



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:49 PM UTC

PDB ID : 8PIU / pdb_00008piu
EMDB ID : EMD-17691
Title : 60-meric complex of dihydrolipoamide acetyltransferase (E2) of the human pyruvate dehydrogenase complex
Authors : Zdanowicz, R.; Afanasyev, P.; Boehringer, D.; Glockshuber, R.
Deposited on : 2023-06-22
Resolution : 2.90 Å(reported)
Based on initial model : 6CT0

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:

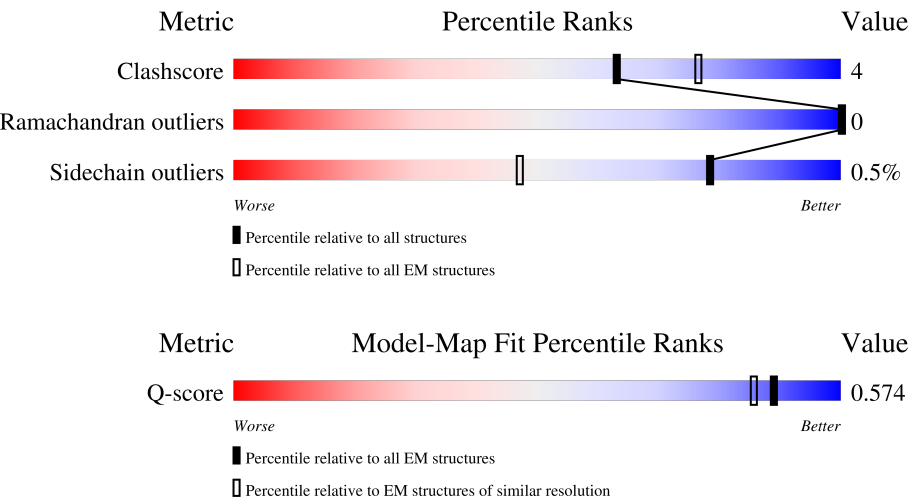
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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.



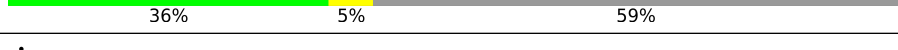
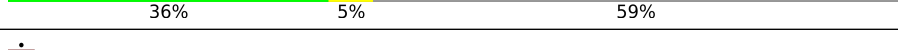
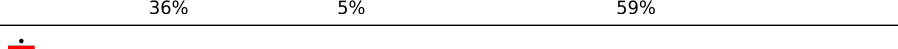
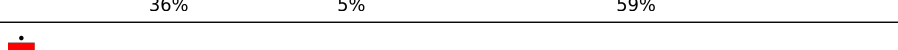
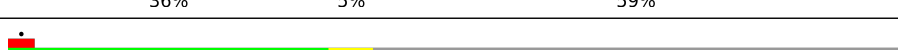
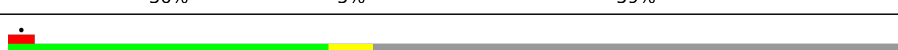
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	A	562	36%5%59%
1	AA	562	36%5%59%
1	AB	562	36%5%59%
1	B	562	36%5%59%

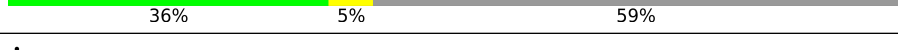
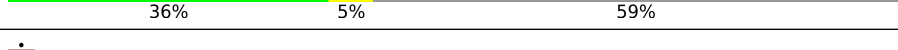
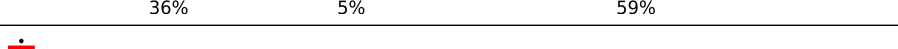
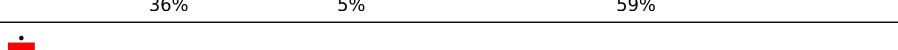
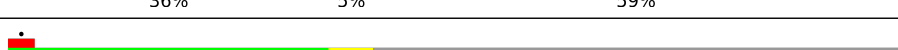
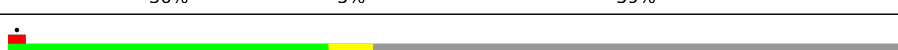
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Mol	Chain	Length	Quality of chain
1	BA	562	
1	BB	562	
1	C	562	
1	CA	562	
1	CB	562	
1	D	562	
1	DA	562	
1	DB	562	
1	E	562	
1	EA	562	
1	EB	562	
1	F	562	
1	FA	562	
1	FB	562	
1	G	562	
1	GA	562	
1	GB	562	
1	H	562	
1	HA	562	
1	HB	562	
1	I	562	
1	IA	562	
1	IB	562	
1	J	562	
1	JA	562	

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Mol	Chain	Length	Quality of chain
1	K	562	
1	KA	562	
1	L	562	
1	LA	562	
1	M	562	
1	MA	562	
1	N	562	
1	NA	562	
1	O	562	
1	OA	562	
1	P	562	
1	PA	562	
1	Q	562	
1	QA	562	
1	R	562	
1	RA	562	
1	S	562	
1	SA	562	
1	T	562	
1	TA	562	
1	UA	562	
1	V	562	
1	VA	562	
1	W	562	
1	WA	562	

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Mol	Chain	Length	Quality of chain
1	X	562	
1	XA	562	
1	Y	562	
1	YA	562	
1	Z	562	
1	ZA	562	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 106140 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 Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	AB	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	A	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	BB	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	CB	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	DB	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	EB	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	FB	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	GB	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	HB	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	IB	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	C	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	D	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	E	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	F	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	G	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	I	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	J	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	K	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	L	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	M	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	N	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	O	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	P	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	Q	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	R	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	BA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	S	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	T	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	V	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	W	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	X	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	Y	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	Z	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	AA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	CA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	DA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	EA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	FA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	GA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	HA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	IA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	JA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	KA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	LA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	MA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	NA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	OA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	PA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	QA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	RA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	SA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	TA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	UA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	VA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	WA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	XA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	YA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		
1	ZA	231	Total	C	N	O	S	0	0
			1769	1127	304	328	10		

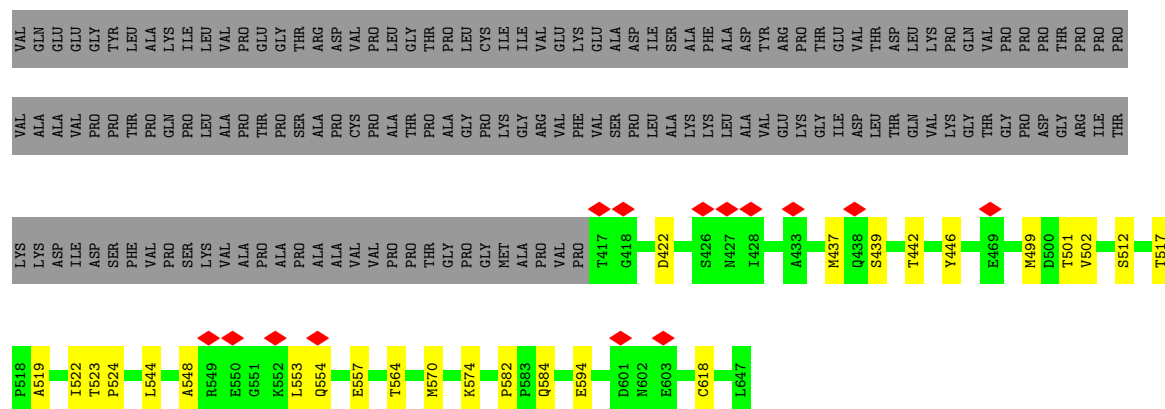
There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	86	MET	-	initiating methionine	UNP P10515
AB	86	MET	-	initiating methionine	UNP P10515
A	86	MET	-	initiating methionine	UNP P10515
BB	86	MET	-	initiating methionine	UNP P10515
CB	86	MET	-	initiating methionine	UNP P10515
DB	86	MET	-	initiating methionine	UNP P10515
EB	86	MET	-	initiating methionine	UNP P10515
FB	86	MET	-	initiating methionine	UNP P10515
GB	86	MET	-	initiating methionine	UNP P10515
HB	86	MET	-	initiating methionine	UNP P10515
IB	86	MET	-	initiating methionine	UNP P10515
C	86	MET	-	initiating methionine	UNP P10515
D	86	MET	-	initiating methionine	UNP P10515
E	86	MET	-	initiating methionine	UNP P10515
F	86	MET	-	initiating methionine	UNP P10515
G	86	MET	-	initiating methionine	UNP P10515
H	86	MET	-	initiating methionine	UNP P10515
I	86	MET	-	initiating methionine	UNP P10515
J	86	MET	-	initiating methionine	UNP P10515
K	86	MET	-	initiating methionine	UNP P10515
L	86	MET	-	initiating methionine	UNP P10515
M	86	MET	-	initiating methionine	UNP P10515
N	86	MET	-	initiating methionine	UNP P10515
O	86	MET	-	initiating methionine	UNP P10515
P	86	MET	-	initiating methionine	UNP P10515
Q	86	MET	-	initiating methionine	UNP P10515
R	86	MET	-	initiating methionine	UNP P10515
BA	86	MET	-	initiating methionine	UNP P10515
S	86	MET	-	initiating methionine	UNP P10515
T	86	MET	-	initiating methionine	UNP P10515
V	86	MET	-	initiating methionine	UNP P10515
W	86	MET	-	initiating methionine	UNP P10515
X	86	MET	-	initiating methionine	UNP P10515
Y	86	MET	-	initiating methionine	UNP P10515

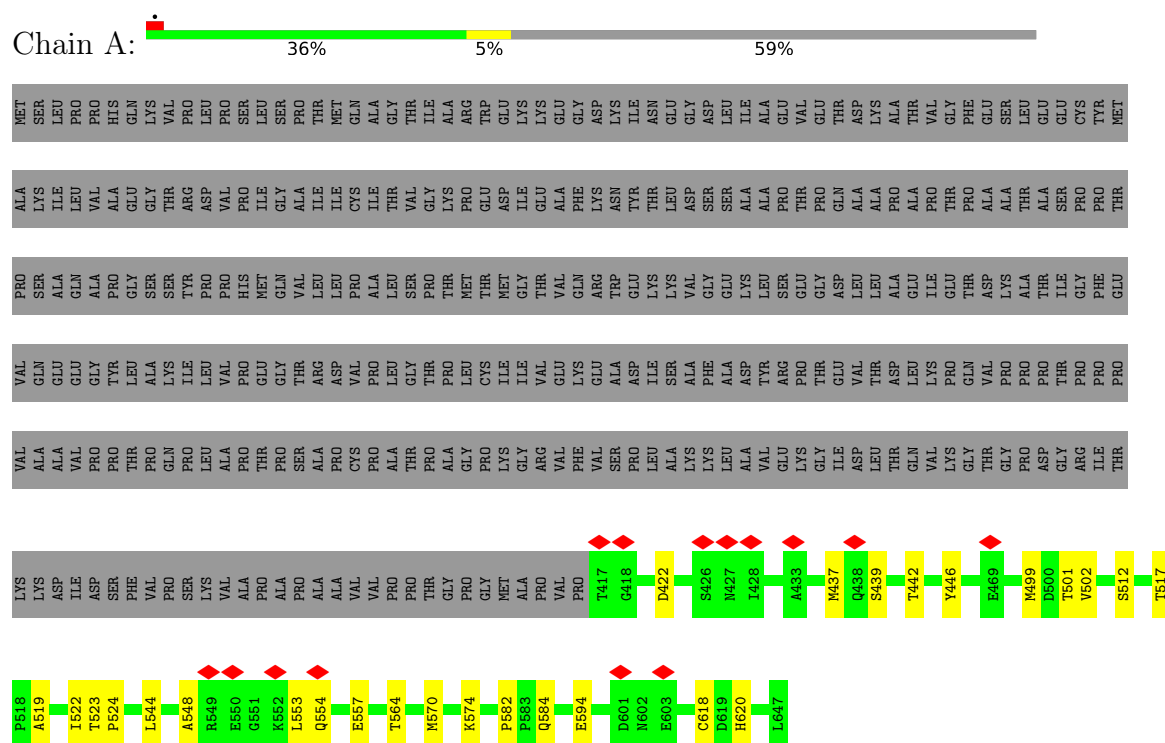
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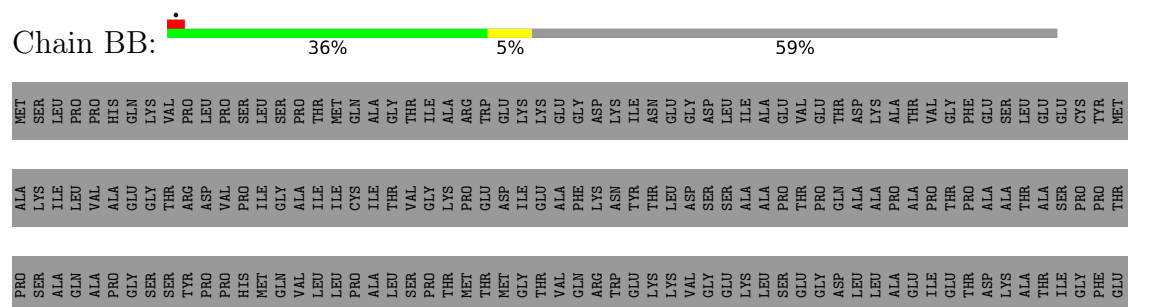
Chain	Residue	Modelled	Actual	Comment	Reference
Z	86	MET	-	initiating methionine	UNP P10515
AA	86	MET	-	initiating methionine	UNP P10515
CA	86	MET	-	initiating methionine	UNP P10515
DA	86	MET	-	initiating methionine	UNP P10515
EA	86	MET	-	initiating methionine	UNP P10515
FA	86	MET	-	initiating methionine	UNP P10515
GA	86	MET	-	initiating methionine	UNP P10515
HA	86	MET	-	initiating methionine	UNP P10515
IA	86	MET	-	initiating methionine	UNP P10515
JA	86	MET	-	initiating methionine	UNP P10515
KA	86	MET	-	initiating methionine	UNP P10515
LA	86	MET	-	initiating methionine	UNP P10515
MA	86	MET	-	initiating methionine	UNP P10515
NA	86	MET	-	initiating methionine	UNP P10515
OA	86	MET	-	initiating methionine	UNP P10515
PA	86	MET	-	initiating methionine	UNP P10515
QA	86	MET	-	initiating methionine	UNP P10515
RA	86	MET	-	initiating methionine	UNP P10515
SA	86	MET	-	initiating methionine	UNP P10515
TA	86	MET	-	initiating methionine	UNP P10515
UA	86	MET	-	initiating methionine	UNP P10515
VA	86	MET	-	initiating methionine	UNP P10515
WA	86	MET	-	initiating methionine	UNP P10515
XA	86	MET	-	initiating methionine	UNP P10515
YA	86	MET	-	initiating methionine	UNP P10515
ZA	86	MET	-	initiating methionine	UNP P10515

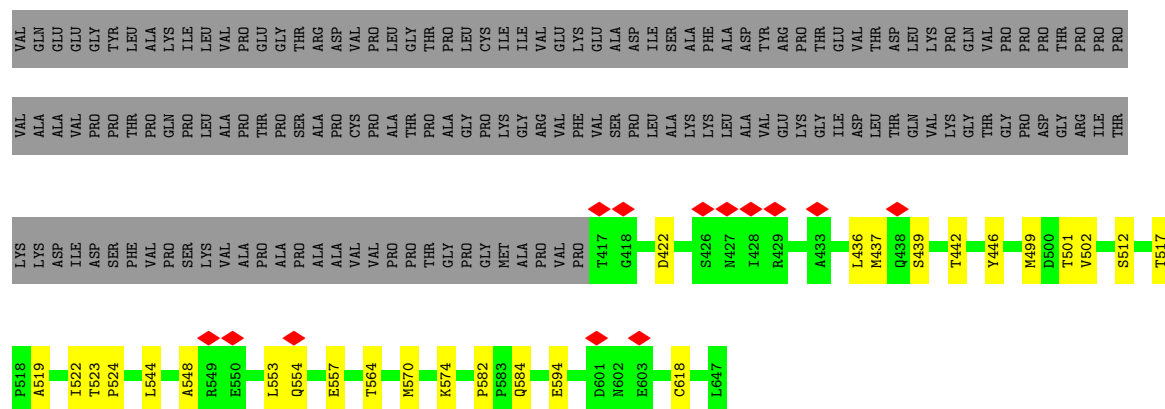


- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



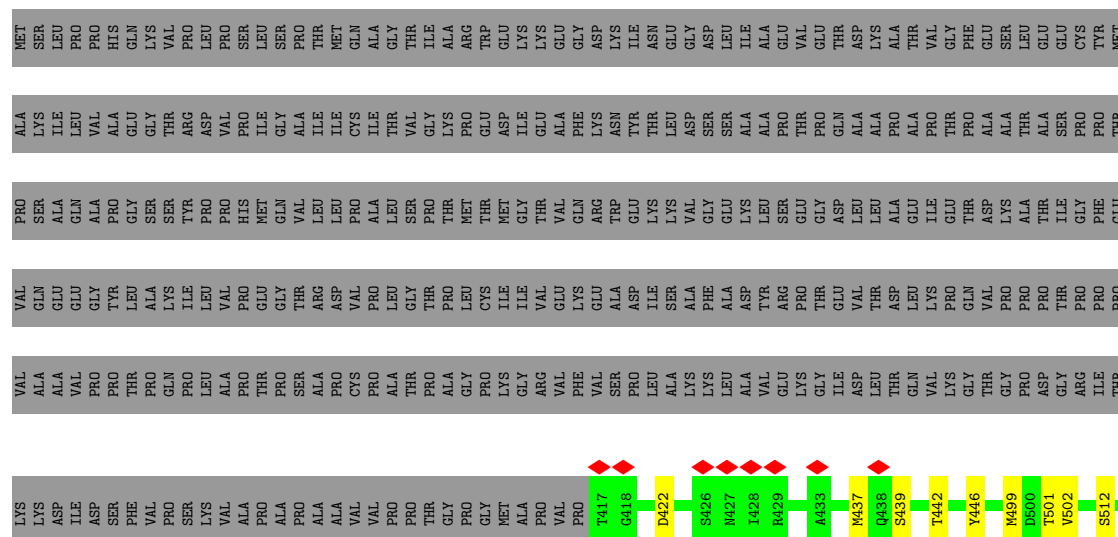
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial





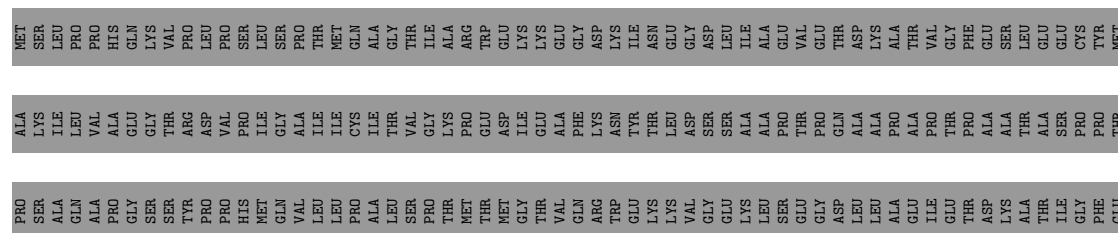
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

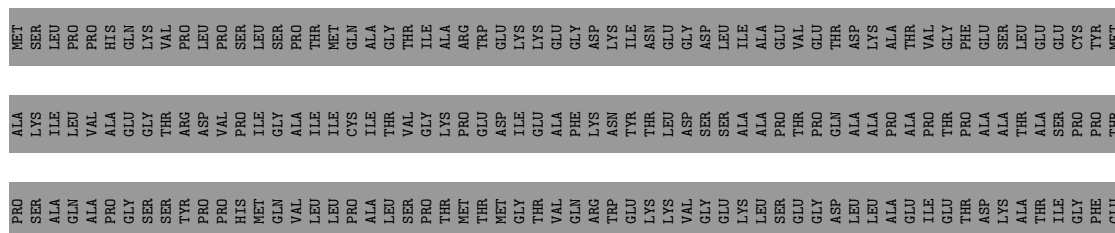
Chain CB: 36% 5% 59%

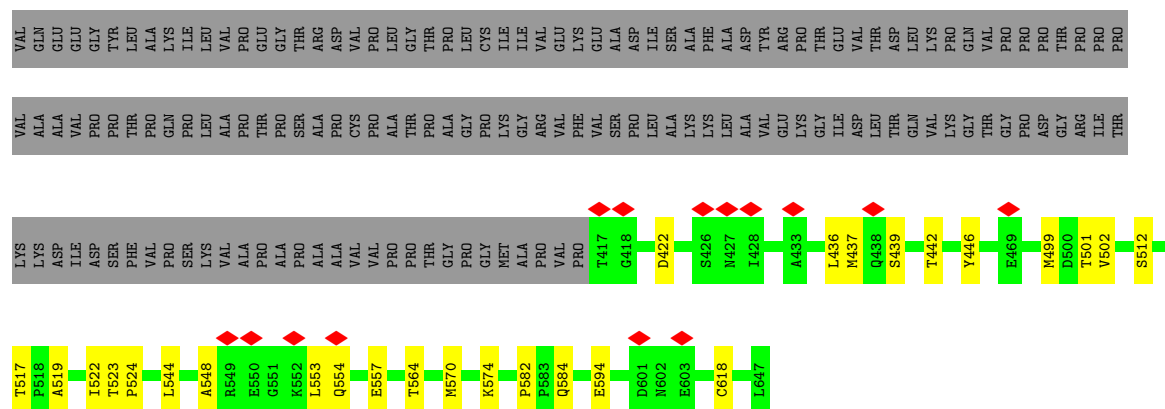


- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

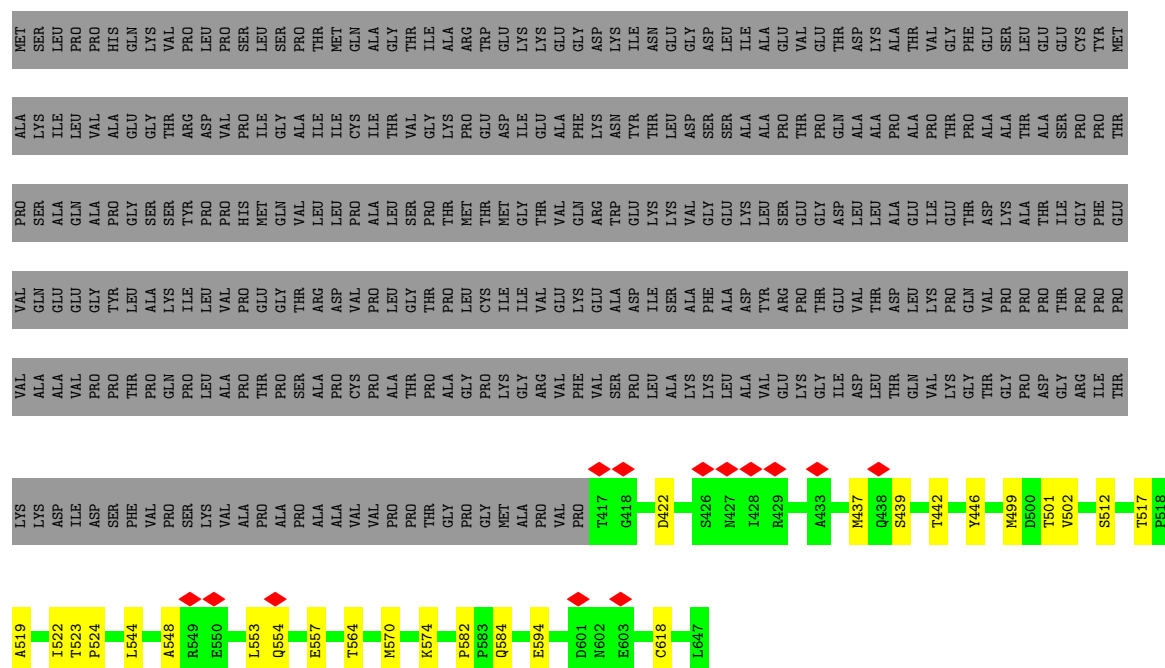
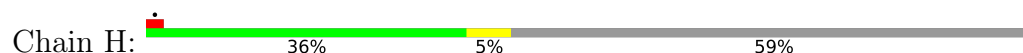
Chain DB: 36% 5% 59%



