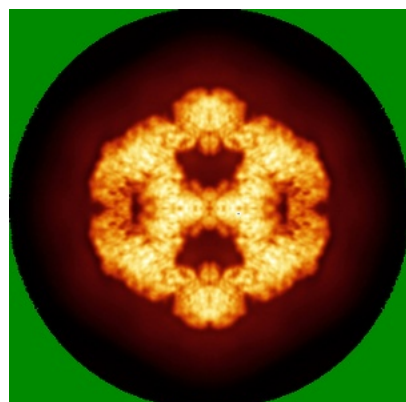


Y

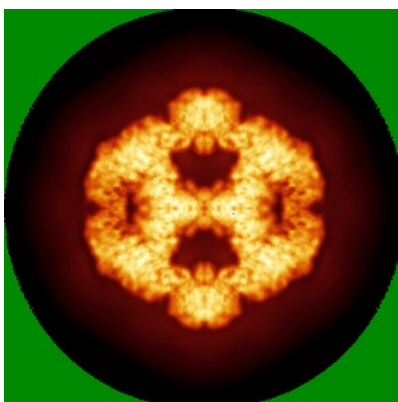


Z

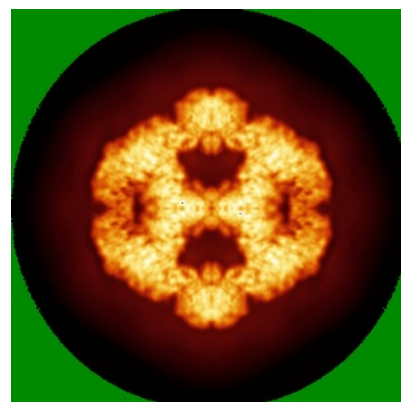
6.4.2 Raw map



X



Y

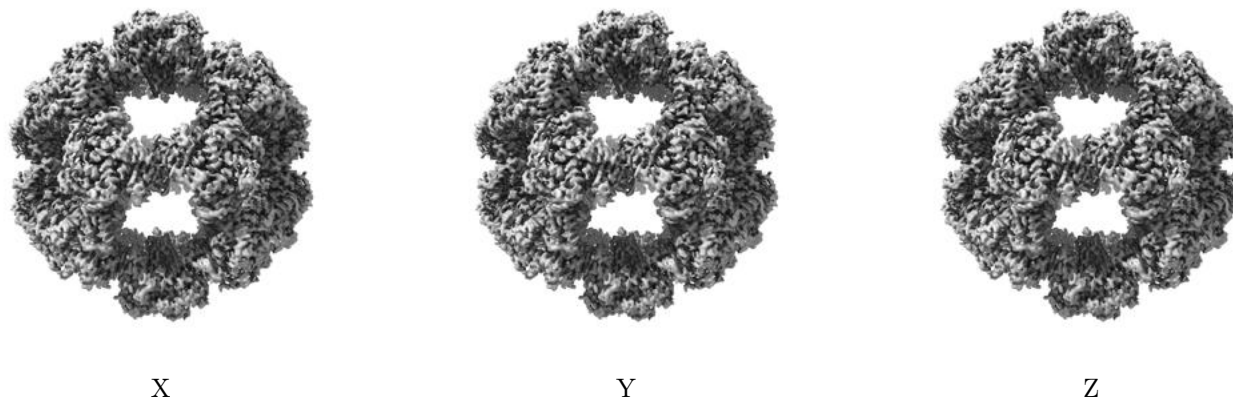


Z

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.