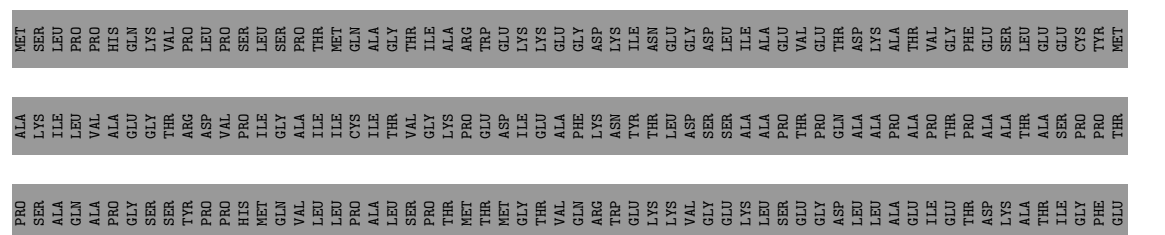


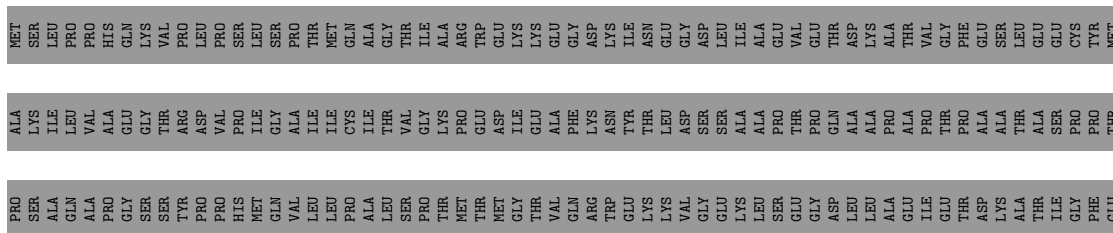


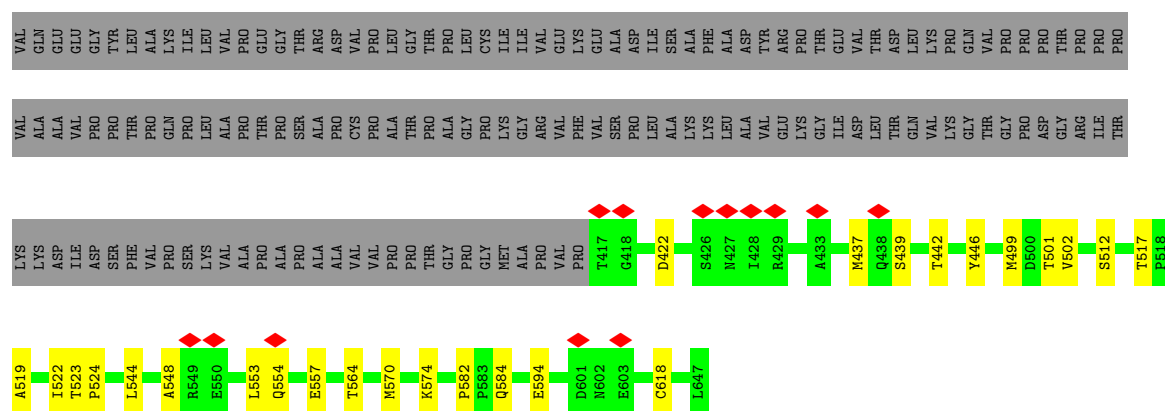
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



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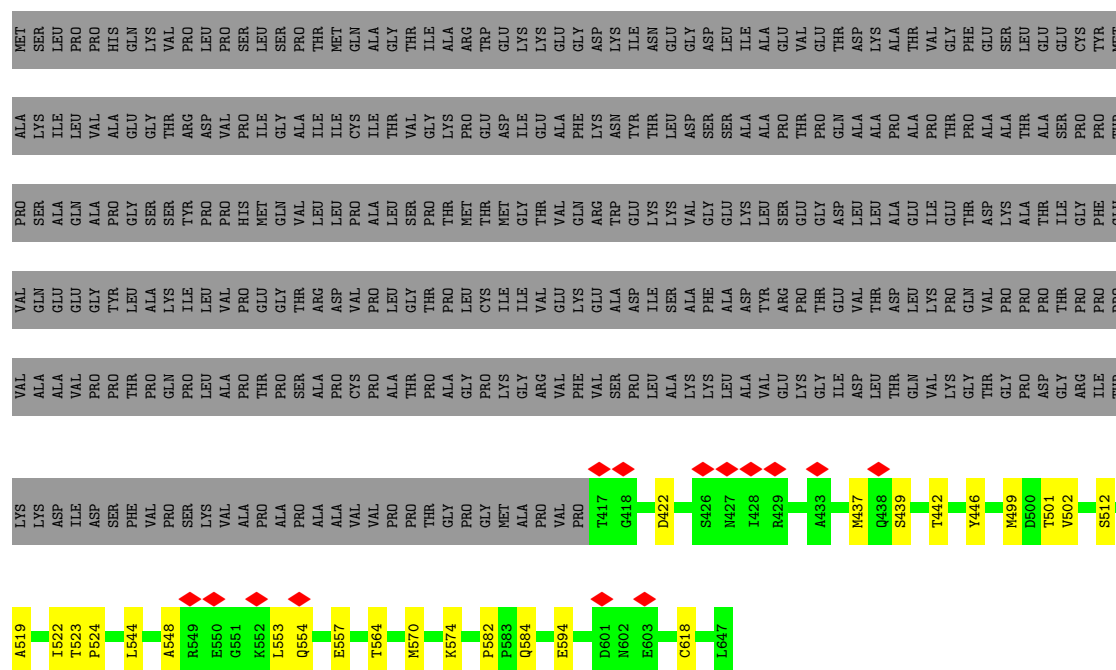






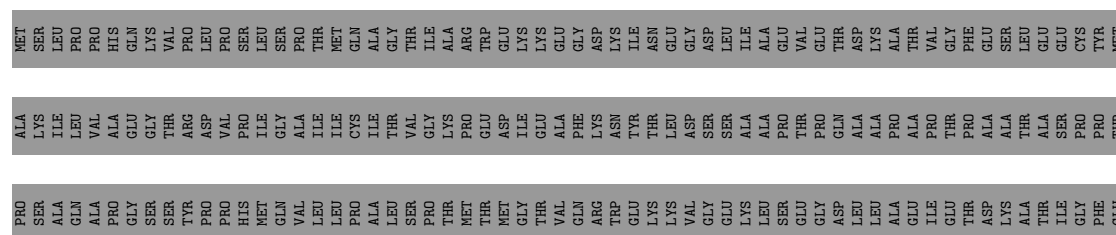
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

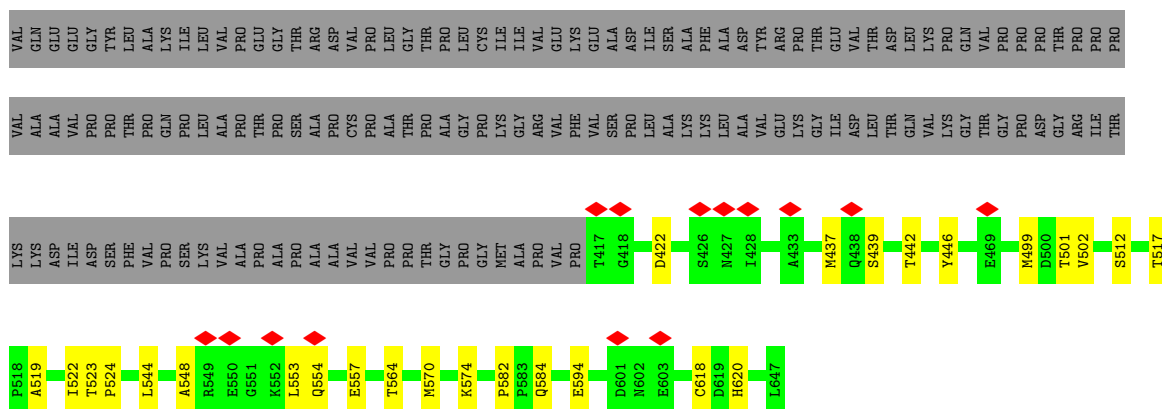
Chain N: 36% 5%



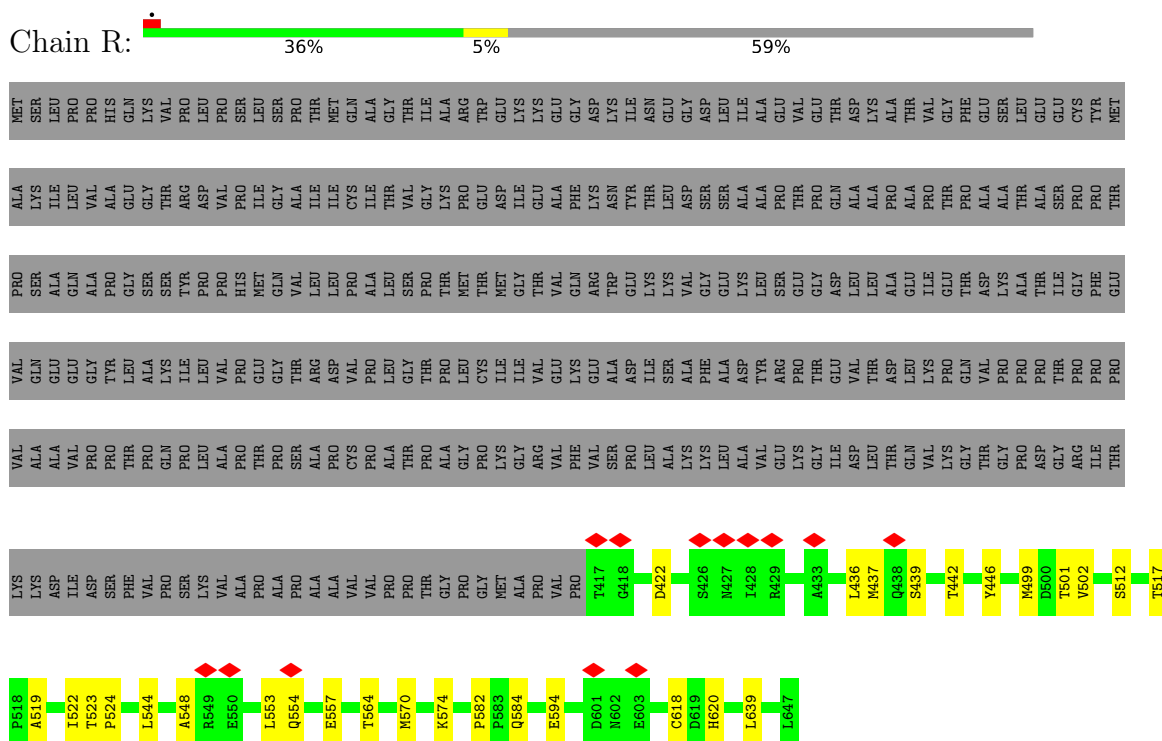
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain O: 36% 5%

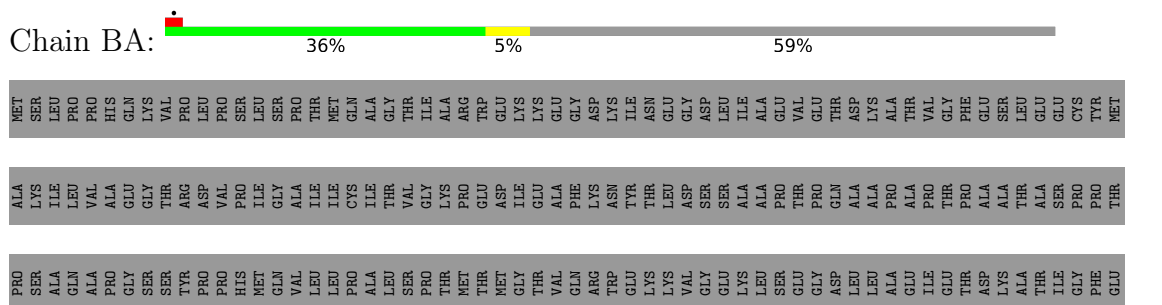


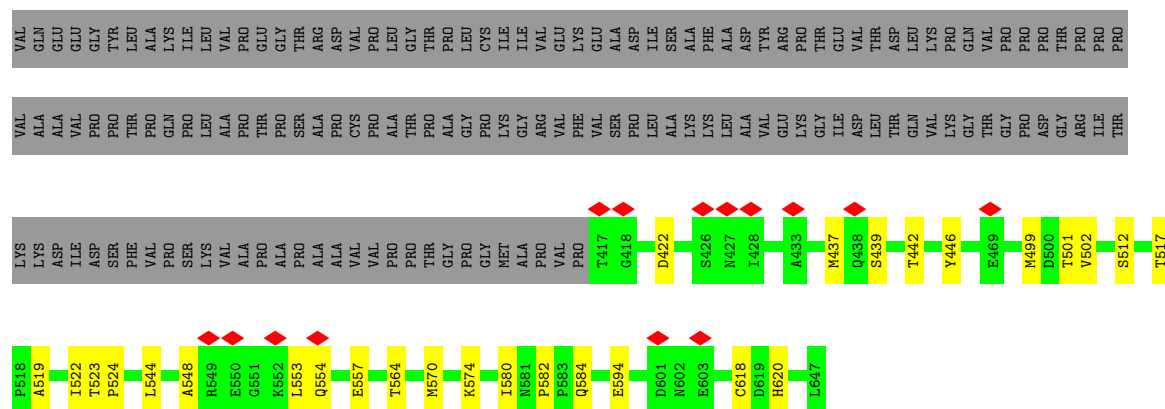


- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



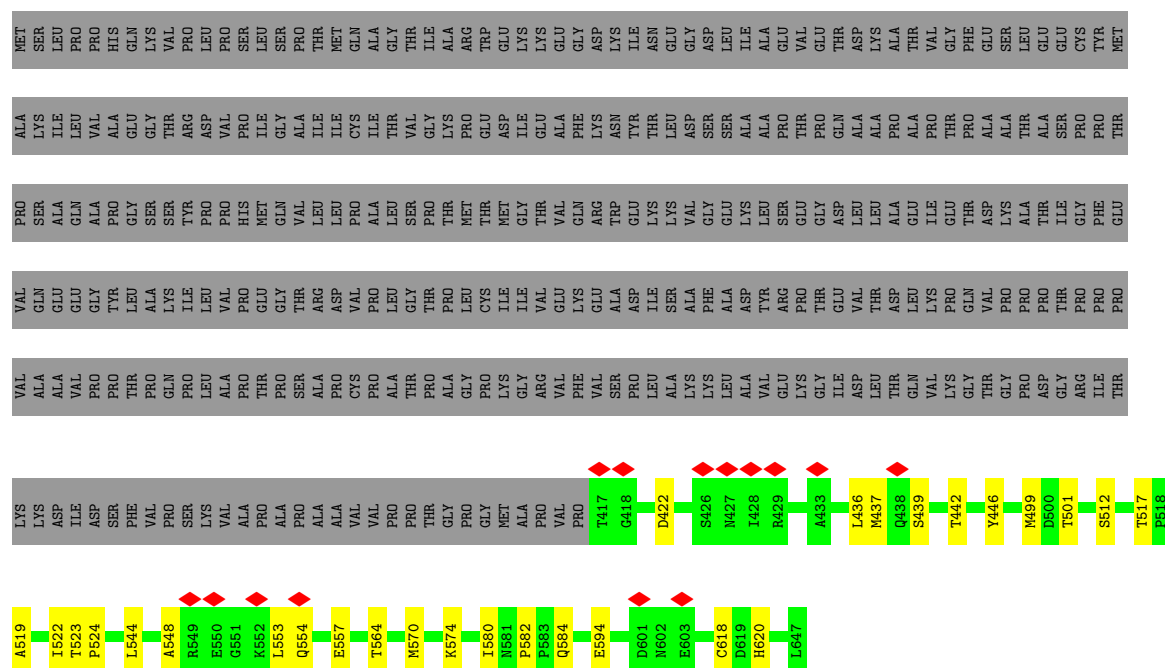
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial





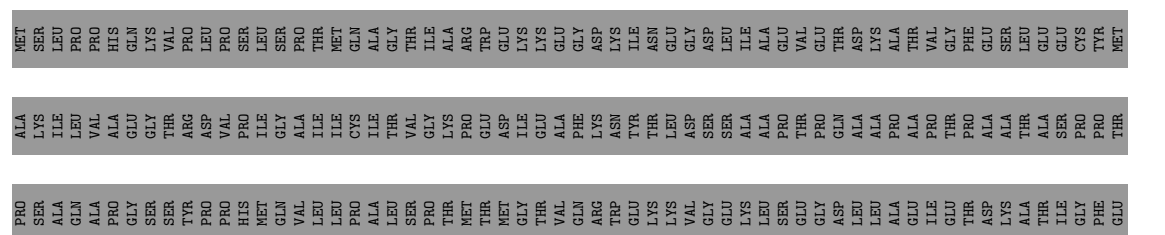
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain S: 36% 5% 59%

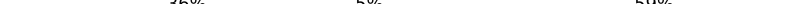


- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

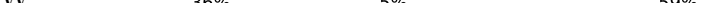
Chain T: 36% 5% 59%

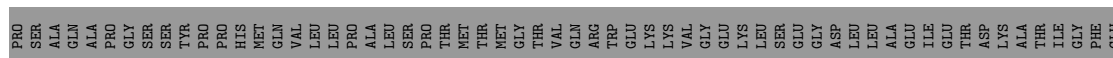


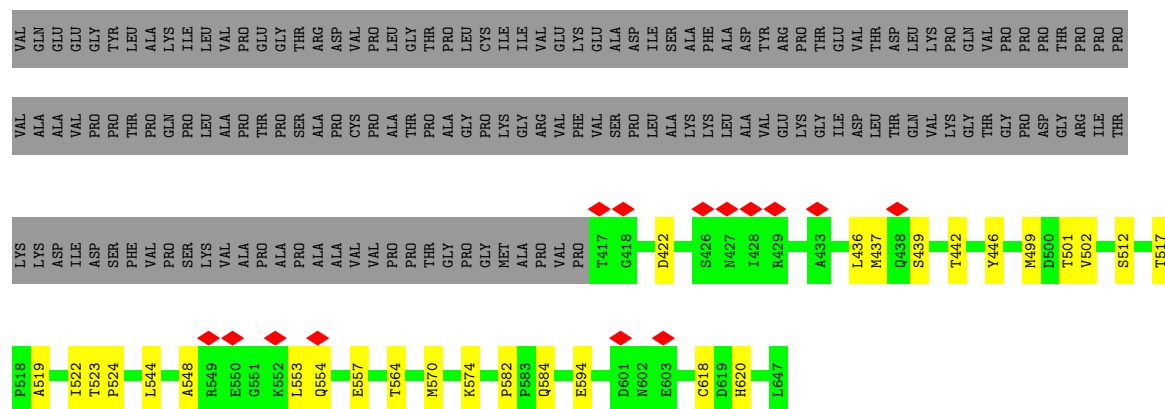


- Chain V: 



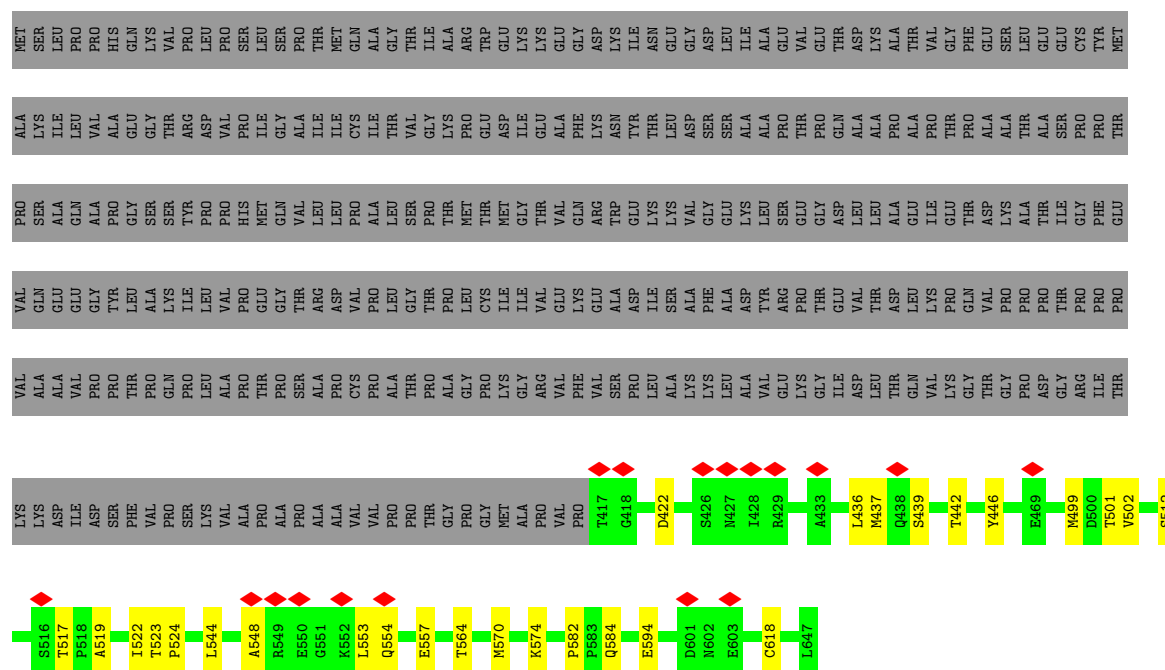
- Chain W: 





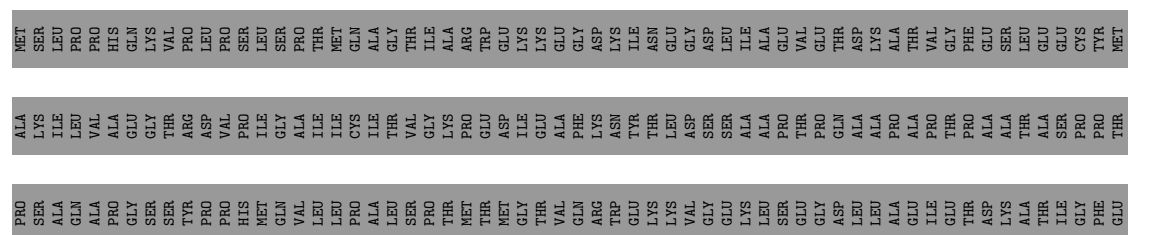
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

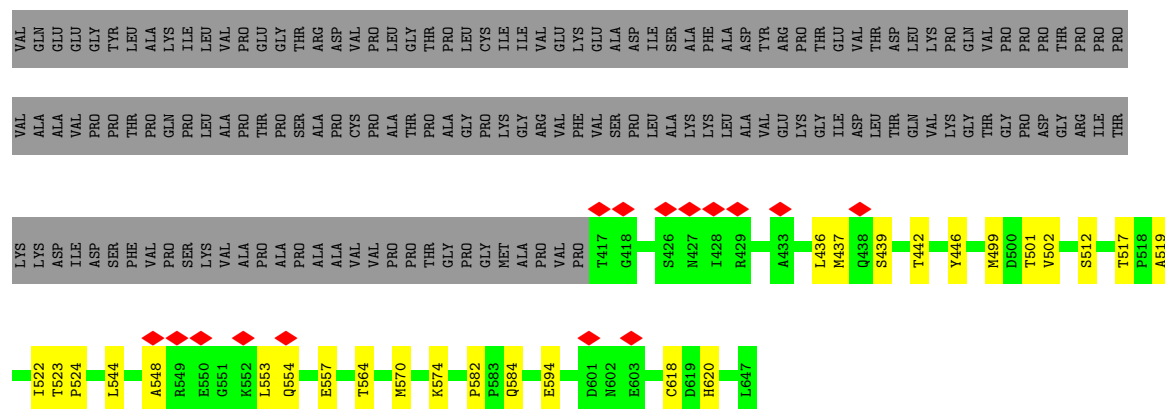
Chain EA: 36% 5% 59%



- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

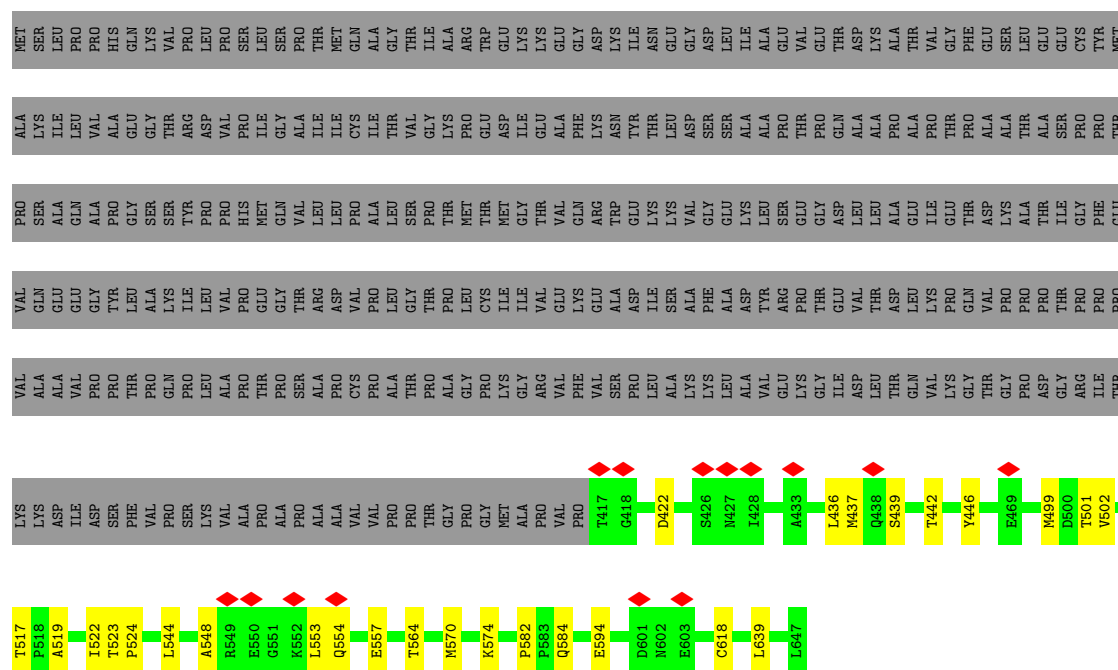
Chain FA: 36% 5% 59%





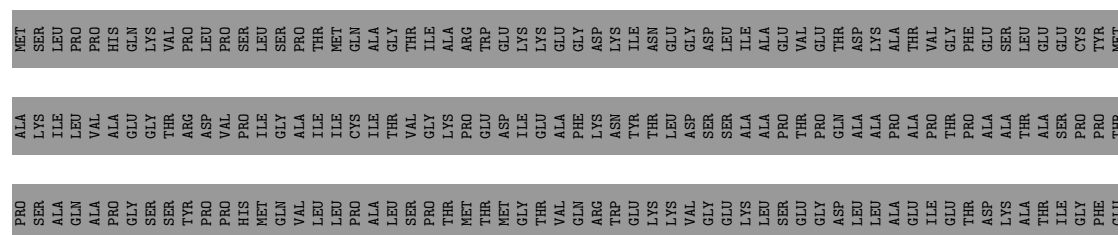
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