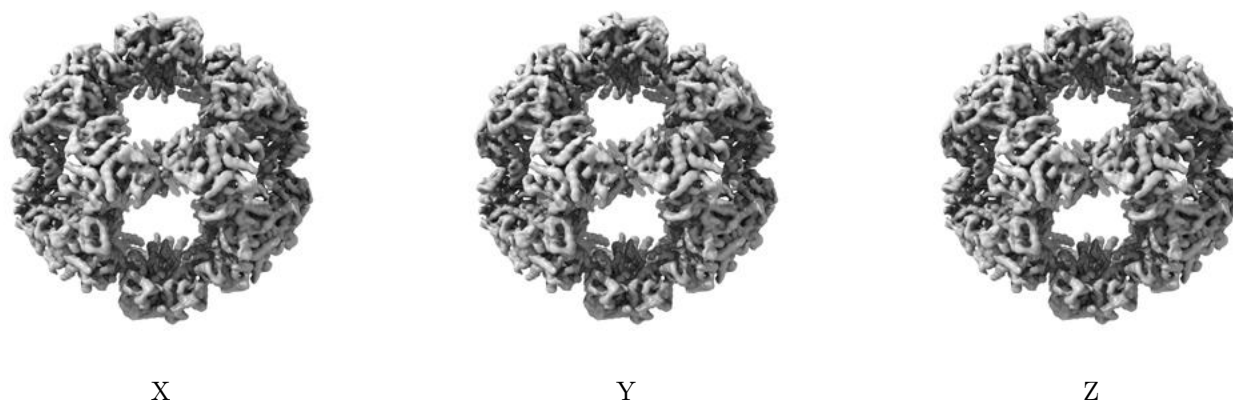
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.019. 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



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.

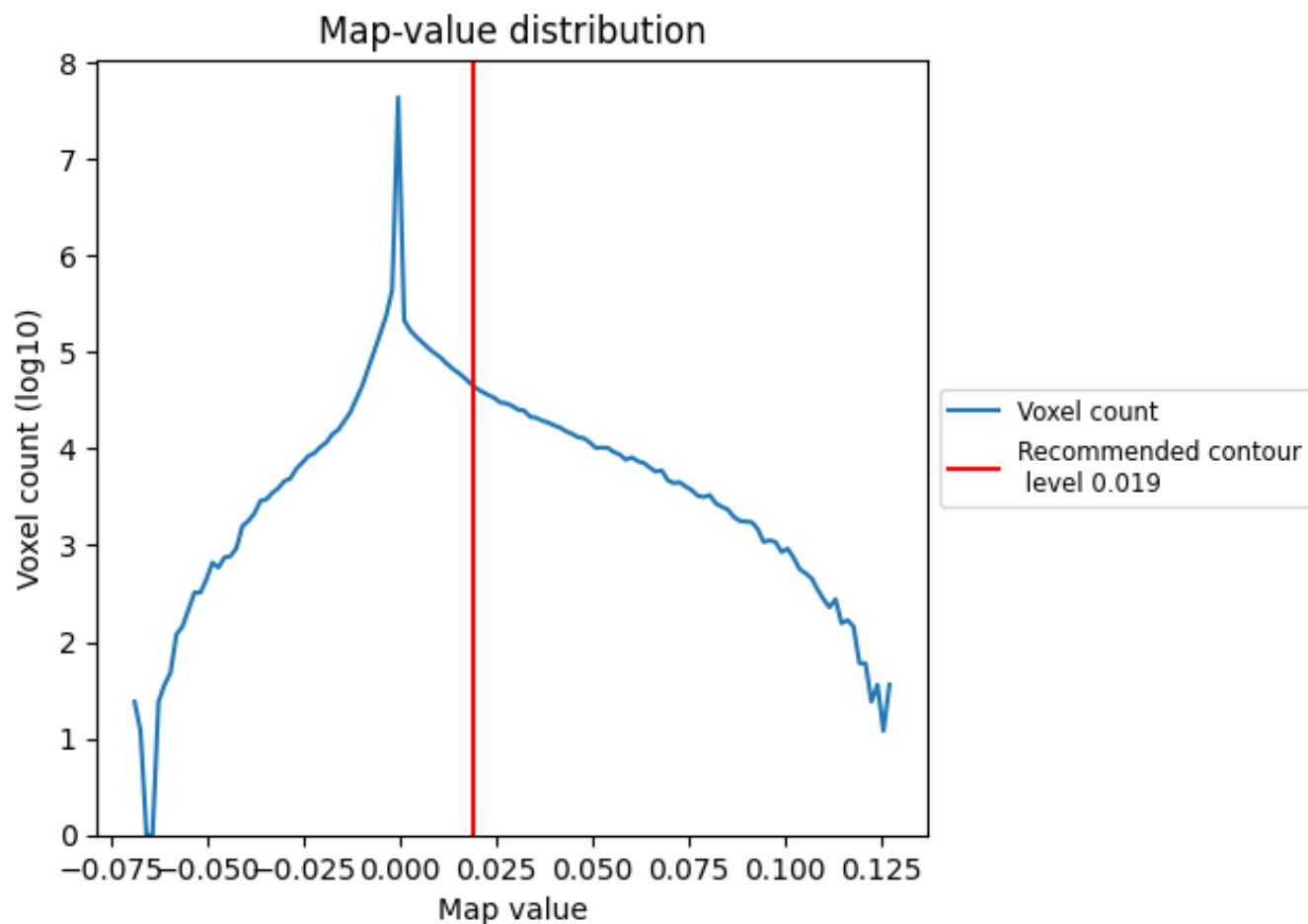
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