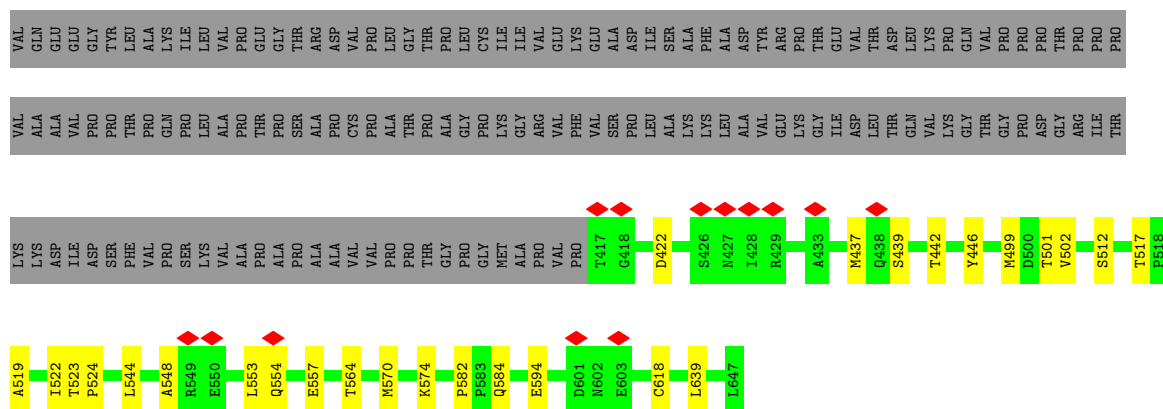
Chain GA: 36% 5% 59%



- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

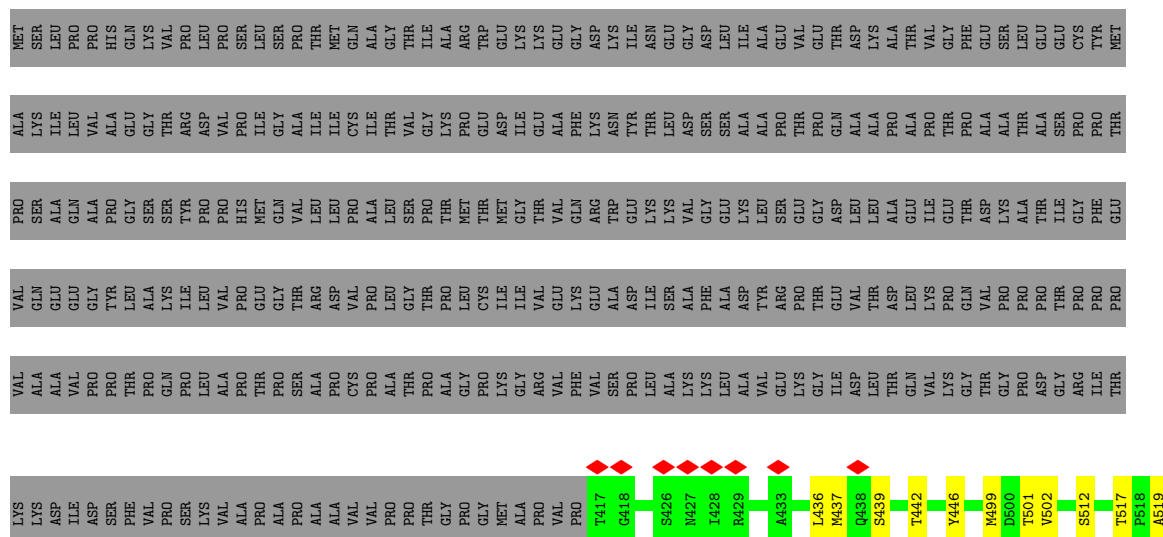
Chain HA: 36% 5% 59%





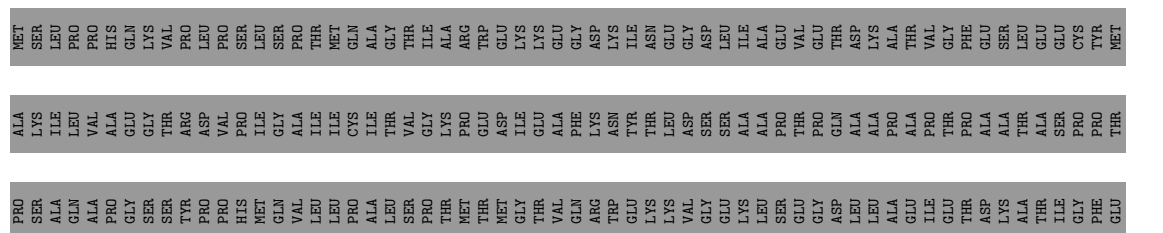
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

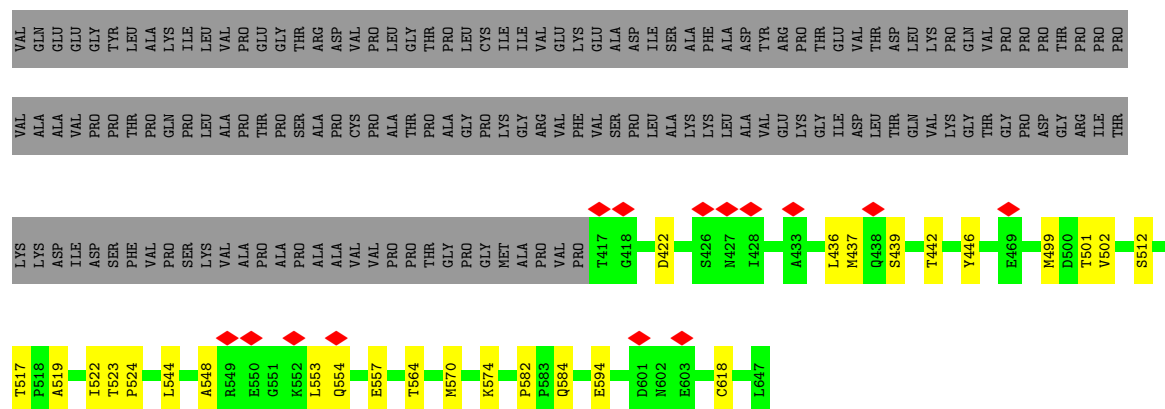
Chain IA: 36% 5% 59%



- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

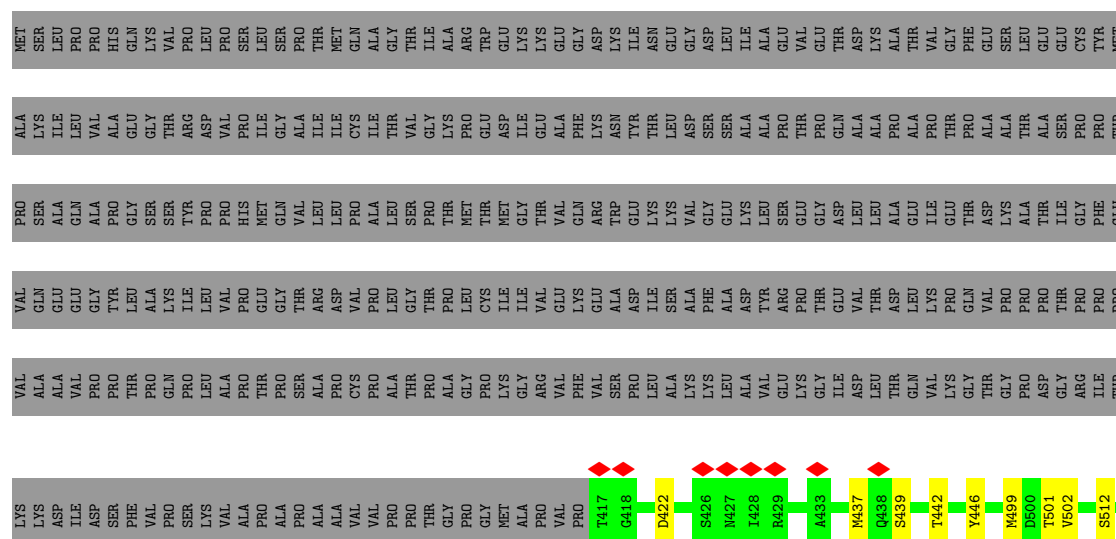
Chain JA: 36% 5% 59%





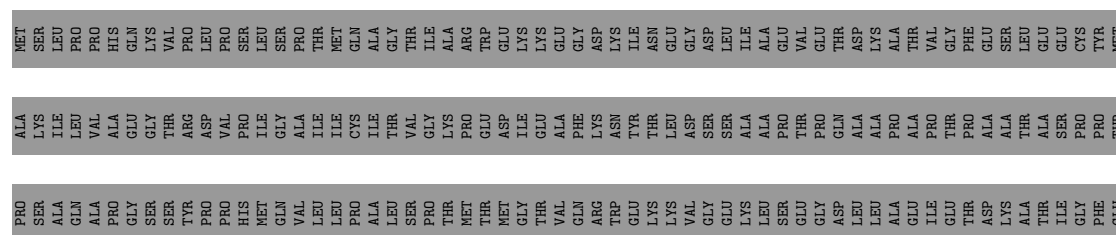
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

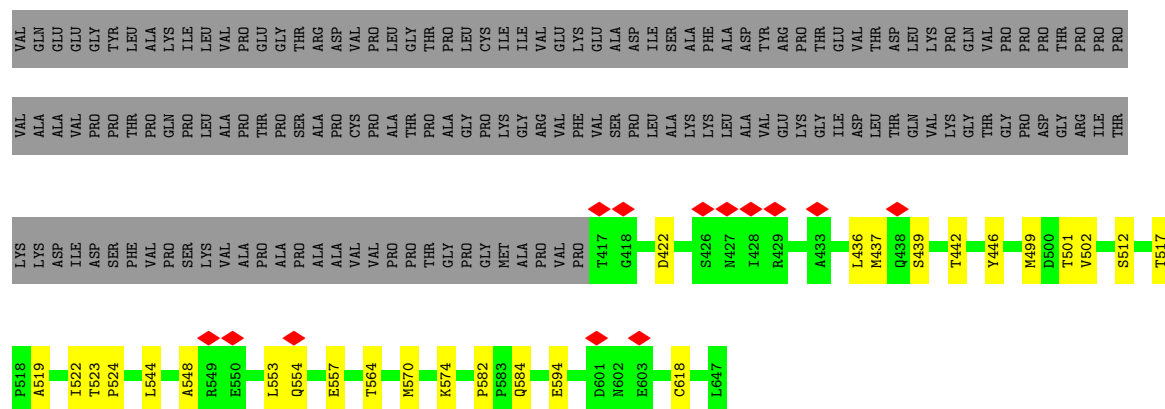
Chain MA: 36% 5% 59%



- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

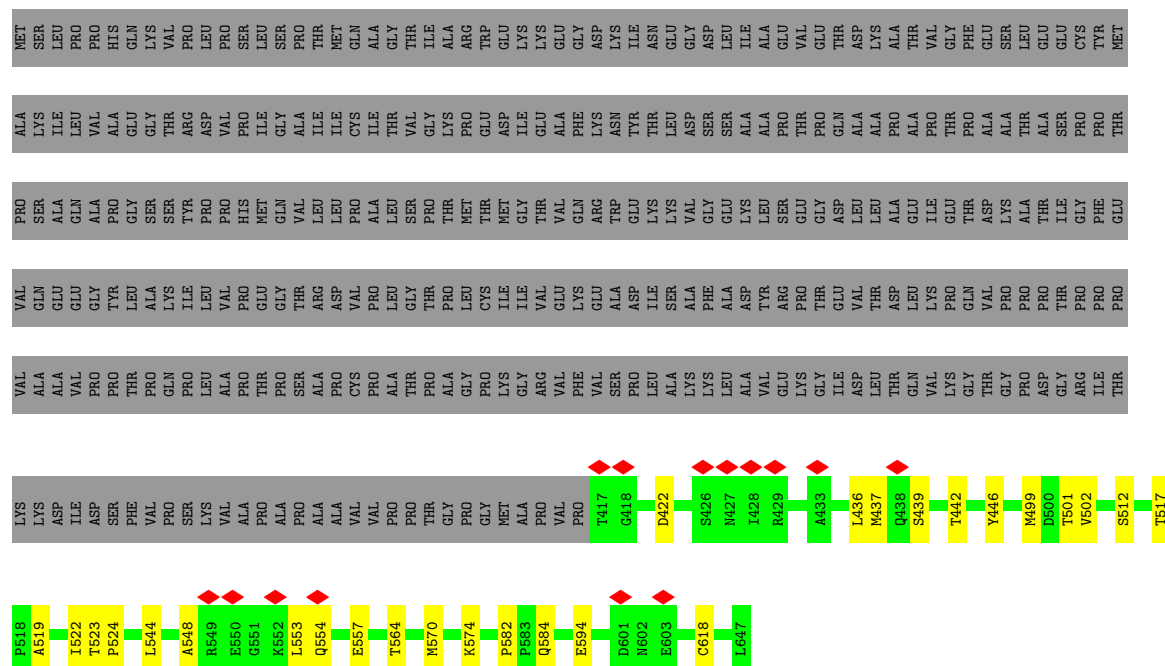
Chain NA: 36% 5% 59%





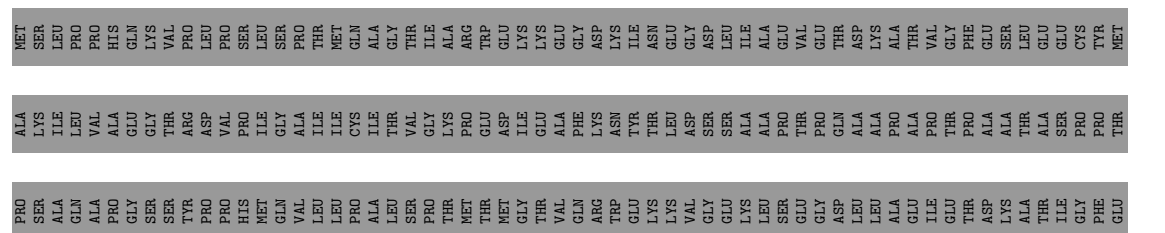
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain SA: 36% 5% 59%

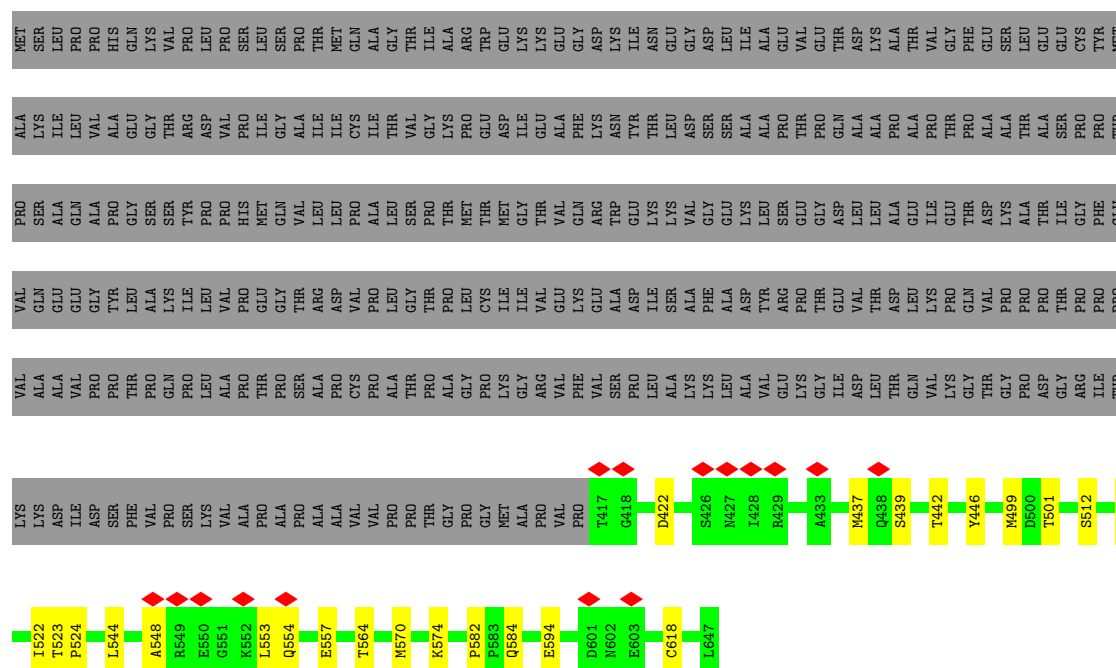


- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

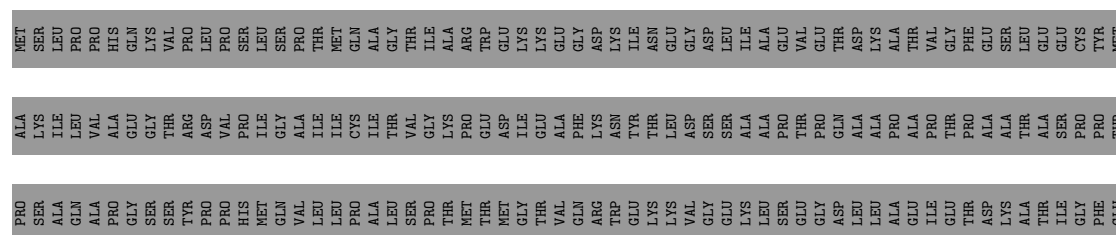
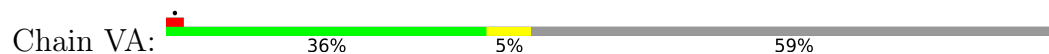
Chain TA: 36% 5% 59%

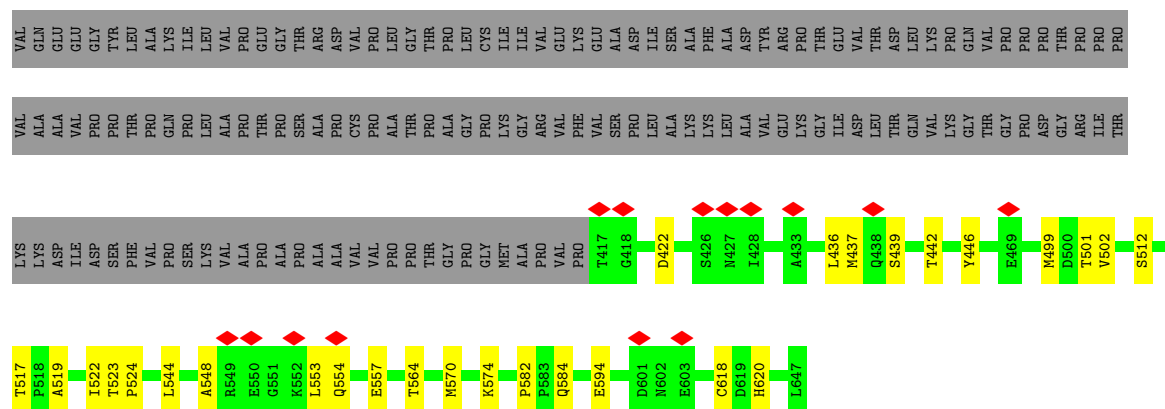


- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



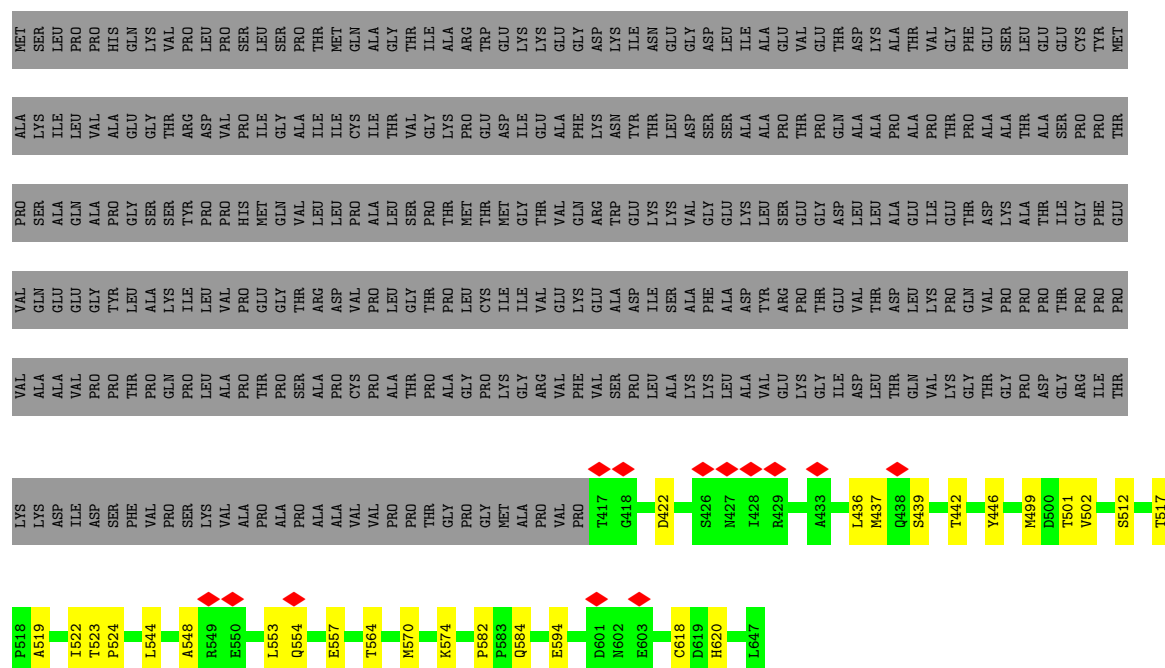
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial





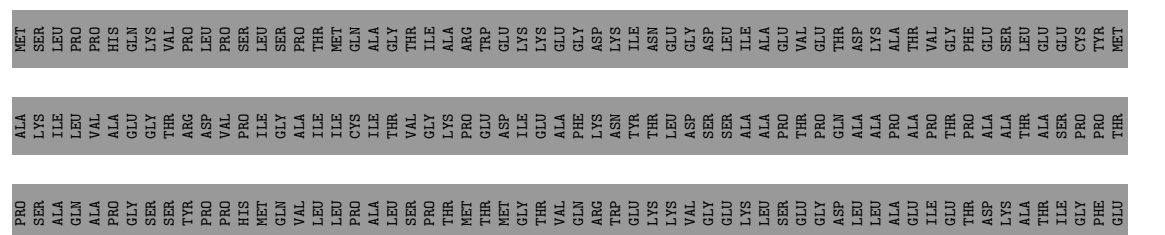
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain WA: 36% 5% 59%



- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain XA: 36% 5% 59%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	83959	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.433	Depositor
Minimum map value	-2.642	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.141	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	386.4, 386.4, 386.4	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.84, 0.84, 0.84	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	0.14	0/1799	0.28	0/2438
1	AA	0.14	0/1799	0.28	0/2438
1	AB	0.14	0/1799	0.28	0/2438
1	B	0.14	0/1799	0.28	0/2438
1	BA	0.14	0/1799	0.28	0/2438
1	BB	0.14	0/1799	0.28	0/2438
1	C	0.14	0/1799	0.28	0/2438
1	CA	0.14	0/1799	0.28	0/2438
1	CB	0.14	0/1799	0.28	0/2438
1	D	0.14	0/1799	0.28	0/2438
1	DA	0.14	0/1799	0.28	0/2438
1	DB	0.14	0/1799	0.28	0/2438
1	E	0.14	0/1799	0.28	0/2438
1	EA	0.14	0/1799	0.28	0/2438
1	EB	0.14	0/1799	0.28	0/2438
1	F	0.14	0/1799	0.28	0/2438
1	FA	0.14	0/1799	0.28	0/2438
1	FB	0.14	0/1799	0.28	0/2438
1	G	0.14	0/1799	0.28	0/2438
1	GA	0.14	0/1799	0.28	0/2438
1	GB	0.14	0/1799	0.28	0/2438
1	H	0.14	0/1799	0.28	0/2438
1	HA	0.14	0/1799	0.28	0/2438
1	HB	0.14	0/1799	0.28	0/2438
1	I	0.14	0/1799	0.28	0/2438
1	IA	0.14	0/1799	0.28	0/2438
1	IB	0.14	0/1799	0.28	0/2438
1	J	0.14	0/1799	0.28	0/2438
1	JA	0.14	0/1799	0.28	0/2438
1	K	0.14	0/1799	0.28	0/2438
1	KA	0.14	0/1799	0.28	0/2438
1	L	0.14	0/1799	0.28	0/2438
1	LA	0.14	0/1799	0.28	0/2438
1	M	0.14	0/1799	0.28	0/2438

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	MA	0.14	0/1799	0.28	0/2438
1	N	0.14	0/1799	0.28	0/2438
1	NA	0.14	0/1799	0.28	0/2438
1	O	0.14	0/1799	0.28	0/2438
1	OA	0.14	0/1799	0.28	0/2438
1	P	0.14	0/1799	0.28	0/2438
1	PA	0.14	0/1799	0.28	0/2438
1	Q	0.14	0/1799	0.28	0/2438
1	QA	0.14	0/1799	0.28	0/2438
1	R	0.14	0/1799	0.28	0/2438
1	RA	0.14	0/1799	0.28	0/2438
1	S	0.14	0/1799	0.28	0/2438
1	SA	0.14	0/1799	0.28	0/2438
1	T	0.14	0/1799	0.28	0/2438
1	TA	0.14	0/1799	0.28	0/2438
1	UA	0.14	0/1799	0.28	0/2438
1	V	0.14	0/1799	0.28	0/2438
1	VA	0.14	0/1799	0.28	0/2438
1	W	0.14	0/1799	0.28	0/2438
1	WA	0.14	0/1799	0.28	0/2438
1	X	0.14	0/1799	0.28	0/2438
1	XA	0.14	0/1799	0.28	0/2438
1	Y	0.14	0/1799	0.28	0/2438
1	YA	0.14	0/1799	0.28	0/2438
1	Z	0.14	0/1799	0.28	0/2438
1	ZA	0.14	0/1799	0.28	0/2438
All	All	0.14	0/107940	0.28	0/146280

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1769	0	1824	17	0
1	AA	1769	0	1824	18	0
1	AB	1769	0	1824	16	0
1	B	1769	0	1824	16	0
1	BA	1769	0	1824	19	0
1	BB	1769	0	1824	17	0
1	C	1769	0	1824	18	0
1	CA	1769	0	1824	17	0
1	CB	1769	0	1824	17	0
1	D	1769	0	1824	18	0
1	DA	1769	0	1824	17	0
1	DB	1769	0	1824	17	0
1	E	1769	0	1824	17	0
1	EA	1769	0	1824	17	0
1	EB	1769	0	1824	17	0
1	F	1769	0	1824	18	0
1	FA	1769	0	1824	17	0
1	FB	1769	0	1824	19	0
1	G	1769	0	1824	18	0
1	GA	1769	0	1824	20	0
1	GB	1769	0	1824	18	0
1	H	1769	0	1824	17	0
1	HA	1769	0	1824	17	0
1	HB	1769	0	1824	16	0
1	I	1769	0	1824	16	0
1	IA	1769	0	1824	18	0
1	IB	1769	0	1824	18	0
1	J	1769	0	1824	18	0
1	JA	1769	0	1824	18	0
1	K	1769	0	1824	18	0
1	KA	1769	0	1824	17	0
1	L	1769	0	1824	20	0
1	LA	1769	0	1824	19	0
1	M	1769	0	1824	17	0
1	MA	1769	0	1824	17	0
1	N	1769	0	1824	16	0
1	NA	1769	0	1824	18	0
1	O	1769	0	1824	18	0
1	OA	1769	0	1824	18	0
1	P	1769	0	1824	16	0
1	PA	1769	0	1824	16	0
1	Q	1769	0	1824	17	0
1	QA	1769	0	1824	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	1769	0	1824	19	0
1	RA	1769	0	1824	17	0
1	S	1769	0	1824	18	0
1	SA	1769	0	1824	18	0
1	T	1769	0	1824	18	0
1	TA	1769	0	1824	18	0
1	UA	1769	0	1824	15	0
1	V	1769	0	1824	18	0
1	VA	1769	0	1824	19	0
1	W	1769	0	1824	19	0
1	WA	1769	0	1824	18	0
1	X	1769	0	1824	17	0
1	XA	1769	0	1824	17	0
1	Y	1769	0	1824	18	0
1	YA	1769	0	1824	18	0
1	Z	1769	0	1824	16	0
1	ZA	1769	0	1824	16	0
All	All	106140	0	109440	911	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 4.