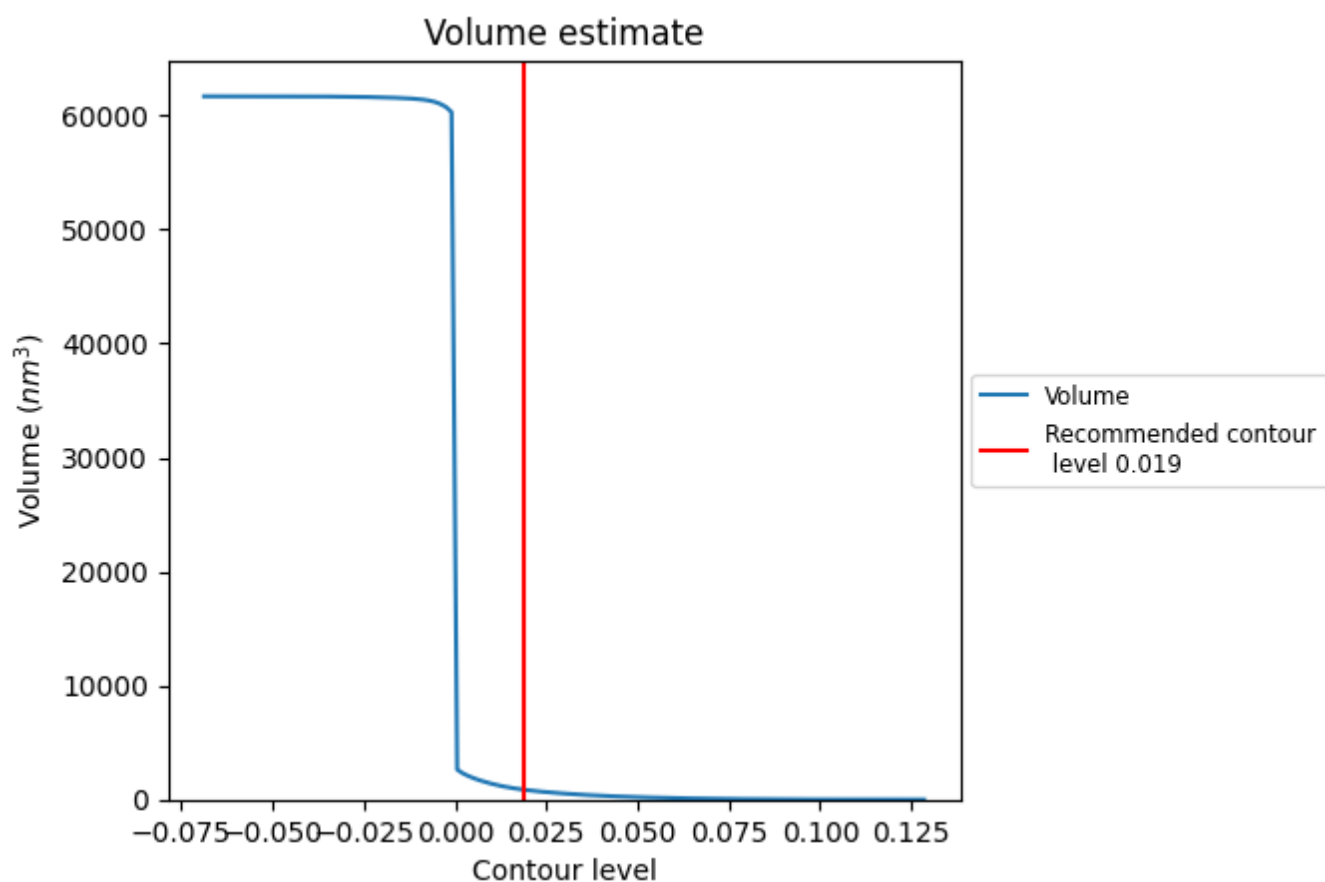
This section contains the results of statistical analysis of the map.

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.

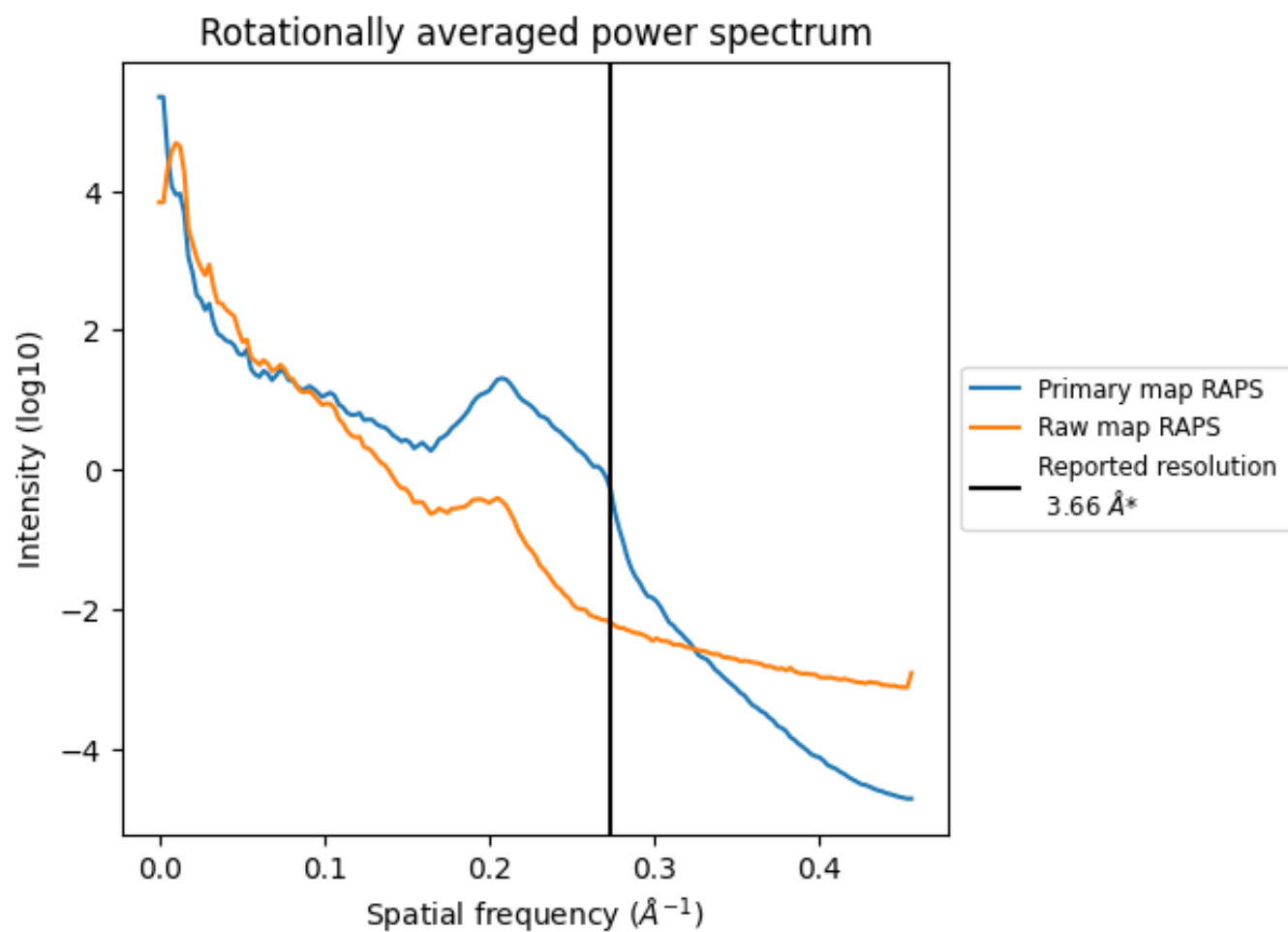
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 855 nm³; this corresponds to an approximate mass of 772 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 ⓘ