All (911) 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:GA:548:ALA:HA	1:GA:553:LEU:HD11	1.74	0.69
1:FA:548:ALA:HA	1:FA:553:LEU:HD11	1.74	0.69
1:KA:548:ALA:HA	1:KA:553:LEU:HD11	1.74	0.69
1:LA:548:ALA:HA	1:LA:553:LEU:HD11	1.75	0.69
1:CB:548:ALA:HA	1:CB:553:LEU:HD11	1.74	0.69
1:L:548:ALA:HA	1:L:553:LEU:HD11	1.75	0.69
1:IA:548:ALA:HA	1:IA:553:LEU:HD11	1.75	0.69
1:NA:548:ALA:HA	1:NA:553:LEU:HD11	1.75	0.69
1:SA:548:ALA:HA	1:SA:553:LEU:HD11	1.74	0.69
1:G:548:ALA:HA	1:G:553:LEU:HD11	1.75	0.69
1:B:548:ALA:HA	1:B:553:LEU:HD11	1.74	0.69
1:P:548:ALA:HA	1:P:553:LEU:HD11	1.74	0.69
1:BA:548:ALA:HA	1:BA:553:LEU:HD11	1.74	0.69
1:W:548:ALA:HA	1:W:553:LEU:HD11	1.75	0.69
1:DB:548:ALA:HA	1:DB:553:LEU:HD11	1.75	0.69
1:C:548:ALA:HA	1:C:553:LEU:HD11	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:548:ALA:HA	1:J:553:LEU:HD11	1.75	0.69
1:O:548:ALA:HA	1:O:553:LEU:HD11	1.75	0.69
1:R:548:ALA:HA	1:R:553:LEU:HD11	1.74	0.69
1:JA:548:ALA:HA	1:JA:553:LEU:HD11	1.74	0.69
1:A:548:ALA:HA	1:A:553:LEU:HD11	1.75	0.69
1:E:548:ALA:HA	1:E:553:LEU:HD11	1.75	0.69
1:T:548:ALA:HA	1:T:553:LEU:HD11	1.74	0.69
1:X:548:ALA:HA	1:X:553:LEU:HD11	1.74	0.69
1:HA:548:ALA:HA	1:HA:553:LEU:HD11	1.75	0.69
1:TA:548:ALA:HA	1:TA:553:LEU:HD11	1.75	0.69
1:BB:548:ALA:HA	1:BB:553:LEU:HD11	1.75	0.69
1:Q:548:ALA:HA	1:Q:553:LEU:HD11	1.75	0.69
1:S:548:ALA:HA	1:S:553:LEU:HD11	1.74	0.69
1:MA:548:ALA:HA	1:MA:553:LEU:HD11	1.75	0.69
1:OA:548:ALA:HA	1:OA:553:LEU:HD11	1.75	0.69
1:CA:548:ALA:HA	1:CA:553:LEU:HD11	1.75	0.68
1:RA:548:ALA:HA	1:RA:553:LEU:HD11	1.74	0.68
1:F:548:ALA:HA	1:F:553:LEU:HD11	1.74	0.68
1:K:548:ALA:HA	1:K:553:LEU:HD11	1.74	0.68
1:V:548:ALA:HA	1:V:553:LEU:HD11	1.74	0.68
1:Z:548:ALA:HA	1:Z:553:LEU:HD11	1.75	0.68
1:QA:548:ALA:HA	1:QA:553:LEU:HD11	1.75	0.68
1:AA:548:ALA:HA	1:AA:553:LEU:HD11	1.74	0.68
1:AB:548:ALA:HA	1:AB:553:LEU:HD11	1.75	0.68
1:HB:548:ALA:HA	1:HB:553:LEU:HD11	1.75	0.68
1:D:548:ALA:HA	1:D:553:LEU:HD11	1.75	0.68
1:EA:548:ALA:HA	1:EA:553:LEU:HD11	1.75	0.68
1:I:548:ALA:HA	1:I:553:LEU:HD11	1.75	0.68
1:N:548:ALA:HA	1:N:553:LEU:HD11	1.75	0.68
1:XA:548:ALA:HA	1:XA:553:LEU:HD11	1.75	0.68
1:EB:548:ALA:HA	1:EB:553:LEU:HD11	1.74	0.68
1:IB:548:ALA:HA	1:IB:553:LEU:HD11	1.75	0.68
1:UA:548:ALA:HA	1:UA:553:LEU:HD11	1.74	0.68
1:WA:548:ALA:HA	1:WA:553:LEU:HD11	1.75	0.68
1:GB:548:ALA:HA	1:GB:553:LEU:HD11	1.75	0.67
1:Y:548:ALA:HA	1:Y:553:LEU:HD11	1.74	0.67
1:DA:548:ALA:HA	1:DA:553:LEU:HD11	1.75	0.67
1:YA:548:ALA:HA	1:YA:553:LEU:HD11	1.75	0.67
1:FB:548:ALA:HA	1:FB:553:LEU:HD11	1.75	0.67
1:VA:548:ALA:HA	1:VA:553:LEU:HD11	1.74	0.67
1:H:548:ALA:HA	1:H:553:LEU:HD11	1.74	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZA:548:ALA:HA	1:ZA:553:LEU:HD11	1.74	0.66
1:PA:548:ALA:HA	1:PA:553:LEU:HD11	1.74	0.66
1:M:548:ALA:HA	1:M:553:LEU:HD11	1.75	0.66
1:AB:439:SER:HB2	1:AB:582:PRO:HG3	1.83	0.61
1:QA:439:SER:HB2	1:QA:582:PRO:HG3	1.83	0.61
1:E:439:SER:HB2	1:E:582:PRO:HG3	1.83	0.61
1:T:439:SER:HB2	1:T:582:PRO:HG3	1.83	0.61
1:EB:439:SER:HB2	1:EB:582:PRO:HG3	1.83	0.61
1:UA:439:SER:HB2	1:UA:582:PRO:HG3	1.83	0.61
1:DB:439:SER:HB2	1:DB:582:PRO:HG3	1.83	0.61
1:HB:439:SER:HB2	1:HB:582:PRO:HG3	1.83	0.61
1:J:439:SER:HB2	1:J:582:PRO:HG3	1.83	0.61
1:O:439:SER:HB2	1:O:582:PRO:HG3	1.83	0.61
1:GA:439:SER:HB2	1:GA:582:PRO:HG3	1.83	0.61
1:LA:439:SER:HB2	1:LA:582:PRO:HG3	1.83	0.61
1:TA:439:SER:HB2	1:TA:582:PRO:HG3	1.83	0.61
1:N:439:SER:HB2	1:N:582:PRO:HG3	1.83	0.61
1:R:439:SER:HB2	1:R:582:PRO:HG3	1.83	0.61
1:IA:439:SER:HB2	1:IA:582:PRO:HG3	1.83	0.61
1:BA:439:SER:HB2	1:BA:582:PRO:HG3	1.83	0.60
1:W:439:SER:HB2	1:W:582:PRO:HG3	1.83	0.60
1:PA:439:SER:HB2	1:PA:582:PRO:HG3	1.83	0.60
1:XA:439:SER:HB2	1:XA:582:PRO:HG3	1.83	0.60
1:FB:439:SER:HB2	1:FB:582:PRO:HG3	1.83	0.60
1:CA:439:SER:HB2	1:CA:582:PRO:HG3	1.83	0.60
1:EA:439:SER:HB2	1:EA:582:PRO:HG3	1.83	0.60
1:NA:439:SER:HB2	1:NA:582:PRO:HG3	1.83	0.60
1:VA:439:SER:HB2	1:VA:582:PRO:HG3	1.83	0.60
1:ZA:439:SER:HB2	1:ZA:582:PRO:HG3	1.83	0.60
1:BB:439:SER:HB2	1:BB:582:PRO:HG3	1.83	0.60
1:C:439:SER:HB2	1:C:582:PRO:HG3	1.83	0.60
1:I:439:SER:HB2	1:I:582:PRO:HG3	1.83	0.60
1:Z:439:SER:HB2	1:Z:582:PRO:HG3	1.83	0.60
1:FA:439:SER:HB2	1:FA:582:PRO:HG3	1.83	0.60
1:KA:439:SER:HB2	1:KA:582:PRO:HG3	1.83	0.60
1:WA:439:SER:HB2	1:WA:582:PRO:HG3	1.83	0.60
1:B:439:SER:HB2	1:B:582:PRO:HG3	1.83	0.60
1:A:439:SER:HB2	1:A:582:PRO:HG3	1.83	0.60
1:X:439:SER:HB2	1:X:582:PRO:HG3	1.83	0.60
1:RA:439:SER:HB2	1:RA:582:PRO:HG3	1.83	0.60
1:GB:439:SER:HB2	1:GB:582:PRO:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:439:SER:HB2	1:P:582:PRO:HG3	1.83	0.60
1:Q:439:SER:HB2	1:Q:582:PRO:HG3	1.83	0.60
1:G:439:SER:HB2	1:G:582:PRO:HG3	1.83	0.60
1:H:439:SER:HB2	1:H:582:PRO:HG3	1.83	0.60
1:L:439:SER:HB2	1:L:582:PRO:HG3	1.83	0.60
1:PA:524:PRO:HB3	1:PA:544:LEU:HB3	1.84	0.60
1:ZA:524:PRO:HB3	1:ZA:544:LEU:HB3	1.84	0.60
1:BA:524:PRO:HB3	1:BA:544:LEU:HB3	1.84	0.60
1:YA:439:SER:HB2	1:YA:582:PRO:HG3	1.83	0.60
1:EB:524:PRO:HB3	1:EB:544:LEU:HB3	1.84	0.59
1:IB:439:SER:HB2	1:IB:582:PRO:HG3	1.83	0.59
1:D:439:SER:HB2	1:D:582:PRO:HG3	1.83	0.59
1:M:439:SER:HB2	1:M:582:PRO:HG3	1.83	0.59
1:S:439:SER:HB2	1:S:582:PRO:HG3	1.83	0.59
1:W:524:PRO:HB3	1:W:544:LEU:HB3	1.84	0.59
1:Y:439:SER:HB2	1:Y:582:PRO:HG3	1.83	0.59
1:DA:439:SER:HB2	1:DA:582:PRO:HG3	1.83	0.59
1:UA:524:PRO:HB3	1:UA:544:LEU:HB3	1.84	0.59
1:V:439:SER:HB2	1:V:582:PRO:HG3	1.83	0.59
1:GA:524:PRO:HB3	1:GA:544:LEU:HB3	1.84	0.59
1:LA:524:PRO:HB3	1:LA:544:LEU:HB3	1.84	0.59
1:MA:439:SER:HB2	1:MA:582:PRO:HG3	1.83	0.59
1:OA:439:SER:HB2	1:OA:582:PRO:HG3	1.83	0.59
1:SA:524:PRO:HB3	1:SA:544:LEU:HB3	1.84	0.59
1:FB:524:PRO:HB3	1:FB:544:LEU:HB3	1.84	0.59
1:N:524:PRO:HB3	1:N:544:LEU:HB3	1.84	0.59
1:AA:439:SER:HB2	1:AA:582:PRO:HG3	1.83	0.59
1:HA:439:SER:HB2	1:HA:582:PRO:HG3	1.83	0.59
1:JA:439:SER:HB2	1:JA:582:PRO:HG3	1.83	0.59
1:JA:524:PRO:HB3	1:JA:544:LEU:HB3	1.84	0.59
1:OA:524:PRO:HB3	1:OA:544:LEU:HB3	1.84	0.59
1:CB:439:SER:HB2	1:CB:582:PRO:HG3	1.83	0.59
1:CB:524:PRO:HB3	1:CB:544:LEU:HB3	1.84	0.59
1:E:524:PRO:HB3	1:E:544:LEU:HB3	1.84	0.59
1:I:524:PRO:HB3	1:I:544:LEU:HB3	1.84	0.59
1:P:524:PRO:HB3	1:P:544:LEU:HB3	1.84	0.59
1:SA:439:SER:HB2	1:SA:582:PRO:HG3	1.83	0.59
1:VA:524:PRO:HB3	1:VA:544:LEU:HB3	1.84	0.59
1:B:524:PRO:HB3	1:B:544:LEU:HB3	1.84	0.59
1:F:439:SER:HB2	1:F:582:PRO:HG3	1.83	0.59
1:T:524:PRO:HB3	1:T:544:LEU:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:524:PRO:HB3	1:C:544:LEU:HB3	1.84	0.59
1:R:524:PRO:HB3	1:R:544:LEU:HB3	1.84	0.59
1:K:439:SER:HB2	1:K:582:PRO:HG3	1.83	0.59
1:H:524:PRO:HB3	1:H:544:LEU:HB3	1.84	0.59
1:M:524:PRO:HB3	1:M:544:LEU:HB3	1.84	0.59
1:HB:524:PRO:HB3	1:HB:544:LEU:HB3	1.84	0.59
1:BB:524:PRO:HB3	1:BB:544:LEU:HB3	1.84	0.59
1:Y:524:PRO:HB3	1:Y:544:LEU:HB3	1.84	0.59
1:TA:524:PRO:HB3	1:TA:544:LEU:HB3	1.84	0.59
1:XA:524:PRO:HB3	1:XA:544:LEU:HB3	1.84	0.59
1:DB:524:PRO:HB3	1:DB:544:LEU:HB3	1.84	0.58
1:GB:524:PRO:HB3	1:GB:544:LEU:HB3	1.84	0.58
1:IB:524:PRO:HB3	1:IB:544:LEU:HB3	1.84	0.58
1:RA:524:PRO:HB3	1:RA:544:LEU:HB3	1.84	0.58
1:Q:524:PRO:HB3	1:Q:544:LEU:HB3	1.84	0.58
1:WA:524:PRO:HB3	1:WA:544:LEU:HB3	1.84	0.58
1:A:524:PRO:HB3	1:A:544:LEU:HB3	1.84	0.58
1:J:524:PRO:HB3	1:J:544:LEU:HB3	1.84	0.58
1:O:524:PRO:HB3	1:O:544:LEU:HB3	1.84	0.58
1:X:524:PRO:HB3	1:X:544:LEU:HB3	1.84	0.58
1:DA:524:PRO:HB3	1:DA:544:LEU:HB3	1.84	0.58
1:IA:524:PRO:HB3	1:IA:544:LEU:HB3	1.84	0.58
1:KA:524:PRO:HB3	1:KA:544:LEU:HB3	1.84	0.58
1:YA:524:PRO:HB3	1:YA:544:LEU:HB3	1.84	0.58
1:FA:524:PRO:HB3	1:FA:544:LEU:HB3	1.84	0.58
1:F:524:PRO:HB3	1:F:544:LEU:HB3	1.84	0.58
1:CA:524:PRO:HB3	1:CA:544:LEU:HB3	1.84	0.58
1:AB:524:PRO:HB3	1:AB:544:LEU:HB3	1.84	0.58
1:K:524:PRO:HB3	1:K:544:LEU:HB3	1.84	0.58
1:EA:524:PRO:HB3	1:EA:544:LEU:HB3	1.84	0.58
1:NA:524:PRO:HB3	1:NA:544:LEU:HB3	1.84	0.58
1:L:524:PRO:HB3	1:L:544:LEU:HB3	1.84	0.58
1:Z:524:PRO:HB3	1:Z:544:LEU:HB3	1.84	0.58
1:D:524:PRO:HB3	1:D:544:LEU:HB3	1.84	0.58
1:G:524:PRO:HB3	1:G:544:LEU:HB3	1.84	0.58
1:S:524:PRO:HB3	1:S:544:LEU:HB3	1.84	0.58
1:V:524:PRO:HB3	1:V:544:LEU:HB3	1.84	0.57
1:AA:524:PRO:HB3	1:AA:544:LEU:HB3	1.84	0.57
1:QA:524:PRO:HB3	1:QA:544:LEU:HB3	1.84	0.57
1:HA:524:PRO:HB3	1:HA:544:LEU:HB3	1.84	0.57
1:MA:524:PRO:HB3	1:MA:544:LEU:HB3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:564:THR:OG1	1:F:584:GLN:OE1	2.22	0.57
1:DB:574:LYS:NZ	1:DB:594:GLU:OE1	2.38	0.56
1:G:574:LYS:NZ	1:G:594:GLU:OE1	2.39	0.56
1:K:564:THR:OG1	1:K:584:GLN:OE1	2.22	0.56
1:FA:574:LYS:NZ	1:FA:594:GLU:OE1	2.39	0.56
1:JA:574:LYS:NZ	1:JA:594:GLU:OE1	2.39	0.56
1:KA:574:LYS:NZ	1:KA:594:GLU:OE1	2.39	0.56
1:TA:574:LYS:NZ	1:TA:594:GLU:OE1	2.39	0.56
1:YA:574:LYS:NZ	1:YA:594:GLU:OE1	2.39	0.56
1:IB:574:LYS:NZ	1:IB:594:GLU:OE1	2.39	0.56
1:D:574:LYS:NZ	1:D:594:GLU:OE1	2.39	0.56
1:J:574:LYS:NZ	1:J:594:GLU:OE1	2.38	0.56
1:L:574:LYS:NZ	1:L:594:GLU:OE1	2.39	0.56
1:S:574:LYS:NZ	1:S:594:GLU:OE1	2.39	0.56
1:OA:574:LYS:NZ	1:OA:594:GLU:OE1	2.39	0.56
1:SA:574:LYS:NZ	1:SA:594:GLU:OE1	2.39	0.56
1:CB:574:LYS:NZ	1:CB:594:GLU:OE1	2.39	0.56
1:O:574:LYS:NZ	1:O:594:GLU:OE1	2.39	0.56
1:GA:574:LYS:NZ	1:GA:594:GLU:OE1	2.39	0.56
1:HA:574:LYS:NZ	1:HA:594:GLU:OE1	2.39	0.56
1:MA:574:LYS:NZ	1:MA:594:GLU:OE1	2.39	0.56
1:ZA:574:LYS:NZ	1:ZA:594:GLU:OE1	2.39	0.56
1:BB:574:LYS:NZ	1:BB:594:GLU:OE1	2.39	0.56
1:GB:574:LYS:NZ	1:GB:594:GLU:OE1	2.39	0.56
1:HB:574:LYS:NZ	1:HB:594:GLU:OE1	2.39	0.56
1:X:574:LYS:NZ	1:X:594:GLU:OE1	2.39	0.56
1:Z:564:THR:OG1	1:Z:584:GLN:OE1	2.22	0.56
1:CA:574:LYS:NZ	1:CA:594:GLU:OE1	2.39	0.56
1:EA:564:THR:OG1	1:EA:584:GLN:OE1	2.22	0.56
1:PA:574:LYS:NZ	1:PA:594:GLU:OE1	2.39	0.56
1:RA:574:LYS:NZ	1:RA:594:GLU:OE1	2.39	0.56
1:XA:574:LYS:NZ	1:XA:594:GLU:OE1	2.38	0.56
1:C:574:LYS:NZ	1:C:594:GLU:OE1	2.39	0.56
1:DA:574:LYS:NZ	1:DA:594:GLU:OE1	2.38	0.56
1:LA:574:LYS:NZ	1:LA:594:GLU:OE1	2.39	0.56
1:WA:574:LYS:NZ	1:WA:594:GLU:OE1	2.39	0.56
1:R:574:LYS:NZ	1:R:594:GLU:OE1	2.39	0.56
1:Y:574:LYS:NZ	1:Y:594:GLU:OE1	2.39	0.56
1:IA:574:LYS:NZ	1:IA:594:GLU:OE1	2.39	0.56
1:UA:574:LYS:NZ	1:UA:594:GLU:OE1	2.39	0.56
1:B:574:LYS:NZ	1:B:594:GLU:OE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CB:564:THR:OG1	1:CB:584:GLN:OE1	2.22	0.56
1:EB:574:LYS:NZ	1:EB:594:GLU:OE1	2.39	0.56
1:E:574:LYS:NZ	1:E:594:GLU:OE1	2.38	0.56
1:X:564:THR:OG1	1:X:584:GLN:OE1	2.22	0.56
1:NA:574:LYS:NZ	1:NA:594:GLU:OE1	2.39	0.56
1:P:574:LYS:NZ	1:P:594:GLU:OE1	2.39	0.56
1:T:574:LYS:NZ	1:T:594:GLU:OE1	2.39	0.56
1:V:574:LYS:NZ	1:V:594:GLU:OE1	2.39	0.56
1:SA:564:THR:OG1	1:SA:584:GLN:OE1	2.22	0.56
1:A:574:LYS:NZ	1:A:594:GLU:OE1	2.39	0.56
1:AA:574:LYS:NZ	1:AA:594:GLU:OE1	2.39	0.56
1:N:574:LYS:NZ	1:N:594:GLU:OE1	2.39	0.55
1:BA:574:LYS:NZ	1:BA:594:GLU:OE1	2.39	0.55
1:EA:574:LYS:NZ	1:EA:594:GLU:OE1	2.38	0.55
1:K:574:LYS:NZ	1:K:594:GLU:OE1	2.39	0.55
1:W:574:LYS:NZ	1:W:594:GLU:OE1	2.39	0.55
1:Z:574:LYS:NZ	1:Z:594:GLU:OE1	2.39	0.55
1:CA:564:THR:OG1	1:CA:584:GLN:OE1	2.22	0.55
1:QA:574:LYS:NZ	1:QA:594:GLU:OE1	2.39	0.55
1:M:574:LYS:NZ	1:M:594:GLU:OE1	2.39	0.55
1:Q:574:LYS:NZ	1:Q:594:GLU:OE1	2.39	0.55
1:F:574:LYS:NZ	1:F:594:GLU:OE1	2.39	0.55
1:H:574:LYS:NZ	1:H:594:GLU:OE1	2.39	0.55
1:I:574:LYS:NZ	1:I:594:GLU:OE1	2.39	0.55
1:VA:574:LYS:NZ	1:VA:594:GLU:OE1	2.39	0.55
1:AB:574:LYS:NZ	1:AB:594:GLU:OE1	2.39	0.55
1:FB:574:LYS:NZ	1:FB:594:GLU:OE1	2.39	0.55
1:IA:564:THR:OG1	1:IA:584:GLN:OE1	2.22	0.55
1:NA:564:THR:OG1	1:NA:584:GLN:OE1	2.22	0.55
1:A:564:THR:OG1	1:A:584:GLN:OE1	2.22	0.55
1:Q:564:THR:OG1	1:Q:584:GLN:OE1	2.22	0.55
1:FA:564:THR:OG1	1:FA:584:GLN:OE1	2.22	0.54
1:C:564:THR:OG1	1:C:584:GLN:OE1	2.22	0.54
1:KA:564:THR:OG1	1:KA:584:GLN:OE1	2.22	0.54
1:R:564:THR:OG1	1:R:584:GLN:OE1	2.22	0.54
1:J:564:THR:OG1	1:J:584:GLN:OE1	2.22	0.54
1:O:564:THR:OG1	1:O:584:GLN:OE1	2.22	0.54
1:IB:564:THR:OG1	1:IB:584:GLN:OE1	2.22	0.54
1:GA:564:THR:OG1	1:GA:584:GLN:OE1	2.22	0.54
1:HA:564:THR:OG1	1:HA:584:GLN:OE1	2.22	0.54
1:YA:564:THR:OG1	1:YA:584:GLN:OE1	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:564:THR:OG1	1:LA:584:GLN:OE1	2.22	0.53
1:WA:564:THR:OG1	1:WA:584:GLN:OE1	2.22	0.53
1:GB:564:THR:OG1	1:GB:584:GLN:OE1	2.22	0.53
1:MA:564:THR:OG1	1:MA:584:GLN:OE1	2.22	0.53
1:DB:564:THR:OG1	1:DB:584:GLN:OE1	2.22	0.53
1:FB:564:THR:OG1	1:FB:584:GLN:OE1	2.22	0.53
1:QA:564:THR:OG1	1:QA:584:GLN:OE1	2.22	0.53
1:AB:564:THR:OG1	1:AB:584:GLN:OE1	2.22	0.53
1:E:564:THR:OG1	1:E:584:GLN:OE1	2.22	0.53
1:W:564:THR:OG1	1:W:584:GLN:OE1	2.22	0.53
1:PA:564:THR:OG1	1:PA:584:GLN:OE1	2.22	0.53
1:BA:564:THR:OG1	1:BA:584:GLN:OE1	2.22	0.52
1:TA:564:THR:OG1	1:TA:584:GLN:OE1	2.22	0.52
1:VA:564:THR:OG1	1:VA:584:GLN:OE1	2.22	0.52
1:T:564:THR:OG1	1:T:584:GLN:OE1	2.22	0.52
1:ZA:564:THR:OG1	1:ZA:584:GLN:OE1	2.22	0.52
1:G:564:THR:OG1	1:G:584:GLN:OE1	2.22	0.52
1:L:564:THR:OG1	1:L:584:GLN:OE1	2.22	0.52
1:XA:564:THR:OG1	1:XA:584:GLN:OE1	2.22	0.52
1:P:437:MET:HE1	1:YA:442:THR:HA	1.92	0.52
1:R:442:THR:HA	1:WA:437:MET:HE1	1.92	0.52
1:GB:437:MET:HE1	1:C:442:THR:HA	1.92	0.52
1:B:437:MET:HE1	1:IB:442:THR:HA	1.92	0.52
1:BB:442:THR:HA	1:HA:437:MET:HE1	1.92	0.52
1:HB:564:THR:OG1	1:HB:584:GLN:OE1	2.22	0.52
1:I:437:MET:HE1	1:P:442:THR:HA	1.92	0.52
1:MA:437:MET:HE1	1:RA:442:THR:HA	1.92	0.52
1:B:442:THR:HA	1:N:437:MET:HE1	1.92	0.52
1:AB:437:MET:HE1	1:LA:442:THR:HA	1.92	0.52
1:AA:442:THR:HA	1:NA:437:MET:HE1	1.92	0.52
1:GA:442:THR:HA	1:QA:437:MET:HE1	1.92	0.52
1:G:442:THR:HA	1:BA:437:MET:HE1	1.92	0.52
1:L:442:THR:HA	1:W:437:MET:HE1	1.92	0.52
1:X:437:MET:HE1	1:WA:442:THR:HA	1.92	0.52
1:EA:437:MET:HE1	1:XA:442:THR:HA	1.92	0.52
1:EB:437:MET:HE1	1:EA:442:THR:HA	1.92	0.51
1:FB:437:MET:HE1	1:W:442:THR:HA	1.92	0.51
1:FB:442:THR:HA	1:L:437:MET:HE1	1.92	0.51
1:GB:442:THR:HA	1:CA:437:MET:HE1	1.92	0.51
1:HB:442:THR:HA	1:Z:437:MET:HE1	1.92	0.51
1:G:437:MET:HE1	1:VA:442:THR:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:442:THR:HA	1:IA:437:MET:HE1	1.92	0.51
1:Y:564:THR:OG1	1:Y:584:GLN:OE1	2.22	0.51
1:O:437:MET:HE1	1:Y:442:THR:HA	1.92	0.51
1:O:442:THR:HA	1:FA:437:MET:HE1	1.92	0.51
1:BA:442:THR:HA	1:VA:437:MET:HE1	1.92	0.51
1:S:442:THR:HA	1:TA:437:MET:HE1	1.92	0.51
1:Z:442:THR:HA	1:UA:437:MET:HE1	1.92	0.51
1:DB:437:MET:HE1	1:D:442:THR:HA	1.92	0.51
1:EB:442:THR:HA	1:XA:437:MET:HE1	1.92	0.51
1:HB:437:MET:HE1	1:UA:442:THR:HA	1.92	0.51
1:J:437:MET:HE1	1:DA:442:THR:HA	1.92	0.51
1:BB:437:MET:HE1	1:M:442:THR:HA	1.92	0.51
1:DB:442:THR:HA	1:K:437:MET:HE1	1.92	0.51
1:C:437:MET:HE1	1:CA:442:THR:HA	1.92	0.51
1:H:442:THR:HA	1:RA:437:MET:HE1	1.92	0.51
1:J:442:THR:HA	1:KA:437:MET:HE1	1.92	0.51
1:E:437:MET:HE1	1:NA:442:THR:HA	1.92	0.51
1:F:437:MET:HE1	1:TA:442:THR:HA	1.92	0.51
1:R:437:MET:HE1	1:X:442:THR:HA	1.92	0.51
1:DA:564:THR:OG1	1:DA:584:GLN:OE1	2.22	0.51
1:I:564:THR:OG1	1:I:584:GLN:OE1	2.22	0.51
1:CB:437:MET:HE1	1:PA:442:THR:HA	1.92	0.51
1:D:437:MET:HE1	1:K:442:THR:HA	1.92	0.51
1:T:437:MET:HE1	1:IA:442:THR:HA	1.92	0.51
1:H:437:MET:HE1	1:MA:442:THR:HA	1.92	0.51
1:M:437:MET:HE1	1:HA:442:THR:HA	1.92	0.51
1:SA:437:MET:HE1	1:ZA:442:THR:HA	1.92	0.51
1:F:442:THR:HA	1:S:437:MET:HE1	1.92	0.51
1:N:564:THR:OG1	1:N:584:GLN:OE1	2.22	0.51
1:Q:437:MET:HE1	1:QA:442:THR:HA	1.92	0.51
1:V:564:THR:OG1	1:V:584:GLN:OE1	2.22	0.51
1:JA:437:MET:HE1	1:SA:442:THR:HA	1.92	0.51
1:AB:442:THR:HA	1:A:437:MET:HE1	1.92	0.51
1:CB:442:THR:HA	1:OA:437:MET:HE1	1.92	0.51
1:A:442:THR:HA	1:LA:437:MET:HE1	1.92	0.50
1:IB:437:MET:HE1	1:N:442:THR:HA	1.92	0.50
1:H:564:THR:OG1	1:H:584:GLN:OE1	2.22	0.50
1:I:442:THR:HA	1:YA:437:MET:HE1	1.92	0.50
1:Q:442:THR:HA	1:GA:437:MET:HE1	1.92	0.50
1:AA:564:THR:OG1	1:AA:584:GLN:OE1	2.22	0.50
1:DA:437:MET:HE1	1:KA:442:THR:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JA:442:THR:HA	1:ZA:437:MET:HE1	1.92	0.50
1:B:564:THR:OG1	1:B:584:GLN:OE1	2.22	0.50
1:Y:437:MET:HE1	1:FA:442:THR:HA	1.92	0.50
1:OA:442:THR:HA	1:PA:437:MET:HE1	1.92	0.50
1:M:564:THR:OG1	1:M:584:GLN:OE1	2.22	0.50
1:T:442:THR:HA	1:V:437:MET:HE1	1.92	0.50
1:BB:564:THR:OG1	1:BB:584:GLN:OE1	2.22	0.50
1:E:442:THR:HA	1:AA:437:MET:HE1	1.92	0.50
1:P:564:THR:OG1	1:P:584:GLN:OE1	2.22	0.50
1:D:564:THR:OG1	1:D:584:GLN:OE1	2.22	0.50
1:RA:564:THR:OG1	1:RA:584:GLN:OE1	2.22	0.49
1:UA:564:THR:OG1	1:UA:584:GLN:OE1	2.22	0.49
1:EB:564:THR:OG1	1:EB:584:GLN:OE1	2.22	0.49
1:JA:564:THR:OG1	1:JA:584:GLN:OE1	2.22	0.49
1:S:564:THR:OG1	1:S:584:GLN:OE1	2.22	0.49
1:OA:564:THR:OG1	1:OA:584:GLN:OE1	2.22	0.49
1:CB:446:TYR:CE1	1:CB:618:CYS:HB2	2.49	0.48
1:XA:446:TYR:CE1	1:XA:618:CYS:HB2	2.49	0.48
1:HB:446:TYR:CE1	1:HB:618:CYS:HB2	2.49	0.47
1:F:446:TYR:CE1	1:F:618:CYS:HB2	2.49	0.47
1:K:446:TYR:CE1	1:K:618:CYS:HB2	2.49	0.47
1:Q:446:TYR:CE1	1:Q:618:CYS:HB2	2.49	0.47
1:SA:446:TYR:CE1	1:SA:618:CYS:HB2	2.49	0.47
1:A:446:TYR:CE1	1:A:618:CYS:HB2	2.50	0.47
1:DB:446:TYR:CE1	1:DB:618:CYS:HB2	2.49	0.47
1:IA:446:TYR:CE1	1:IA:618:CYS:HB2	2.49	0.47
1:TA:446:TYR:CE1	1:TA:618:CYS:HB2	2.49	0.47
1:I:446:TYR:CE1	1:I:618:CYS:HB2	2.49	0.47
1:N:446:TYR:CE1	1:N:618:CYS:HB2	2.49	0.47
1:NA:446:TYR:CE1	1:NA:618:CYS:HB2	2.49	0.47
1:BB:446:TYR:CE1	1:BB:618:CYS:HB2	2.49	0.47
1:IB:446:TYR:CE1	1:IB:618:CYS:HB2	2.49	0.47
1:J:446:TYR:CE1	1:J:618:CYS:HB2	2.49	0.47
1:L:446:TYR:CE1	1:L:618:CYS:HB2	2.49	0.47
1:O:446:TYR:CE1	1:O:618:CYS:HB2	2.49	0.47
1:R:446:TYR:CE1	1:R:618:CYS:HB2	2.49	0.47
1:Y:512:SER:OG	1:Y:523:THR:HB	2.15	0.47
1:Z:446:TYR:CE1	1:Z:618:CYS:HB2	2.49	0.47
1:DA:512:SER:OG	1:DA:523:THR:HB	2.15	0.47
1:OA:512:SER:OG	1:OA:523:THR:HB	2.15	0.47
1:RA:446:TYR:CE1	1:RA:618:CYS:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:VA:446:TYR:CE1	1:VA:618:CYS:HB2	2.49	0.47
1:YA:446:TYR:CE1	1:YA:618:CYS:HB2	2.49	0.47
1:YA:512:SER:OG	1:YA:523:THR:HB	2.15	0.47
1:FB:446:TYR:CE1	1:FB:618:CYS:HB2	2.49	0.47
1:GB:512:SER:OG	1:GB:523:THR:HB	2.15	0.47
1:IB:512:SER:OG	1:IB:523:THR:HB	2.15	0.47
1:G:446:TYR:CE1	1:G:618:CYS:HB2	2.49	0.47
1:H:512:SER:OG	1:H:523:THR:HB	2.15	0.47
1:M:512:SER:OG	1:M:523:THR:HB	2.15	0.47
1:BA:446:TYR:CE1	1:BA:618:CYS:HB2	2.49	0.47
1:T:512:SER:OG	1:T:523:THR:HB	2.15	0.47
1:CA:512:SER:OG	1:CA:523:THR:HB	2.15	0.47
1:JA:512:SER:OG	1:JA:523:THR:HB	2.15	0.47
1:MA:446:TYR:CE1	1:MA:618:CYS:HB2	2.49	0.47
1:OA:446:TYR:CE1	1:OA:618:CYS:HB2	2.49	0.47
1:WA:512:SER:OG	1:WA:523:THR:HB	2.15	0.47
1:XA:512:SER:OG	1:XA:523:THR:HB	2.15	0.47
1:AB:446:TYR:CE1	1:AB:618:CYS:HB2	2.49	0.47
1:AB:512:SER:OG	1:AB:523:THR:HB	2.15	0.47
1:HB:512:SER:OG	1:HB:523:THR:HB	2.15	0.47
1:C:446:TYR:CE1	1:C:618:CYS:HB2	2.49	0.47
1:D:446:TYR:CE1	1:D:618:CYS:HB2	2.49	0.47
1:E:512:SER:OG	1:E:523:THR:HB	2.15	0.47
1:F:512:SER:OG	1:F:523:THR:HB	2.15	0.47
1:K:512:SER:OG	1:K:523:THR:HB	2.15	0.47
1:BA:512:SER:OG	1:BA:523:THR:HB	2.15	0.47
1:S:446:TYR:CE1	1:S:618:CYS:HB2	2.49	0.47
1:V:512:SER:OG	1:V:523:THR:HB	2.15	0.47
1:W:446:TYR:CE1	1:W:618:CYS:HB2	2.50	0.47
1:X:512:SER:OG	1:X:523:THR:HB	2.15	0.47
1:AA:512:SER:OG	1:AA:523:THR:HB	2.15	0.47
1:EA:446:TYR:CE1	1:EA:618:CYS:HB2	2.49	0.47
1:GA:446:TYR:CE1	1:GA:618:CYS:HB2	2.49	0.47
1:HA:446:TYR:CE1	1:HA:618:CYS:HB2	2.50	0.47
1:IA:512:SER:OG	1:IA:523:THR:HB	2.15	0.47
1:JA:446:TYR:CE1	1:JA:618:CYS:HB2	2.49	0.47
1:LA:446:TYR:CE1	1:LA:618:CYS:HB2	2.49	0.47
1:NA:512:SER:OG	1:NA:523:THR:HB	2.15	0.47
1:QA:446:TYR:CE1	1:QA:618:CYS:HB2	2.49	0.47
1:QA:512:SER:OG	1:QA:523:THR:HB	2.15	0.47
1:UA:446:TYR:CE1	1:UA:618:CYS:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EB:446:TYR:CE1	1:EB:618:CYS:HB2	2.49	0.47
1:GB:446:TYR:CE1	1:GB:618:CYS:HB2	2.49	0.47
1:H:446:TYR:CE1	1:H:618:CYS:HB2	2.49	0.47
1:R:512:SER:OG	1:R:523:THR:HB	2.15	0.47
1:W:512:SER:OG	1:W:523:THR:HB	2.15	0.47
1:FA:446:TYR:CE1	1:FA:618:CYS:HB2	2.49	0.47
1:L:512:SER:OG	1:L:523:THR:HB	2.15	0.47
1:M:446:TYR:CE1	1:M:618:CYS:HB2	2.49	0.47
1:M:499:MET:O	1:M:501:THR:N	2.48	0.47
1:O:512:SER:OG	1:O:523:THR:HB	2.15	0.47
1:V:446:TYR:CE1	1:V:618:CYS:HB2	2.49	0.47
1:Z:499:MET:O	1:Z:501:THR:N	2.48	0.47
1:AA:446:TYR:CE1	1:AA:618:CYS:HB2	2.49	0.47
1:CA:499:MET:O	1:CA:501:THR:N	2.48	0.47
1:EA:499:MET:O	1:EA:501:THR:N	2.48	0.47
1:GA:499:MET:O	1:GA:501:THR:N	2.48	0.47
1:GA:512:SER:OG	1:GA:523:THR:HB	2.15	0.47
1:KA:446:TYR:CE1	1:KA:618:CYS:HB2	2.49	0.47
1:LA:499:MET:O	1:LA:501:THR:N	2.48	0.47
1:LA:512:SER:OG	1:LA:523:THR:HB	2.15	0.47
1:PA:446:TYR:CE1	1:PA:618:CYS:HB2	2.49	0.47
1:WA:446:TYR:CE1	1:WA:618:CYS:HB2	2.49	0.47
1:ZA:446:TYR:CE1	1:ZA:618:CYS:HB2	2.49	0.47
1:EB:512:SER:OG	1:EB:523:THR:HB	2.15	0.47
1:C:512:SER:OG	1:C:523:THR:HB	2.15	0.47
1:G:512:SER:OG	1:G:523:THR:HB	2.15	0.47
1:H:499:MET:O	1:H:501:THR:N	2.48	0.47
1:J:512:SER:OG	1:J:523:THR:HB	2.15	0.47
1:P:446:TYR:CE1	1:P:618:CYS:HB2	2.49	0.47
1:X:499:MET:O	1:X:501:THR:N	2.48	0.47
1:B:446:TYR:CE1	1:B:618:CYS:HB2	2.49	0.46
1:A:512:SER:OG	1:A:523:THR:HB	2.15	0.46
1:DB:499:MET:O	1:DB:501:THR:N	2.48	0.46
1:D:512:SER:OG	1:D:523:THR:HB	2.15	0.46
1:P:512:SER:OG	1:P:523:THR:HB	2.15	0.46
1:S:512:SER:OG	1:S:523:THR:HB	2.15	0.46
1:T:446:TYR:CE1	1:T:618:CYS:HB2	2.49	0.46
1:TA:499:MET:O	1:TA:501:THR:N	2.48	0.46
1:UA:499:MET:O	1:UA:501:THR:N	2.48	0.46
1:UA:512:SER:OG	1:UA:523:THR:HB	2.15	0.46
1:B:512:SER:OG	1:B:523:THR:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EB:499:MET:O	1:EB:501:THR:N	2.48	0.46
1:CA:446:TYR:CE1	1:CA:618:CYS:HB2	2.49	0.46
1:FA:499:MET:O	1:FA:501:THR:N	2.48	0.46
1:KA:499:MET:O	1:KA:501:THR:N	2.48	0.46
1:FB:499:MET:O	1:FB:501:THR:N	2.48	0.46
1:GB:499:MET:O	1:GB:501:THR:N	2.48	0.46
1:E:446:TYR:CE1	1:E:618:CYS:HB2	2.49	0.46
1:J:499:MET:O	1:J:501:THR:N	2.48	0.46
1:O:499:MET:O	1:O:501:THR:N	2.48	0.46
1:Q:512:SER:OG	1:Q:523:THR:HB	2.15	0.46
1:X:446:TYR:CE1	1:X:618:CYS:HB2	2.49	0.46
1:EA:512:SER:OG	1:EA:523:THR:HB	2.15	0.46
1:TA:512:SER:OG	1:TA:523:THR:HB	2.15	0.46
1:WA:499:MET:O	1:WA:501:THR:N	2.48	0.46
1:G:499:MET:O	1:G:501:THR:N	2.48	0.46
1:I:512:SER:OG	1:I:523:THR:HB	2.15	0.46
1:Q:499:MET:O	1:Q:501:THR:N	2.48	0.46
1:Y:446:TYR:CE1	1:Y:618:CYS:HB2	2.49	0.46
1:Z:512:SER:OG	1:Z:523:THR:HB	2.15	0.46
1:NA:499:MET:O	1:NA:501:THR:N	2.48	0.46
1:E:499:MET:O	1:E:501:THR:N	2.48	0.46
1:L:499:MET:O	1:L:501:THR:N	2.48	0.46
1:N:512:SER:OG	1:N:523:THR:HB	2.15	0.46
1:T:499:MET:O	1:T:501:THR:N	2.48	0.46
1:DA:446:TYR:CE1	1:DA:618:CYS:HB2	2.49	0.46
1:HA:499:MET:O	1:HA:501:THR:N	2.48	0.46
1:IA:499:MET:O	1:IA:501:THR:N	2.48	0.46
1:MA:512:SER:OG	1:MA:523:THR:HB	2.15	0.46
1:PA:512:SER:OG	1:PA:523:THR:HB	2.15	0.46
1:VA:499:MET:O	1:VA:501:THR:N	2.48	0.46
1:ZA:499:MET:O	1:ZA:501:THR:N	2.48	0.46
1:ZA:512:SER:OG	1:ZA:523:THR:HB	2.15	0.46
1:A:499:MET:O	1:A:501:THR:N	2.48	0.46
1:DB:512:SER:OG	1:DB:523:THR:HB	2.15	0.46
1:FB:512:SER:OG	1:FB:523:THR:HB	2.15	0.46
1:MA:499:MET:O	1:MA:501:THR:N	2.48	0.46
1:PA:499:MET:O	1:PA:501:THR:N	2.48	0.46
1:RA:512:SER:OG	1:RA:523:THR:HB	2.15	0.46
1:BB:512:SER:OG	1:BB:523:THR:HB	2.15	0.46
1:F:499:MET:O	1:F:501:THR:N	2.48	0.46
1:AA:499:MET:O	1:AA:501:THR:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HA:512:SER:OG	1:HA:523:THR:HB	2.15	0.46
1:KA:512:SER:OG	1:KA:523:THR:HB	2.15	0.46
1:IB:499:MET:O	1:IB:501:THR:N	2.48	0.46
1:V:499:MET:O	1:V:501:THR:N	2.48	0.46
1:VA:512:SER:OG	1:VA:523:THR:HB	2.15	0.46
1:BB:499:MET:O	1:BB:501:THR:N	2.48	0.46
1:HB:499:MET:O	1:HB:501:THR:N	2.48	0.46
1:K:499:MET:O	1:K:501:THR:N	2.48	0.46
1:N:499:MET:O	1:N:501:THR:N	2.48	0.46
1:FA:512:SER:OG	1:FA:523:THR:HB	2.15	0.46
1:RA:499:MET:O	1:RA:501:THR:N	2.48	0.46
1:YA:499:MET:O	1:YA:501:THR:N	2.48	0.46
1:B:499:MET:O	1:B:501:THR:N	2.48	0.46
1:I:499:MET:O	1:I:501:THR:N	2.48	0.46
1:P:499:MET:O	1:P:501:THR:N	2.48	0.46
1:Y:499:MET:O	1:Y:501:THR:N	2.48	0.46
1:XA:499:MET:O	1:XA:501:THR:N	2.48	0.46
1:CB:499:MET:O	1:CB:501:THR:N	2.48	0.45
1:CB:512:SER:OG	1:CB:523:THR:HB	2.15	0.45
1:DA:499:MET:O	1:DA:501:THR:N	2.48	0.45
1:SA:499:MET:O	1:SA:501:THR:N	2.48	0.45
1:SA:512:SER:OG	1:SA:523:THR:HB	2.15	0.45
1:BA:499:MET:O	1:BA:501:THR:N	2.48	0.45
1:W:439:SER:OG	1:W:580:ILE:O	2.31	0.45
1:W:499:MET:O	1:W:501:THR:N	2.48	0.45
1:B:517:THR:C	1:B:519:ALA:H	2.25	0.45
1:AB:499:MET:O	1:AB:501:THR:N	2.48	0.45