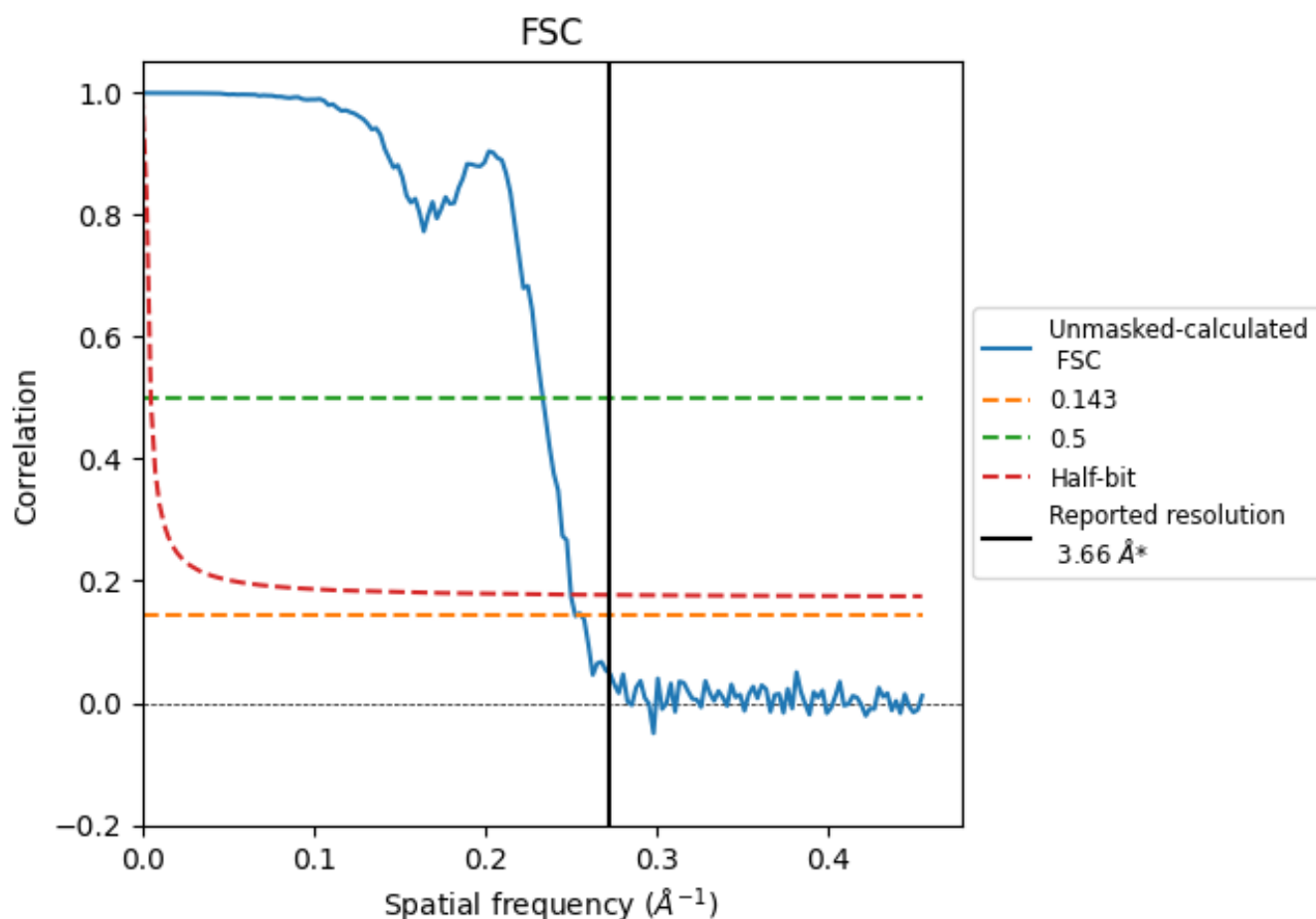


*Reported resolution corresponds to spatial frequency of 0.273 Å⁻¹

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 0.273 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

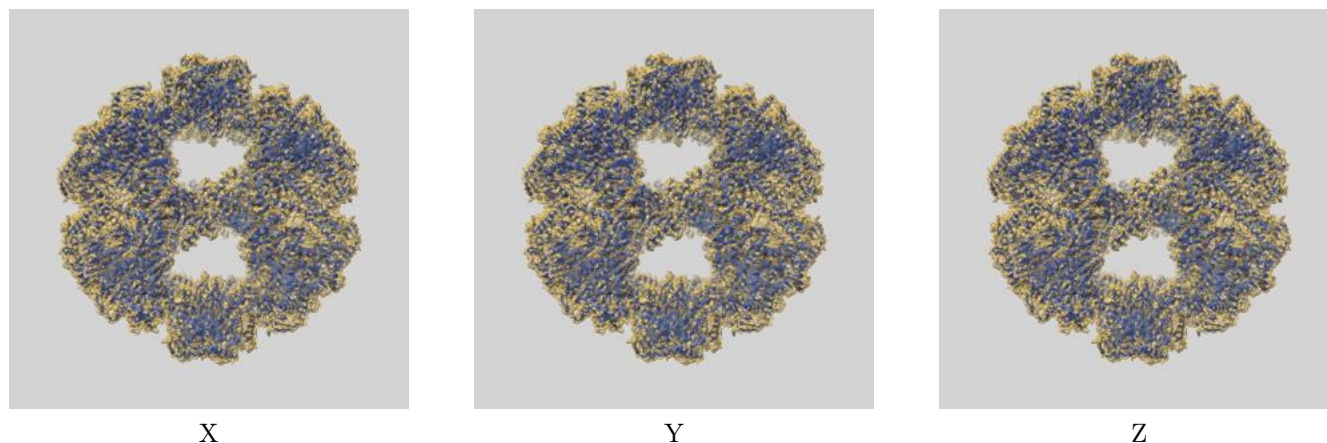
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.66	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.95	4.27	3.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

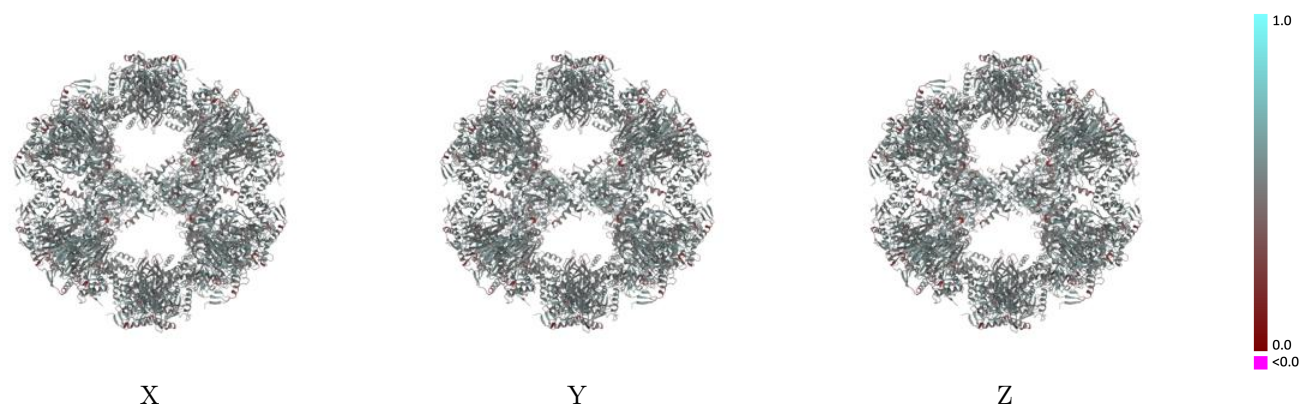
This section contains information regarding the fit between EMDB map EMD-37969 and PDB model 8X03. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