1:AB:522:ILE:HG21	1:AB:548:ALA:HB1	1.99	0.45
1:A:517:THR:C	1:A:519:ALA:H	2.25	0.45
1:P:517:THR:C	1:P:519:ALA:H	2.25	0.45
1:BA:439:SER:OG	1:BA:580:ILE:O	2.31	0.45
1:QA:522:ILE:HG21	1:QA:548:ALA:HB1	1.99	0.45
1:DB:522:ILE:HG21	1:DB:548:ALA:HB1	1.99	0.45
1:C:522:ILE:HG21	1:C:548:ALA:HB1	1.99	0.45
1:D:499:MET:O	1:D:501:THR:N	2.48	0.45
1:Q:517:THR:C	1:Q:519:ALA:H	2.25	0.45
1:EA:522:ILE:HG21	1:EA:548:ALA:HB1	1.99	0.45
1:GA:522:ILE:HG21	1:GA:548:ALA:HB1	1.99	0.45
1:HA:517:THR:C	1:HA:519:ALA:H	2.25	0.45
1:MA:517:THR:C	1:MA:519:ALA:H	2.25	0.45
1:IB:517:THR:C	1:IB:519:ALA:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:517:THR:C	1:G:519:ALA:H	2.25	0.45
1:R:522:ILE:HG21	1:R:548:ALA:HB1	1.99	0.45
1:S:499:MET:O	1:S:501:THR:N	2.48	0.45
1:W:517:THR:C	1:W:519:ALA:H	2.25	0.45
1:Z:522:ILE:HG21	1:Z:548:ALA:HB1	1.99	0.45
1:KA:517:THR:C	1:KA:519:ALA:H	2.25	0.45
1:OA:499:MET:O	1:OA:501:THR:N	2.48	0.45
1:QA:499:MET:O	1:QA:501:THR:N	2.48	0.45
1:J:522:ILE:HG21	1:J:548:ALA:HB1	1.99	0.45
1:L:517:THR:C	1:L:519:ALA:H	2.25	0.45
1:O:522:ILE:HG21	1:O:548:ALA:HB1	1.99	0.45
1:P:522:ILE:HG21	1:P:548:ALA:HB1	1.99	0.45
1:R:517:THR:C	1:R:519:ALA:H	2.25	0.45
1:BA:517:THR:C	1:BA:519:ALA:H	2.25	0.45
1:T:517:THR:C	1:T:519:ALA:H	2.25	0.45
1:FA:517:THR:C	1:FA:519:ALA:H	2.25	0.45
1:LA:522:ILE:HG21	1:LA:548:ALA:HB1	1.99	0.45
1:RA:522:ILE:HG21	1:RA:548:ALA:HB1	1.99	0.45
1:TA:522:ILE:HG21	1:TA:548:ALA:HB1	1.99	0.45
1:UA:517:THR:C	1:UA:519:ALA:H	2.25	0.45
1:YA:517:THR:C	1:YA:519:ALA:H	2.25	0.45
1:B:522:ILE:HG21	1:B:548:ALA:HB1	1.99	0.45
1:CB:517:THR:C	1:CB:519:ALA:H	2.25	0.45
1:EB:517:THR:C	1:EB:519:ALA:H	2.25	0.45
1:HB:522:ILE:HG21	1:HB:548:ALA:HB1	1.99	0.45
1:C:517:THR:C	1:C:519:ALA:H	2.25	0.45
1:E:517:THR:C	1:E:519:ALA:H	2.25	0.45
1:L:522:ILE:HG21	1:L:548:ALA:HB1	1.99	0.45
1:GA:517:THR:C	1:GA:519:ALA:H	2.25	0.45
1:JA:499:MET:O	1:JA:501:THR:N	2.48	0.45
1:KA:522:ILE:HG21	1:KA:548:ALA:HB1	1.99	0.45
1:LA:517:THR:C	1:LA:519:ALA:H	2.25	0.45
1:D:522:ILE:HG21	1:D:548:ALA:HB1	1.99	0.45
1:G:522:ILE:HG21	1:G:548:ALA:HB1	1.99	0.45
1:AA:522:ILE:HG21	1:AA:548:ALA:HB1	1.99	0.45
1:FA:522:ILE:HG21	1:FA:548:ALA:HB1	1.99	0.45
1:IA:517:THR:C	1:IA:519:ALA:H	2.25	0.45
1:IA:522:ILE:HG21	1:IA:548:ALA:HB1	1.99	0.45
1:JA:522:ILE:HG21	1:JA:548:ALA:HB1	1.99	0.45
1:NA:517:THR:C	1:NA:519:ALA:H	2.25	0.45
1:NA:522:ILE:HG21	1:NA:548:ALA:HB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:517:THR:C	1:SA:519:ALA:H	2.25	0.45
1:BB:522:ILE:HG21	1:BB:548:ALA:HB1	1.99	0.44
1:C:499:MET:O	1:C:501:THR:N	2.48	0.44
1:H:517:THR:C	1:H:519:ALA:H	2.25	0.44
1:S:522:ILE:HG21	1:S:548:ALA:HB1	1.99	0.44
1:V:522:ILE:HG21	1:V:548:ALA:HB1	1.99	0.44
1:X:522:ILE:HG21	1:X:548:ALA:HB1	1.99	0.44
1:CA:522:ILE:HG21	1:CA:548:ALA:HB1	1.99	0.44
1:OA:522:ILE:HG21	1:OA:548:ALA:HB1	1.99	0.44
1:TA:517:THR:C	1:TA:519:ALA:H	2.25	0.44
1:XA:522:ILE:HG21	1:XA:548:ALA:HB1	1.99	0.44
1:DB:517:THR:C	1:DB:519:ALA:H	2.25	0.44
1:H:522:ILE:HG21	1:H:548:ALA:HB1	1.99	0.44
1:M:522:ILE:HG21	1:M:548:ALA:HB1	1.99	0.44
1:T:522:ILE:HG21	1:T:548:ALA:HB1	1.99	0.44
1:X:517:THR:C	1:X:519:ALA:H	2.25	0.44
1:IB:522:ILE:HG21	1:IB:548:ALA:HB1	1.99	0.44
1:E:522:ILE:HG21	1:E:548:ALA:HB1	1.99	0.44
1:M:517:THR:C	1:M:519:ALA:H	2.25	0.44
1:W:522:ILE:HG21	1:W:548:ALA:HB1	1.99	0.44
1:CA:517:THR:C	1:CA:519:ALA:H	2.25	0.44
1:YA:522:ILE:HG21	1:YA:548:ALA:HB1	1.99	0.44
1:R:499:MET:O	1:R:501:THR:N	2.48	0.44
1:V:517:THR:C	1:V:519:ALA:H	2.25	0.44
1:EA:517:THR:C	1:EA:519:ALA:H	2.25	0.44
1:JA:517:THR:C	1:JA:519:ALA:H	2.25	0.44
1:SA:522:ILE:HG21	1:SA:548:ALA:HB1	1.99	0.44
1:CB:522:ILE:HG21	1:CB:548:ALA:HB1	1.99	0.44
1:BA:522:ILE:HG21	1:BA:548:ALA:HB1	1.99	0.44
1:Y:517:THR:C	1:Y:519:ALA:H	2.25	0.44
1:Z:517:THR:C	1:Z:519:ALA:H	2.25	0.44
1:AA:517:THR:C	1:AA:519:ALA:H	2.25	0.44
1:OA:517:THR:C	1:OA:519:ALA:H	2.25	0.44
1:HB:517:THR:C	1:HB:519:ALA:H	2.25	0.44
1:D:517:THR:C	1:D:519:ALA:H	2.25	0.44
1:I:517:THR:C	1:I:519:ALA:H	2.25	0.44
1:K:517:THR:C	1:K:519:ALA:H	2.25	0.44
1:S:517:THR:C	1:S:519:ALA:H	2.25	0.44
1:AB:517:THR:C	1:AB:519:ALA:H	2.25	0.44
1:N:517:THR:C	1:N:519:ALA:H	2.25	0.44
1:DA:517:THR:C	1:DA:519:ALA:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NA:439:SER:OG	1:NA:580:ILE:O	2.31	0.44
1:PA:517:THR:C	1:PA:519:ALA:H	2.25	0.44
1:QA:517:THR:C	1:QA:519:ALA:H	2.25	0.44
1:ZA:517:THR:C	1:ZA:519:ALA:H	2.25	0.44
1:ZA:522:ILE:HG21	1:ZA:548:ALA:HB1	1.99	0.44
1:F:517:THR:C	1:F:519:ALA:H	2.25	0.44
1:XA:517:THR:C	1:XA:519:ALA:H	2.25	0.44
1:F:522:ILE:HG21	1:F:548:ALA:HB1	1.99	0.44
1:IA:439:SER:OG	1:IA:580:ILE:O	2.31	0.44
1:PA:522:ILE:HG21	1:PA:548:ALA:HB1	1.99	0.44
1:K:522:ILE:HG21	1:K:548:ALA:HB1	1.99	0.43
1:SA:436:LEU:HD12	1:SA:436:LEU:HA	1.89	0.43
1:BB:517:THR:C	1:BB:519:ALA:H	2.25	0.43
1:FB:522:ILE:HG21	1:FB:548:ALA:HB1	1.99	0.43
1:GB:517:THR:C	1:GB:519:ALA:H	2.25	0.43
1:C:436:LEU:HD12	1:C:436:LEU:HA	1.89	0.43
1:J:517:THR:C	1:J:519:ALA:H	2.25	0.43
1:RA:517:THR:C	1:RA:519:ALA:H	2.25	0.43
1:WA:517:THR:C	1:WA:519:ALA:H	2.25	0.43
1:O:517:THR:C	1:O:519:ALA:H	2.25	0.43
1:HA:522:ILE:HG21	1:HA:548:ALA:HB1	1.99	0.43
1:JA:436:LEU:HD12	1:JA:436:LEU:HA	1.89	0.43
1:MA:522:ILE:HG21	1:MA:548:ALA:HB1	1.99	0.43
1:VA:522:ILE:HG21	1:VA:548:ALA:HB1	1.99	0.43
1:Q:522:ILE:HG21	1:Q:548:ALA:HB1	1.99	0.43
1:R:436:LEU:HD12	1:R:436:LEU:HA	1.89	0.43
1:DA:522:ILE:HG21	1:DA:548:ALA:HB1	1.99	0.43
1:A:522:ILE:HG21	1:A:548:ALA:HB1	1.99	0.43
1:FB:517:THR:C	1:FB:519:ALA:H	2.25	0.43
1:GB:522:ILE:HG21	1:GB:548:ALA:HB1	1.99	0.43
1:I:522:ILE:HG21	1:I:548:ALA:HB1	1.99	0.43
1:N:522:ILE:HG21	1:N:548:ALA:HB1	1.99	0.43
1:Y:522:ILE:HG21	1:Y:548:ALA:HB1	1.99	0.43
1:VA:517:THR:C	1:VA:519:ALA:H	2.25	0.43
1:HB:436:LEU:HD12	1:HB:436:LEU:HA	1.89	0.43
1:D:554:GLN:HB2	1:D:557:GLU:HG3	2.01	0.43
1:E:554:GLN:HB2	1:E:557:GLU:HG3	2.01	0.43
1:T:439:SER:OG	1:T:580:ILE:O	2.31	0.43
1:T:554:GLN:HB2	1:T:557:GLU:HG3	2.01	0.43
1:WA:522:ILE:HG21	1:WA:548:ALA:HB1	1.99	0.43
1:XA:436:LEU:HD12	1:XA:436:LEU:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:554:GLN:HB2	1:LA:557:GLU:HG3	2.01	0.43
1:GA:554:GLN:HB2	1:GA:557:GLU:HG3	2.01	0.43
1:GA:436:LEU:HD12	1:GA:436:LEU:HA	1.89	0.43
1:J:436:LEU:HD12	1:J:436:LEU:HA	1.89	0.42
1:S:554:GLN:HB2	1:S:557:GLU:HG3	2.01	0.42
1:V:554:GLN:HB2	1:V:557:GLU:HG3	2.01	0.42
1:UA:522:ILE:HG21	1:UA:548:ALA:HB1	1.99	0.42
1:AB:554:GLN:HB2	1:AB:557:GLU:HG3	2.01	0.42
1:EB:522:ILE:HG21	1:EB:548:ALA:HB1	1.99	0.42
1:F:554:GLN:HB2	1:F:557:GLU:HG3	2.01	0.42
1:K:554:GLN:HB2	1:K:557:GLU:HG3	2.01	0.42
1:BA:554:GLN:HB2	1:BA:557:GLU:HG3	2.01	0.42
1:Z:554:GLN:HB2	1:Z:557:GLU:HG3	2.01	0.42
1:EA:554:GLN:HB2	1:EA:557:GLU:HG3	2.01	0.42
1:OA:436:LEU:HD12	1:OA:436:LEU:HA	1.89	0.42
1:W:554:GLN:HB2	1:W:557:GLU:HG3	2.01	0.42
1:AA:554:GLN:HB2	1:AA:557:GLU:HG3	2.01	0.42
1:QA:554:GLN:HB2	1:QA:557:GLU:HG3	2.01	0.42
1:D:439:SER:OG	1:D:580:ILE:O	2.31	0.42
1:O:436:LEU:HD12	1:O:436:LEU:HA	1.89	0.42
1:O:554:GLN:HB2	1:O:557:GLU:HG3	2.01	0.42
1:X:554:GLN:HB2	1:X:557:GLU:HG3	2.01	0.42
1:CA:554:GLN:HB2	1:CA:557:GLU:HG3	2.01	0.42
1:LA:436:LEU:HD12	1:LA:436:LEU:HA	1.89	0.42
1:PA:554:GLN:HB2	1:PA:557:GLU:HG3	2.01	0.42
1:SA:554:GLN:HB2	1:SA:557:GLU:HG3	2.01	0.42
1:B:554:GLN:HB2	1:B:557:GLU:HG3	2.01	0.42
1:J:554:GLN:HB2	1:J:557:GLU:HG3	2.01	0.42
1:IA:436:LEU:HD12	1:IA:436:LEU:HA	1.89	0.42
1:ZA:554:GLN:HB2	1:ZA:557:GLU:HG3	2.01	0.42
1:CB:554:GLN:HB2	1:CB:557:GLU:HG3	2.01	0.42
1:DA:554:GLN:HB2	1:DA:557:GLU:HG3	2.01	0.42
1:GB:554:GLN:HB2	1:GB:557:GLU:HG3	2.01	0.42
1:C:517:THR:O	1:C:519:ALA:N	2.52	0.42
1:H:517:THR:O	1:H:519:ALA:N	2.52	0.42
1:H:554:GLN:HB2	1:H:557:GLU:HG3	2.01	0.42
1:M:517:THR:O	1:M:519:ALA:N	2.52	0.42
1:N:554:GLN:HB2	1:N:557:GLU:HG3	2.01	0.42
1:P:554:GLN:HB2	1:P:557:GLU:HG3	2.01	0.42
1:R:517:THR:O	1:R:519:ALA:N	2.52	0.42
1:Y:554:GLN:HB2	1:Y:557:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HA:554:GLN:HB2	1:HA:557:GLU:HG3	2.01	0.42
1:MA:554:GLN:HB2	1:MA:557:GLU:HG3	2.01	0.42
1:RA:554:GLN:HB2	1:RA:557:GLU:HG3	2.01	0.42
1:I:554:GLN:HB2	1:I:557:GLU:HG3	2.01	0.42
1:M:554:GLN:HB2	1:M:557:GLU:HG3	2.01	0.42
1:Q:554:GLN:HB2	1:Q:557:GLU:HG3	2.01	0.42
1:CA:517:THR:O	1:CA:519:ALA:N	2.52	0.42
1:IA:639:LEU:HD23	1:IA:639:LEU:HA	1.90	0.42
1:A:554:GLN:HB2	1:A:557:GLU:HG3	2.01	0.42
1:FB:436:LEU:HD12	1:FB:436:LEU:HA	1.89	0.42
1:IB:517:THR:O	1:IB:519:ALA:N	2.52	0.42
1:C:554:GLN:HB2	1:C:557:GLU:HG3	2.01	0.42
1:S:439:SER:OG	1:S:580:ILE:O	2.31	0.42
1:WA:554:GLN:HB2	1:WA:557:GLU:HG3	2.01	0.42
1:A:502:VAL:HG21	1:LA:422:ASP:HB3	2.02	0.42
1:BB:554:GLN:HB2	1:BB:557:GLU:HG3	2.01	0.42
1:L:554:GLN:HB2	1:L:557:GLU:HG3	2.01	0.42
1:R:639:LEU:HD23	1:R:639:LEU:HA	1.90	0.42
1:X:517:THR:O	1:X:519:ALA:N	2.52	0.42
1:FA:554:GLN:HB2	1:FA:557:GLU:HG3	2.01	0.42
1:JA:502:VAL:HG21	1:ZA:422:ASP:HB3	2.02	0.42
1:KA:554:GLN:HB2	1:KA:557:GLU:HG3	2.01	0.42
1:NA:436:LEU:HD12	1:NA:436:LEU:HA	1.89	0.42
1:NA:639:LEU:HD23	1:NA:639:LEU:HA	1.91	0.42
1:QA:639:LEU:HD23	1:QA:639:LEU:HA	1.91	0.42
1:SA:517:THR:O	1:SA:519:ALA:N	2.52	0.42
1:YA:517:THR:O	1:YA:519:ALA:N	2.52	0.42
1:FB:639:LEU:HD23	1:FB:639:LEU:HA	1.91	0.41
1:GB:502:VAL:HG21	1:CA:422:ASP:HB3	2.02	0.41
1:Q:502:VAL:HG21	1:GA:422:ASP:HB3	2.02	0.41
1:R:554:GLN:HB2	1:R:557:GLU:HG3	2.01	0.41
1:IA:554:GLN:HB2	1:IA:557:GLU:HG3	2.01	0.41
1:MA:517:THR:O	1:MA:519:ALA:N	2.52	0.41
1:OA:502:VAL:HG21	1:PA:422:ASP:HB3	2.03	0.41
1:VA:436:LEU:HD12	1:VA:436:LEU:HA	1.89	0.41
1:CB:502:VAL:HG21	1:OA:422:ASP:HB3	2.02	0.41
1:CB:517:THR:O	1:CB:519:ALA:N	2.52	0.41
1:G:517:THR:O	1:G:519:ALA:N	2.52	0.41
1:G:554:GLN:HB2	1:G:557:GLU:HG3	2.01	0.41
1:V:517:THR:O	1:V:519:ALA:N	2.52	0.41
1:HA:517:THR:O	1:HA:519:ALA:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:436:LEU:HD12	1:RA:436:LEU:HA	1.89	0.41
1:XA:554:GLN:HB2	1:XA:557:GLU:HG3	2.01	0.41
1:BB:422:ASP:HB3	1:M:502:VAL:HG21	2.02	0.41
1:BB:502:VAL:HG21	1:HA:422:ASP:HB3	2.02	0.41
1:F:502:VAL:HG21	1:S:422:ASP:HB3	2.03	0.41
1:L:517:THR:O	1:L:519:ALA:N	2.52	0.41
1:X:422:ASP:HB3	1:WA:502:VAL:HG21	2.02	0.41
1:AA:517:THR:O	1:AA:519:ALA:N	2.52	0.41
1:JA:422:ASP:HB3	1:SA:502:VAL:HG21	2.03	0.41
1:MA:422:ASP:HB3	1:RA:502:VAL:HG21	2.02	0.41
1:NA:554:GLN:HB2	1:NA:557:GLU:HG3	2.01	0.41
1:TA:517:THR:O	1:TA:519:ALA:N	2.52	0.41
1:DB:554:GLN:HB2	1:DB:557:GLU:HG3	2.01	0.41
1:FB:554:GLN:HB2	1:FB:557:GLU:HG3	2.01	0.41
1:HB:554:GLN:HB2	1:HB:557:GLU:HG3	2.01	0.41
1:H:502:VAL:HG21	1:RA:422:ASP:HB3	2.02	0.41
1:EB:639:LEU:HD23	1:EB:639:LEU:HA	1.90	0.41
1:IB:554:GLN:HB2	1:IB:557:GLU:HG3	2.01	0.41
1:G:502:VAL:HG21	1:BA:422:ASP:HB3	2.03	0.41
1:L:502:VAL:HG21	1:W:422:ASP:HB3	2.03	0.41
1:M:422:ASP:HB3	1:HA:502:VAL:HG21	2.02	0.41
1:O:422:ASP:HB3	1:Y:502:VAL:HG21	2.03	0.41
1:FA:436:LEU:HD12	1:FA:436:LEU:HA	1.89	0.41
1:LA:517:THR:O	1:LA:519:ALA:N	2.52	0.41
1:VA:554:GLN:HB2	1:VA:557:GLU:HG3	2.01	0.41
1:BB:436:LEU:HD12	1:BB:436:LEU:HA	1.89	0.41
1:CB:422:ASP:HB3	1:PA:502:VAL:HG21	2.03	0.41
1:DB:517:THR:O	1:DB:519:ALA:N	2.52	0.41
1:EB:422:ASP:HB3	1:EA:502:VAL:HG21	2.03	0.41
1:D:422:ASP:HB3	1:K:502:VAL:HG21	2.03	0.41
1:H:422:ASP:HB3	1:MA:502:VAL:HG21	2.02	0.41
1:J:422:ASP:HB3	1:DA:502:VAL:HG21	2.03	0.41
1:J:548:ALA:HB2	1:J:553:LEU:HD21	2.03	0.41
1:L:548:ALA:HB2	1:L:553:LEU:HD21	2.03	0.41
1:BA:517:THR:O	1:BA:519:ALA:N	2.52	0.41
1:W:517:THR:O	1:W:519:ALA:N	2.52	0.41
1:Z:502:VAL:HG21	1:UA:422:ASP:HB3	2.03	0.41
1:GA:517:THR:O	1:GA:519:ALA:N	2.52	0.41
1:GA:548:ALA:HB2	1:GA:553:LEU:HD21	2.03	0.41
1:JA:554:GLN:HB2	1:JA:557:GLU:HG3	2.01	0.41
1:LA:548:ALA:HB2	1:LA:553:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OA:554:GLN:HB2	1:OA:557:GLU:HG3	2.01	0.41
1:B:422:ASP:HB3	1:IB:502:VAL:HG21	2.02	0.41
1:A:548:ALA:HB2	1:A:553:LEU:HD21	2.03	0.41
1:CB:548:ALA:HB2	1:CB:553:LEU:HD21	2.03	0.41
1:FB:422:ASP:HB3	1:W:502:VAL:HG21	2.02	0.41
1:HB:502:VAL:HG21	1:Z:422:ASP:HB3	2.03	0.41
1:G:548:ALA:HB2	1:G:553:LEU:HD21	2.03	0.41
1:I:548:ALA:HB2	1:I:553:LEU:HD21	2.03	0.41
1:O:548:ALA:HB2	1:O:553:LEU:HD21	2.03	0.41
1:EA:422:ASP:HB3	1:XA:502:VAL:HG21	2.03	0.41
1:HA:639:LEU:HD23	1:HA:639:LEU:HA	1.91	0.41
1:JA:517:THR:O	1:JA:519:ALA:N	2.52	0.41
1:MA:639:LEU:HD23	1:MA:639:LEU:HA	1.91	0.41
1:OA:548:ALA:HB2	1:OA:553:LEU:HD21	2.03	0.41
1:SA:422:ASP:HB3	1:ZA:502:VAL:HG21	2.03	0.41
1:TA:554:GLN:HB2	1:TA:557:GLU:HG3	2.01	0.41
1:YA:554:GLN:HB2	1:YA:557:GLU:HG3	2.01	0.41
1:AB:502:VAL:HG21	1:A:422:ASP:HB3	2.02	0.41
1:DB:502:VAL:HG21	1:K:422:ASP:HB3	2.03	0.41
1:GB:422:ASP:HB3	1:C:502:VAL:HG21	2.02	0.41
1:K:517:THR:O	1:K:519:ALA:N	2.52	0.41
1:M:548:ALA:HB2	1:M:553:LEU:HD21	2.03	0.41
1:N:548:ALA:HB2	1:N:553:LEU:HD21	2.03	0.41
1:P:422:ASP:HB3	1:YA:502:VAL:HG21	2.03	0.41
1:Q:422:ASP:HB3	1:QA:502:VAL:HG21	2.02	0.41
1:R:502:VAL:HG21	1:WA:422:ASP:HB3	2.02	0.41
1:BA:502:VAL:HG21	1:VA:422:ASP:HB3	2.02	0.41
1:S:548:ALA:HB2	1:S:553:LEU:HD21	2.03	0.41
1:FA:548:ALA:HB2	1:FA:553:LEU:HD21	2.03	0.41
1:KA:548:ALA:HB2	1:KA:553:LEU:HD21	2.03	0.41
1:OA:517:THR:O	1:OA:519:ALA:N	2.52	0.41
1:IB:548:ALA:HB2	1:IB:553:LEU:HD21	2.03	0.41
1:E:502:VAL:HG21	1:AA:422:ASP:HB3	2.02	0.41
1:F:422:ASP:HB3	1:TA:502:VAL:HG21	2.03	0.41
1:F:517:THR:O	1:F:519:ALA:N	2.52	0.41
1:H:548:ALA:HB2	1:H:553:LEU:HD21	2.03	0.41
1:I:422:ASP:HB3	1:P:502:VAL:HG21	2.03	0.41
1:L:639:LEU:HD23	1:L:639:LEU:HA	1.91	0.41
1:Q:548:ALA:HB2	1:Q:553:LEU:HD21	2.03	0.41
1:BA:548:ALA:HB2	1:BA:553:LEU:HD21	2.03	0.41
1:T:502:VAL:HG21	1:V:422:ASP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:548:ALA:HB2	1:V:553:LEU:HD21	2.03	0.41
1:W:548:ALA:HB2	1:W:553:LEU:HD21	2.03	0.41
1:Z:548:ALA:HB2	1:Z:553:LEU:HD21	2.03	0.41
1:AA:548:ALA:HB2	1:AA:553:LEU:HD21	2.03	0.41
1:EA:548:ALA:HB2	1:EA:553:LEU:HD21	2.03	0.41
1:JA:548:ALA:HB2	1:JA:553:LEU:HD21	2.03	0.41
1:KA:436:LEU:HD12	1:KA:436:LEU:HA	1.89	0.41
1:SA:548:ALA:HB2	1:SA:553:LEU:HD21	2.03	0.41
1:UA:517:THR:O	1:UA:519:ALA:N	2.52	0.41
1:B:502:VAL:HG21	1:N:422:ASP:HB3	2.03	0.41
1:AB:548:ALA:HB2	1:AB:553:LEU:HD21	2.03	0.41
1:EB:517:THR:O	1:EB:519:ALA:N	2.52	0.41
1:D:548:ALA:HB2	1:D:553:LEU:HD21	2.03	0.41
1:DA:422:ASP:HB3	1:KA:502:VAL:HG21	2.03	0.41
1:TA:548:ALA:HB2	1:TA:553:LEU:HD21	2.03	0.41
1:UA:554:GLN:HB2	1:UA:557:GLU:HG3	2.01	0.41
1:YA:548:ALA:HB2	1:YA:553:LEU:HD21	2.03	0.41
1:ZA:548:ALA:HB2	1:ZA:553:LEU:HD21	2.03	0.41
1:BB:517:THR:O	1:BB:519:ALA:N	2.52	0.40
1:DB:548:ALA:HB2	1:DB:553:LEU:HD21	2.03	0.40
1:EB:554:GLN:HB2	1:EB:557:GLU:HG3	2.01	0.40
1:E:548:ALA:HB2	1:E:553:LEU:HD21	2.03	0.40
1:I:502:VAL:HG21	1:YA:422:ASP:HB3	2.02	0.40
1:Y:422:ASP:HB3	1:FA:502:VAL:HG21	2.03	0.40
1:PA:548:ALA:HB2	1:PA:553:LEU:HD21	2.03	0.40
1:QA:548:ALA:HB2	1:QA:553:LEU:HD21	2.03	0.40
1:VA:548:ALA:HB2	1:VA:553:LEU:HD21	2.03	0.40
1:FB:548:ALA:HB2	1:FB:553:LEU:HD21	2.03	0.40
1:GB:548:ALA:HB2	1:GB:553:LEU:HD21	2.03	0.40
1:IB:422:ASP:HB3	1:N:502:VAL:HG21	2.03	0.40
1:J:517:THR:O	1:J:519:ALA:N	2.52	0.40
1:O:517:THR:O	1:O:519:ALA:N	2.52	0.40
1:P:436:LEU:HD21	1:YA:620:HIS:ND1	2.37	0.40
1:R:422:ASP:HB3	1:X:502:VAL:HG21	2.02	0.40
1:T:548:ALA:HB2	1:T:553:LEU:HD21	2.03	0.40
1:DA:436:LEU:HD21	1:KA:620:HIS:ND1	2.37	0.40
1:RA:517:THR:O	1:RA:519:ALA:N	2.52	0.40
1:B:436:LEU:HD21	1:IB:620:HIS:ND1	2.37	0.40
1:AB:422:ASP:HB3	1:LA:502:VAL:HG21	2.02	0.40
1:FB:502:VAL:HG21	1:L:422:ASP:HB3	2.02	0.40
1:FB:620:HIS:ND1	1:L:436:LEU:HD21	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GB:436:LEU:HD21	1:C:620:HIS:ND1	2.37	0.40
1:GB:620:HIS:ND1	1:CA:436:LEU:HD21	2.37	0.40
1:C:422:ASP:HB3	1:CA:502:VAL:HG21	2.02	0.40
1:D:436:LEU:HD21	1:K:620:HIS:ND1	2.37	0.40
1:G:422:ASP:HB3	1:VA:502:VAL:HG21	2.02	0.40
1:R:620:HIS:ND1	1:WA:436:LEU:HD21	2.37	0.40
1:S:620:HIS:ND1	1:TA:436:LEU:HD21	2.37	0.40
1:T:620:HIS:ND1	1:V:436:LEU:HD21	2.37	0.40
1:X:436:LEU:HD21	1:WA:620:HIS:ND1	2.37	0.40
1:Y:436:LEU:HD21	1:FA:620:HIS:ND1	2.37	0.40
1:TA:639:LEU:HD23	1:TA:639:LEU:HA	1.91	0.40
1:WA:548:ALA:HB2	1:WA:553:LEU:HD21	2.03	0.40
1:A:620:HIS:ND1	1:LA:436:LEU:HD21	2.37	0.40
1:E:620:HIS:ND1	1:AA:436:LEU:HD21	2.37	0.40
1:F:439:SER:OG	1:F:580:ILE:O	2.30	0.40
1:F:620:HIS:ND1	1:S:436:LEU:HD21	2.37	0.40
1:G:436:LEU:HD21	1:VA:620:HIS:ND1	2.37	0.40
1:J:436:LEU:HD21	1:DA:620:HIS:ND1	2.37	0.40
1:K:439:SER:OG	1:K:580:ILE:O	2.31	0.40
1:L:620:HIS:ND1	1:W:436:LEU:HD21	2.37	0.40
1:O:436:LEU:HD21	1:Y:620:HIS:ND1	2.37	0.40
1:Q:620:HIS:ND1	1:GA:436:LEU:HD21	2.37	0.40
1:AA:620:HIS:ND1	1:NA:436:LEU:HD21	2.37	0.40
1:GA:502:VAL:HG21	1:QA:422:ASP:HB3	2.02	0.40
1:GA:639:LEU:HD23	1:GA:639:LEU:HA	1.91	0.40
1:DB:436:LEU:HD21	1:D:620:HIS:ND1	2.37	0.40
1:EB:502:VAL:HG21	1:XA:422:ASP:HB3	2.03	0.40
1:HB:548:ALA:HB2	1:HB:553:LEU:HD21	2.03	0.40
1:E:436:LEU:HD21	1:NA:620:HIS:ND1	2.37	0.40
1:BA:620:HIS:ND1	1:VA:436:LEU:HD21	2.37	0.40
1:T:422:ASP:HB3	1:IA:502:VAL:HG21	2.03	0.40
1:V:620:HIS:ND1	1:IA:436:LEU:HD21	2.37	0.40
1:Y:548:ALA:HB2	1:Y:553:LEU:HD21	2.03	0.40
1:EA:436:LEU:HD21	1:XA:620:HIS:ND1	2.37	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	A	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	AA	229/562 (41%)	223 (97%)	6 (3%)	0	100	100
1	AB	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	B	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	BA	229/562 (41%)	223 (97%)	6 (3%)	0	100	100
1	BB	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	C	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	CA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	CB	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	D	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	DA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	DB	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	E	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	EA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	EB	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	F	229/562 (41%)	223 (97%)	6 (3%)	0	100	100
1	FA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	FB	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	G	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	GA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	GB	229/562 (41%)	223 (97%)	6 (3%)	0	100	100
1	H	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	HA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	HB	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	I	229/562 (41%)	222 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	IA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	IB	229/562 (41%)	223 (97%)	6 (3%)	0	100	100
1	J	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	JA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	K	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	KA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	L	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	LA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	M	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	MA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	N	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	NA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	O	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	OA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	P	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	PA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	Q	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	QA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	R	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	RA	229/562 (41%)	223 (97%)	6 (3%)	0	100	100
1	S	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	SA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	T	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	TA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	UA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	V	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	VA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	W	229/562 (41%)	223 (97%)	6 (3%)	0	100	100
1	WA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	X	229/562 (41%)	223 (97%)	6 (3%)	0	100	100
1	XA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	YA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	Z	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
1	ZA	229/562 (41%)	222 (97%)	7 (3%)	0	100	100
All	All	13740/33720 (41%)	13328 (97%)	412 (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	A	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	AA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	AB	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	B	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	BA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	BB	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	C	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	CA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	CB	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	D	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	DA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	DB	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	E	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	EA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	EB	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	F	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	FA	197/467 (42%)	196 (100%)	1 (0%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FB	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	G	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	GA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	GB	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	H	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	HA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	HB	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	I	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	IA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	IB	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	J	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	JA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	K	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	KA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	L	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	LA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	M	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	MA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	N	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	NA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	O	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	OA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	P	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	PA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	Q	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	QA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	R	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	RA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	S	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	SA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	T	197/467 (42%)	196 (100%)	1 (0%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	TA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	UA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	V	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	VA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	W	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	WA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	X	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	XA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	Y	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	YA	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	Z	197/467 (42%)	196 (100%)	1 (0%)	81	93
1	ZA	197/467 (42%)	196 (100%)	1 (0%)	81	93
All	All	11820/28020 (42%)	11760 (100%)	60 (0%)	78	93