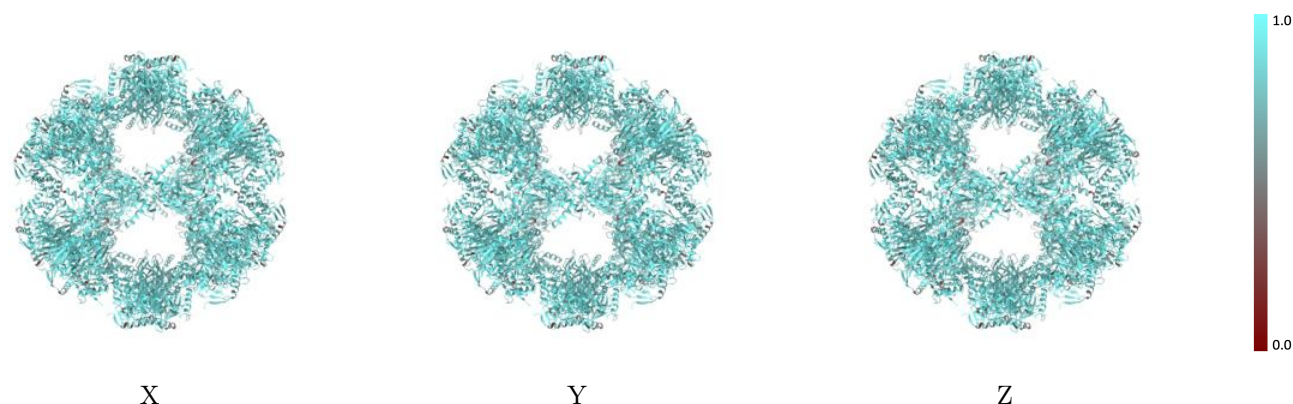
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