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	570	MET
1	AB	570	MET
1	A	570	MET
1	BB	570	MET
1	CB	570	MET
1	DB	570	MET
1	EB	570	MET
1	FB	570	MET
1	GB	570	MET
1	HB	570	MET
1	IB	570	MET
1	C	570	MET
1	D	570	MET
1	E	570	MET
1	F	570	MET
1	G	570	MET
1	H	570	MET
1	I	570	MET
1	J	570	MET
1	K	570	MET
1	L	570	MET

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Mol	Chain	Res	Type
1	M	570	MET
1	N	570	MET
1	O	570	MET
1	P	570	MET
1	Q	570	MET
1	R	570	MET
1	BA	570	MET
1	S	570	MET
1	T	570	MET
1	V	570	MET
1	W	570	MET
1	X	570	MET
1	Y	570	MET
1	Z	570	MET
1	AA	570	MET
1	CA	570	MET
1	DA	570	MET
1	EA	570	MET
1	FA	570	MET
1	GA	570	MET
1	HA	570	MET
1	IA	570	MET
1	JA	570	MET
1	KA	570	MET
1	LA	570	MET
1	MA	570	MET
1	NA	570	MET
1	OA	570	MET
1	PA	570	MET
1	QA	570	MET
1	RA	570	MET
1	SA	570	MET
1	TA	570	MET
1	UA	570	MET
1	VA	570	MET
1	WA	570	MET
1	XA	570	MET
1	YA	570	MET
1	ZA	570	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	438	GLN
1	AB	438	GLN
1	A	438	GLN
1	BB	438	GLN
1	CB	438	GLN
1	DB	438	GLN
1	DB	441	GLN
1	EB	438	GLN
1	FB	438	GLN
1	GB	438	GLN
1	HB	438	GLN
1	IB	438	GLN
1	C	438	GLN
1	D	438	GLN
1	E	438	GLN
1	F	438	GLN
1	G	438	GLN
1	H	438	GLN
1	I	438	GLN
1	J	438	GLN
1	K	438	GLN
1	L	438	GLN
1	M	438	GLN
1	N	438	GLN
1	O	438	GLN
1	P	438	GLN
1	Q	438	GLN
1	R	438	GLN
1	BA	438	GLN
1	S	438	GLN
1	T	438	GLN
1	V	438	GLN
1	W	438	GLN
1	X	438	GLN
1	Y	438	GLN
1	Z	438	GLN
1	AA	438	GLN
1	CA	438	GLN
1	DA	438	GLN
1	EA	438	GLN
1	FA	438	GLN
1	GA	438	GLN
1	HA	438	GLN

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Mol	Chain	Res	Type
1	IA	438	GLN
1	JA	438	GLN
1	JA	441	GLN
1	KA	438	GLN
1	LA	438	GLN
1	MA	438	GLN
1	NA	438	GLN
1	OA	438	GLN
1	OA	441	GLN
1	PA	438	GLN
1	QA	438	GLN
1	RA	438	GLN
1	SA	438	GLN
1	TA	438	GLN
1	UA	438	GLN
1	VA	438	GLN
1	WA	438	GLN
1	XA	438	GLN
1	YA	438	GLN
1	ZA	438	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

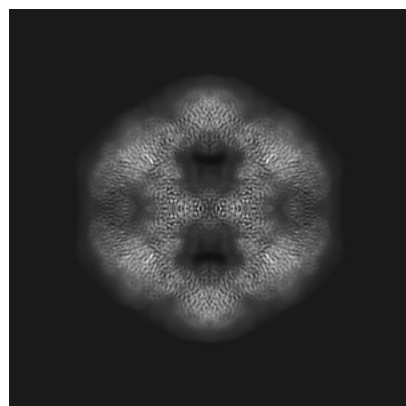
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17691. These allow visual inspection of the internal detail of the map and identification of artifacts.

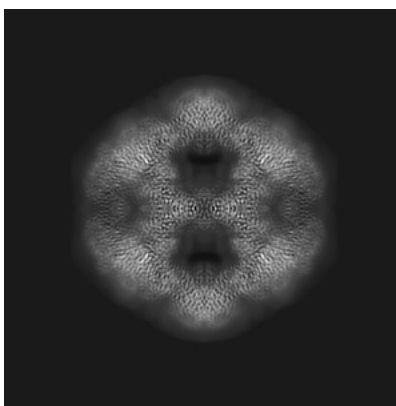
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

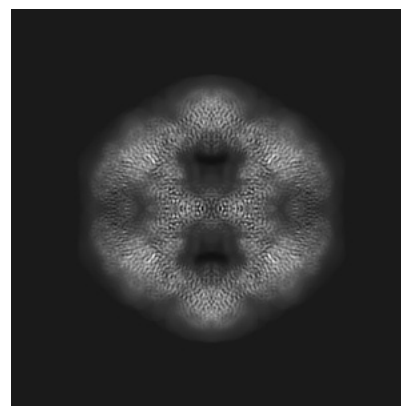
6.1.1 Primary map



X

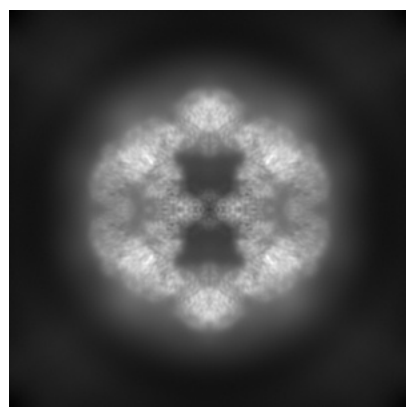


Y

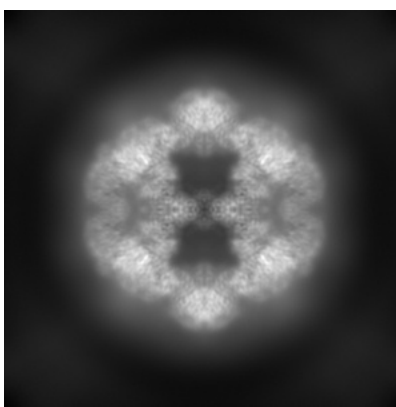


Z

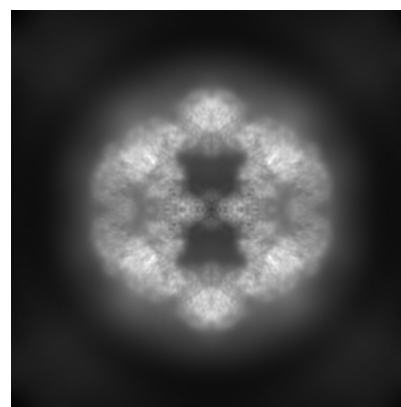
6.1.2 Raw map



X



Y

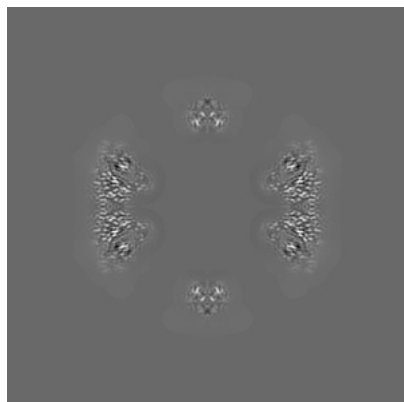


Z

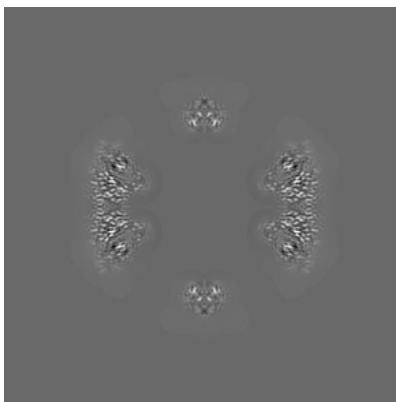
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

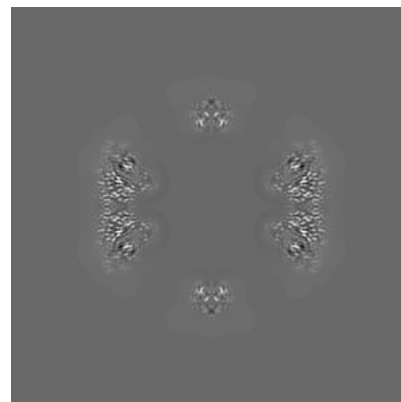
6.2.1 Primary map



X Index: 230

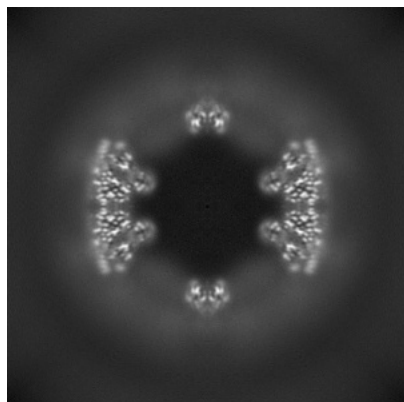


Y Index: 230

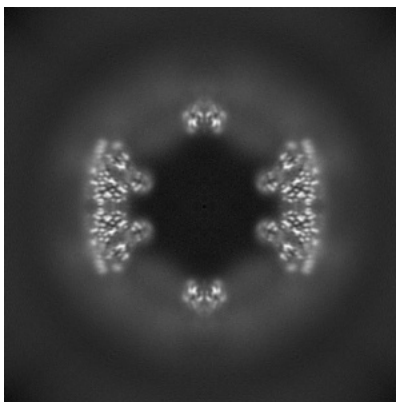


Z Index: 230

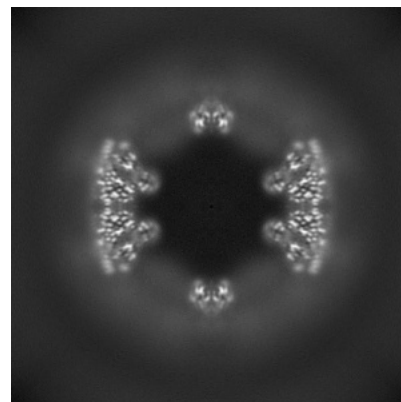
6.2.2 Raw map



X Index: 230



Y Index: 230



Z Index: 230

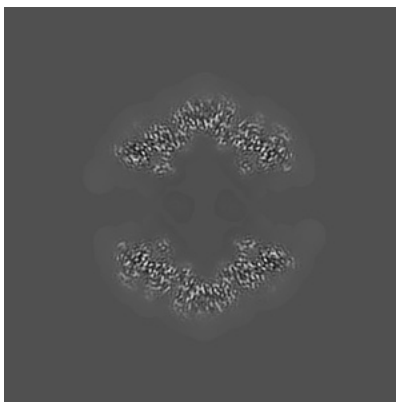
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 285

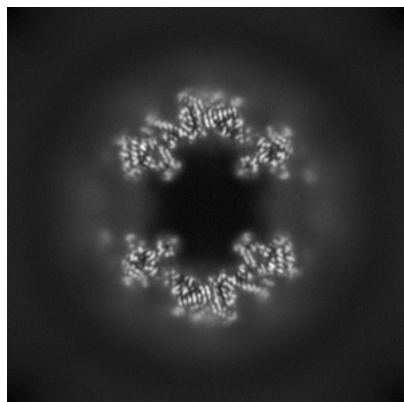


Y Index: 285

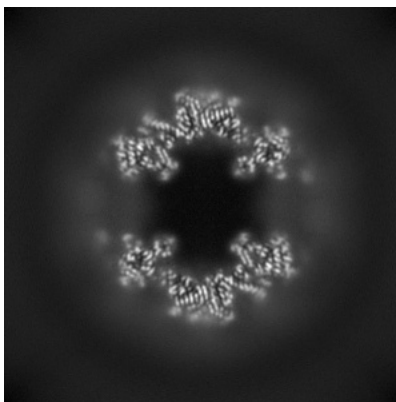


Z Index: 285

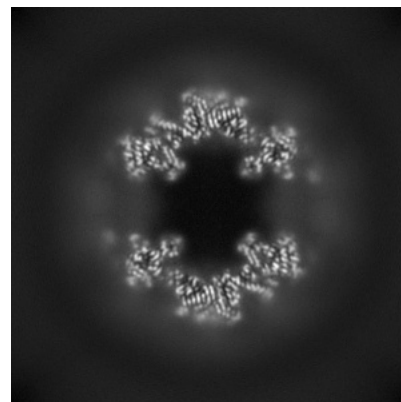
6.3.2 Raw map



X Index: 184



Y Index: 184

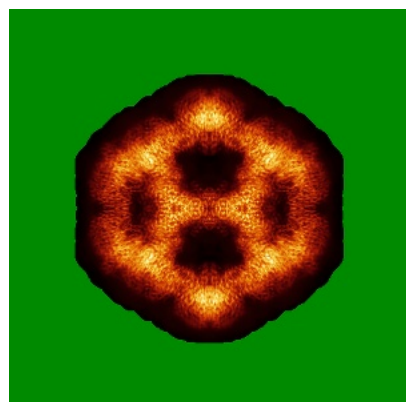


Z Index: 184

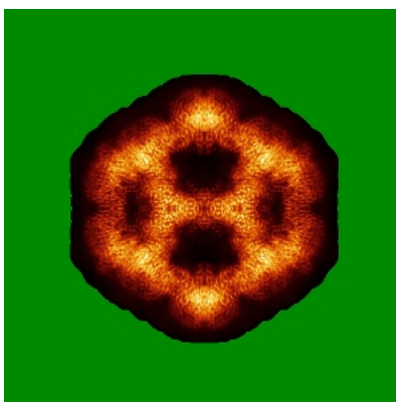
The images above show the largest variance slices of the map in three orthogonal directions.

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

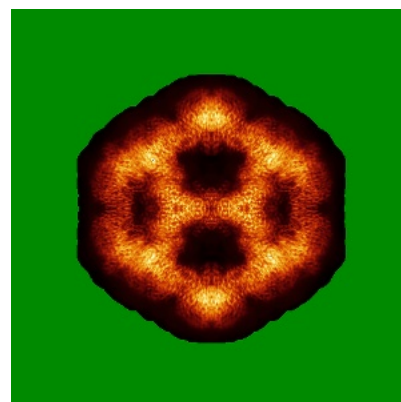
6.4.1 Primary map



X

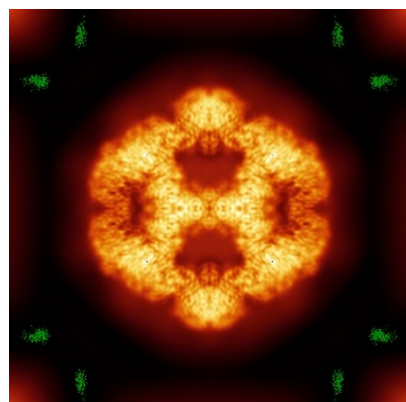


Y

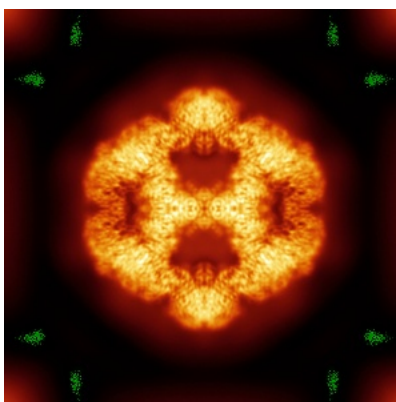


Z

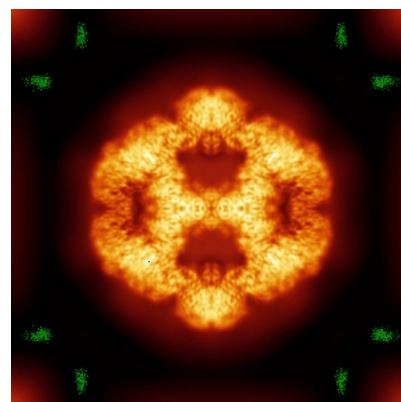
6.4.2 Raw map



X



Y

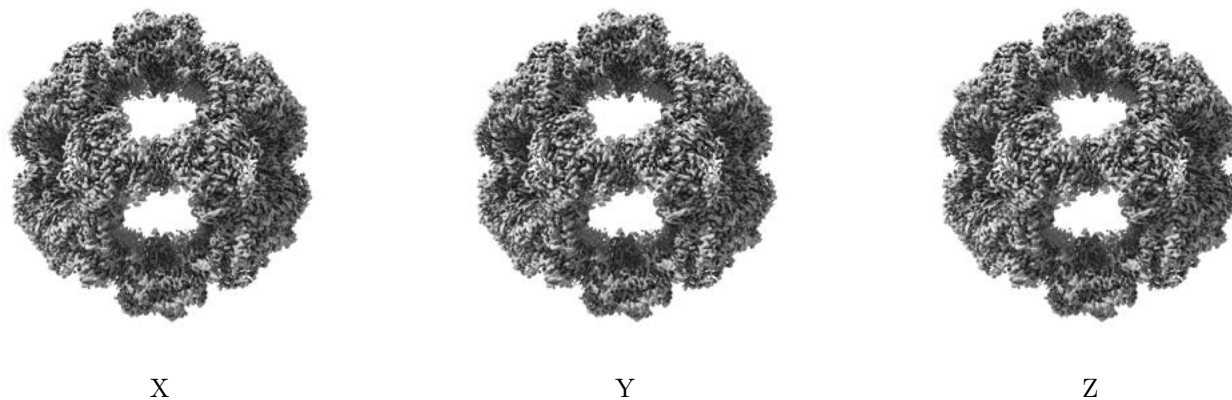


Z

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.