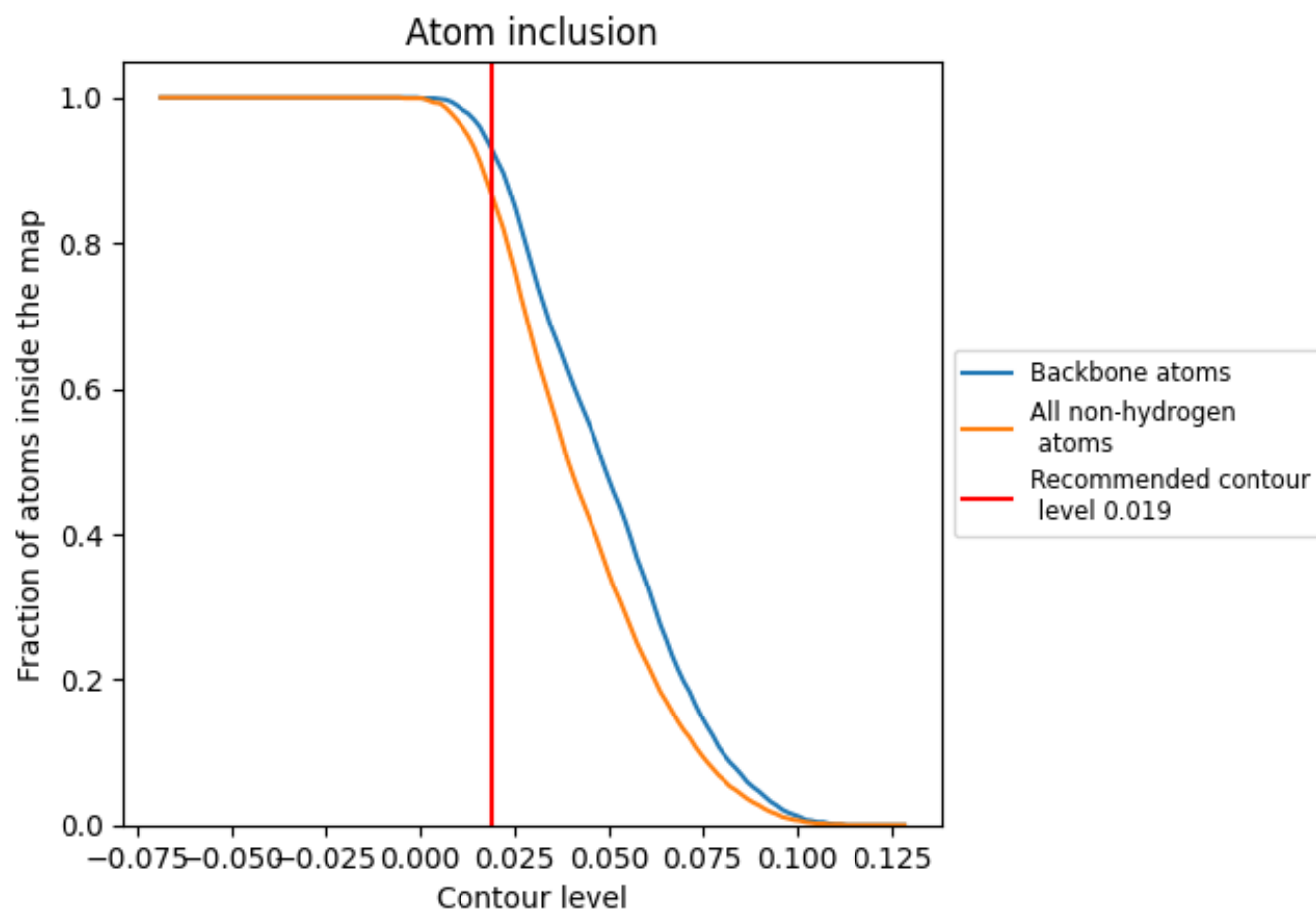
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.019).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 87% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8680	 0.4960
0	 0.8670	 0.4950
1	 0.8650	 0.4960
2	 0.8700	 0.5000
3	 0.8660	 0.4980
4	 0.8700	 0.4940
5	 0.8660	 0.4940
6	 0.8740	 0.4960
7	 0.8740	 0.4950
A	 0.8690	 0.4960
B	 0.8700	 0.4950
C	 0.8700	 0.4960
D	 0.8700	 0.4980
E	 0.8700	 0.4980
F	 0.8690	 0.4980
G	 0.8710	 0.4970
H	 0.8710	 0.4960
I	 0.8700	 0.4950
J	 0.8710	 0.4970
K	 0.8670	 0.4970
L	 0.8720	 0.4940
M	 0.8660	 0.4950
N	 0.8660	 0.4970
O	 0.8640	 0.4970
P	 0.8660	 0.4950
Q	 0.8620	 0.4960
R	 0.8710	 0.4930
S	 0.8670	 0.4980
T	 0.8660	 0.4980
U	 0.8700	 0.4940
V	 0.8720	 0.4950
W	 0.8720	 0.4950
X	 0.8690	 0.4970
Y	 0.8710	 0.4950
Z	 0.8630	 0.4950



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Chain	Atom inclusion	Q-score
a	 0.8660	 0.4950
b	 0.8640	 0.4980
c	 0.8720	 0.4980
d	 0.8710	 0.4950
e	 0.8670	 0.4950
f	 0.8650	 0.4930
g	 0.8660	 0.4940
h	 0.8650	 0.4990
i	 0.8670	 0.4940
j	 0.8640	 0.5010
k	 0.8690	 0.4950
l	 0.8670	 0.4960
m	 0.8650	 0.4930
n	 0.8630	 0.4950
o	 0.8660	 0.4990
p	 0.8690	 0.4970
q	 0.8710	 0.4980
r	 0.8730	 0.4950
s	 0.8700	 0.4960
t	 0.8690	 0.4990
u	 0.8670	 0.4970
v	 0.8670	 0.4960
w	 0.8650	 0.4930
x	 0.8630	 0.4990
y	 0.8740	 0.4960
z	 0.8700	 0.4960