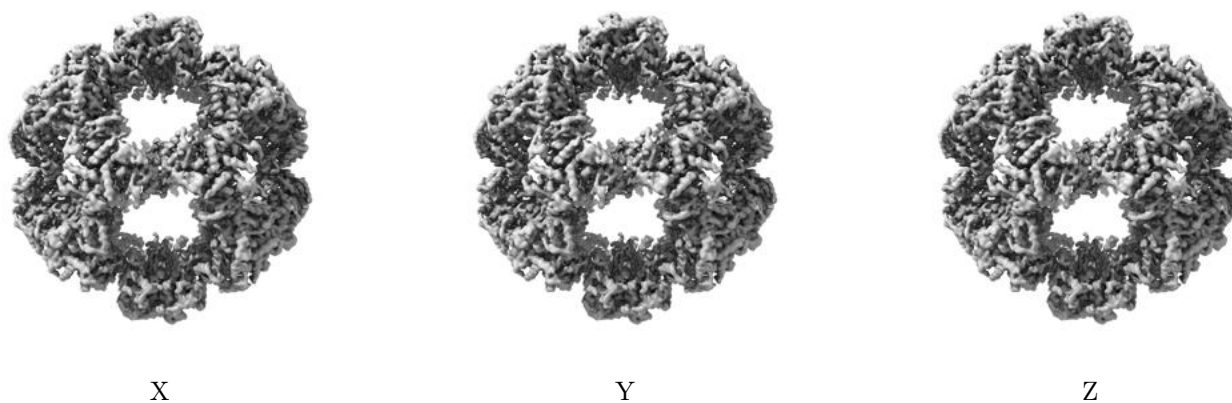
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

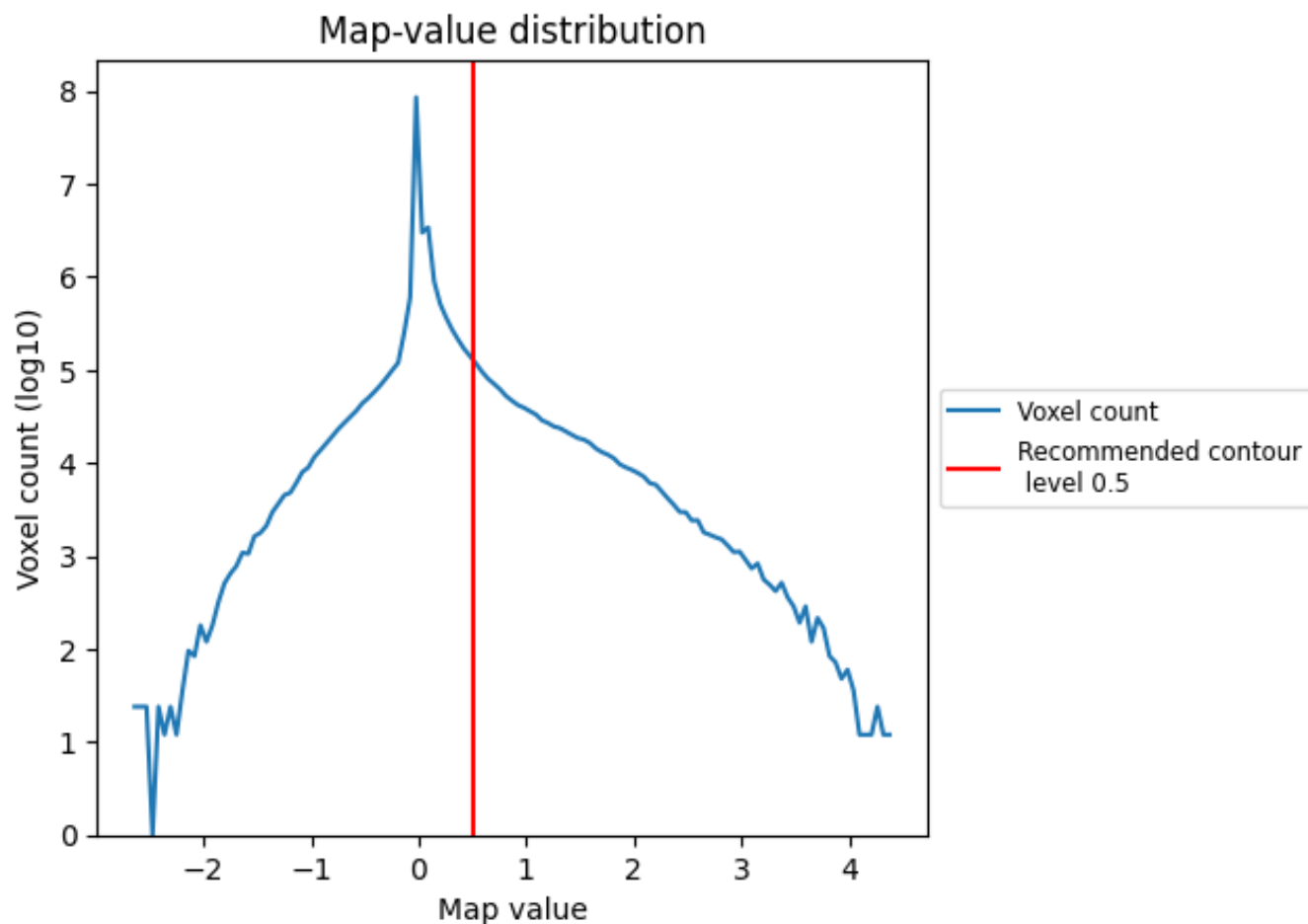
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

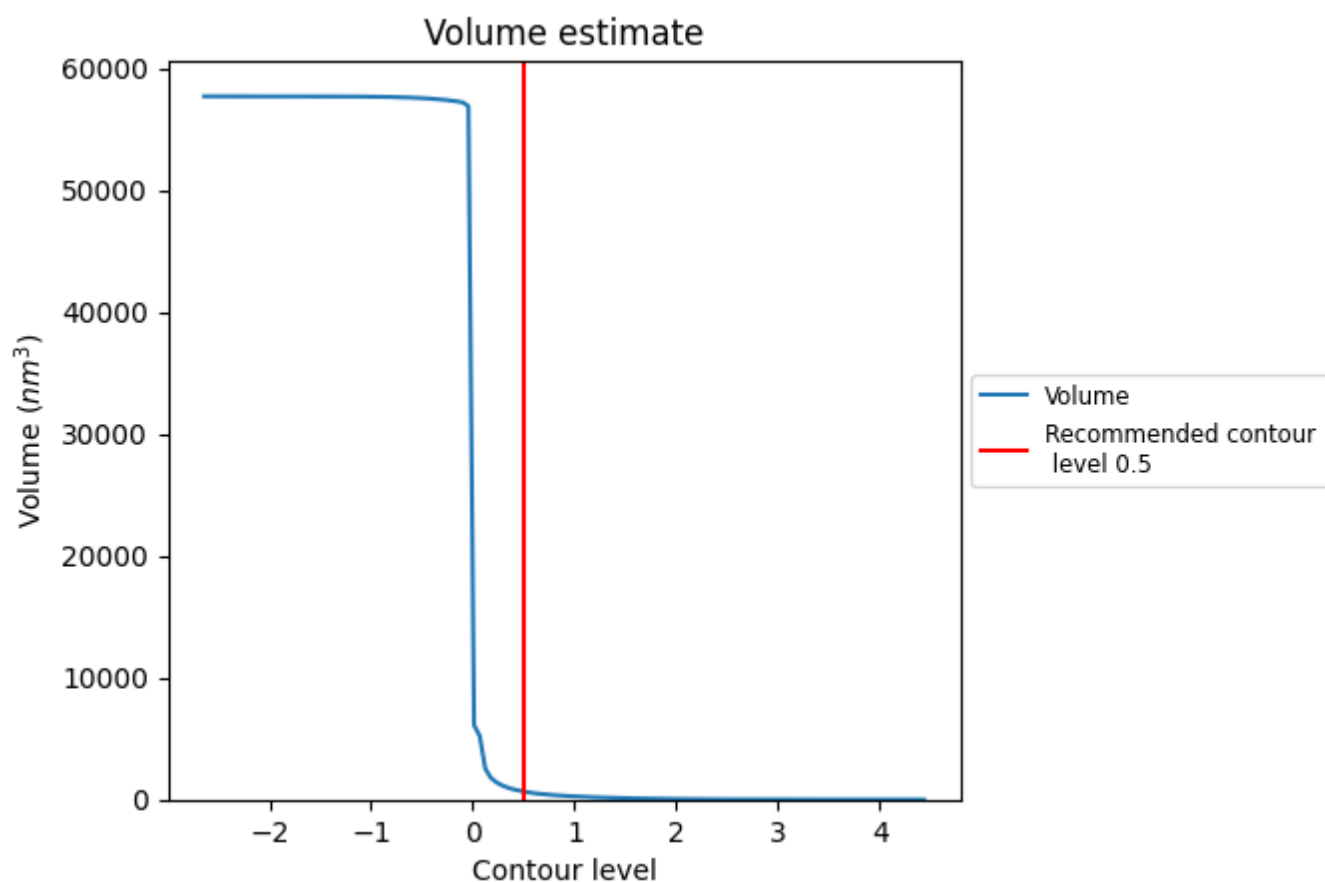
This section contains the results of statistical analysis of the map.

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.

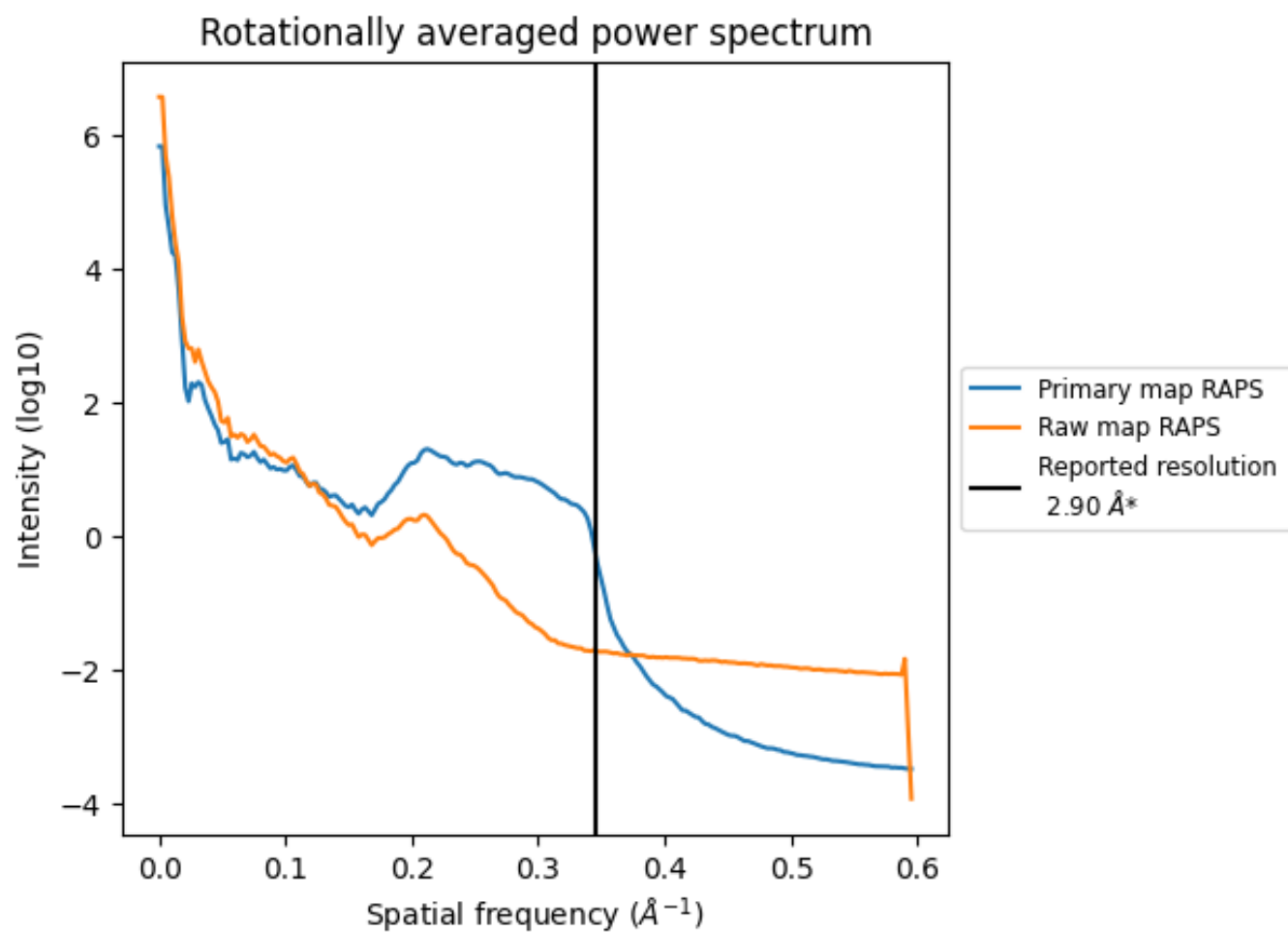
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 654 nm³; this corresponds to an approximate mass of 591 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 ⓘ

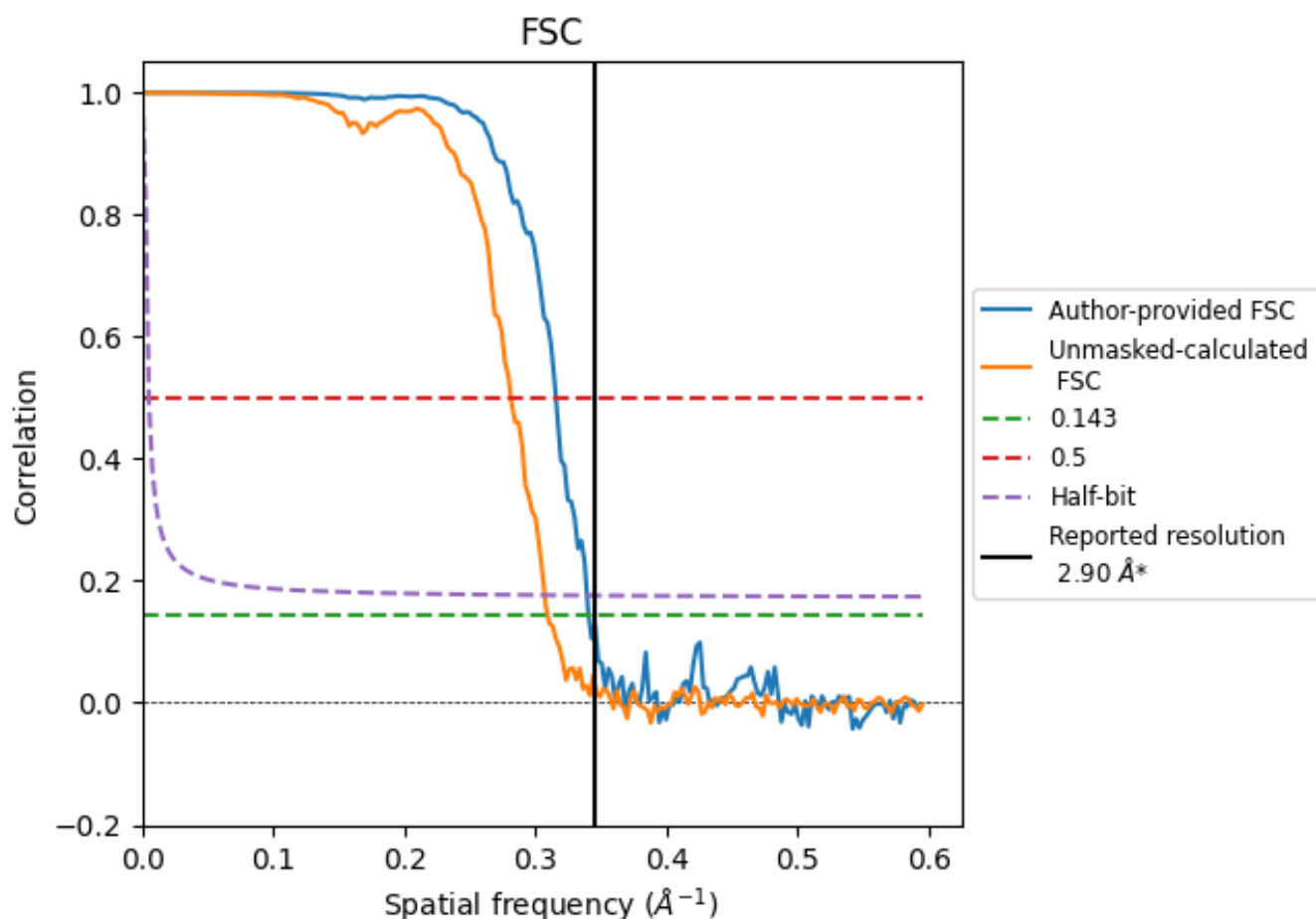


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

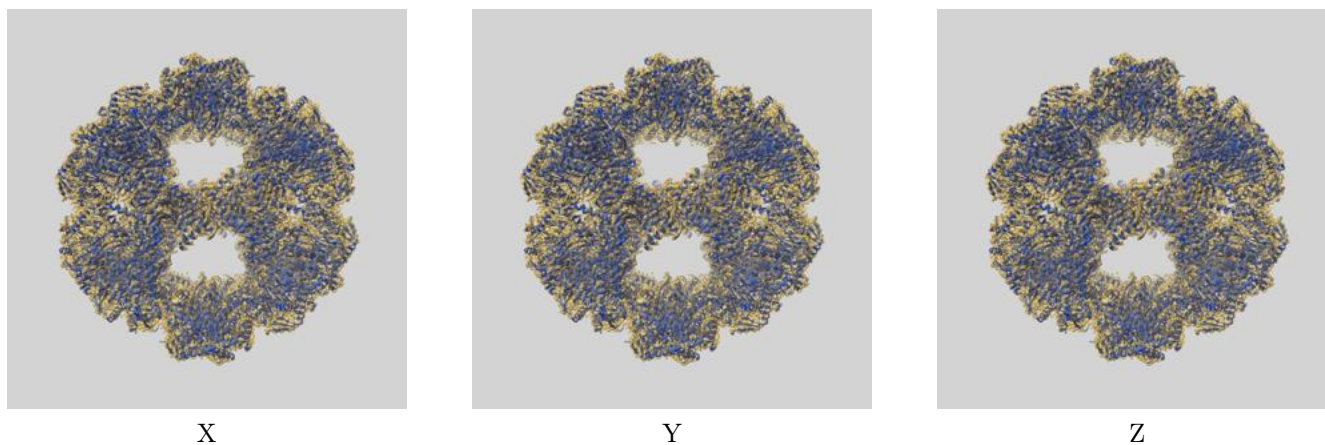
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.94	3.17	2.95
Unmasked-calculated*	3.23	3.55	3.26

*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 3.23 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

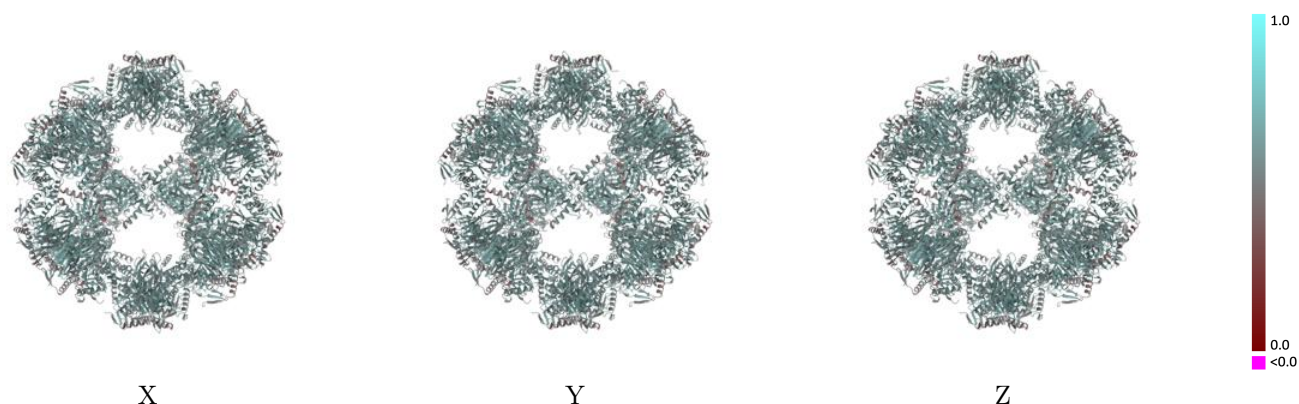
This section contains information regarding the fit between EMDB map EMD-17691 and PDB model 8PIU. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



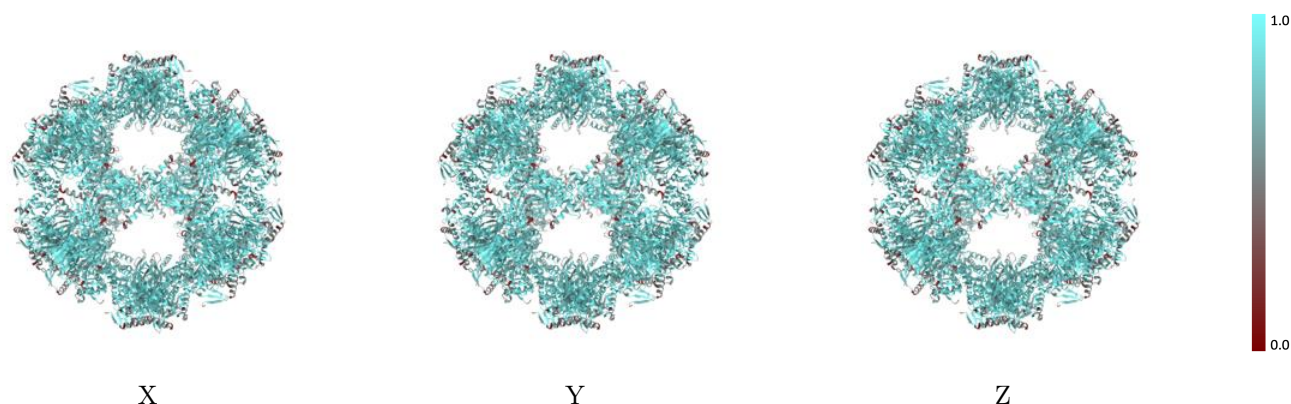
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



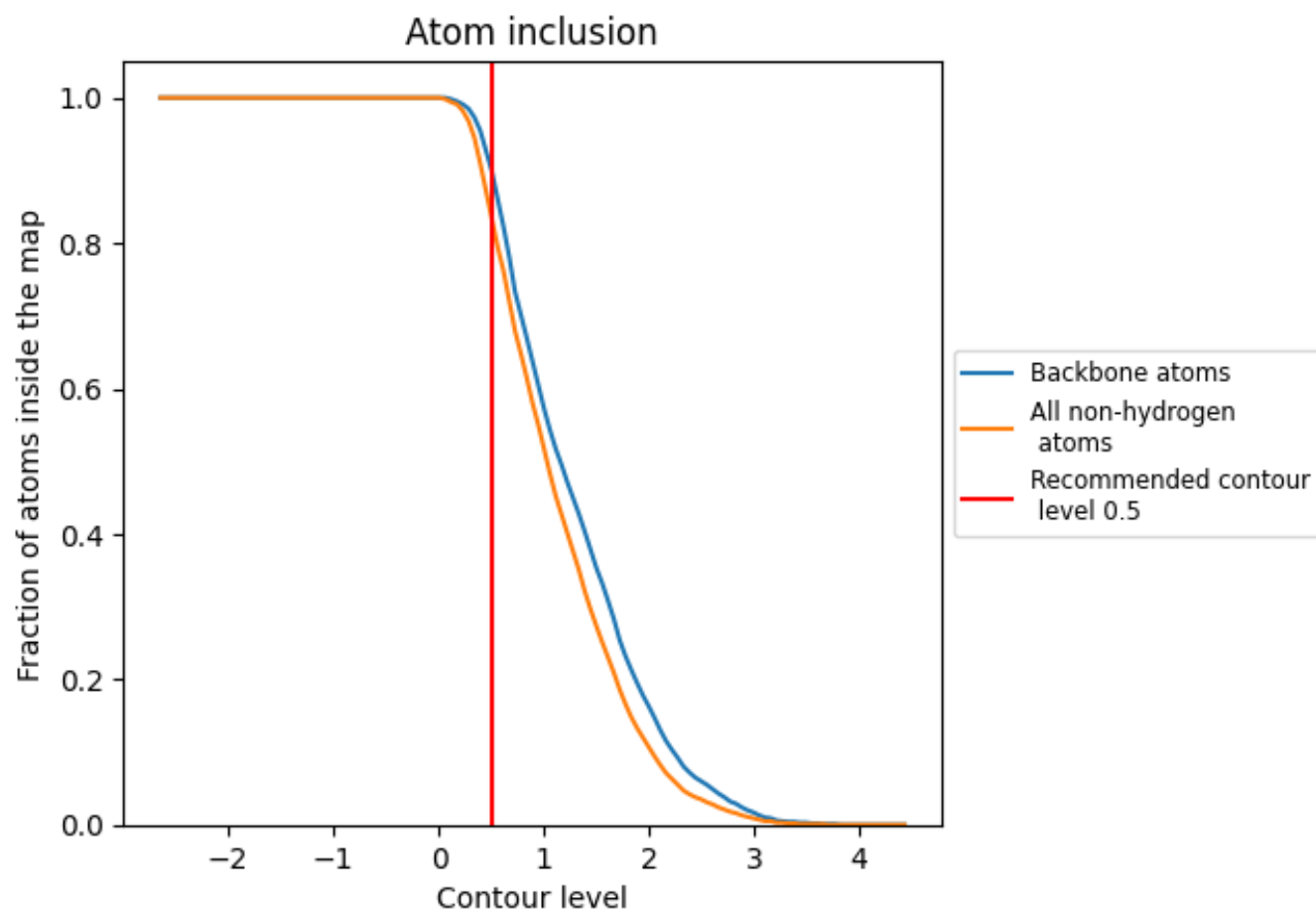
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 84% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8390	 0.5740
A	 0.8390	 0.5740
AA	 0.8390	 0.5750
AB	 0.8380	 0.5730
B	 0.8380	 0.5750
BA	 0.8390	 0.5750
BB	 0.8430	 0.5750
C	 0.8430	 0.5760
CA	 0.8430	 0.5750
CB	 0.8370	 0.5720
D	 0.8370	 0.5770
DA	 0.8370	 0.5740
DB	 0.8360	 0.5750
E	 0.8360	 0.5760
EA	 0.8360	 0.5720
EB	 0.8370	 0.5730
F	 0.8380	 0.5760
FA	 0.8390	 0.5740
FB	 0.8390	 0.5740
G	 0.8380	 0.5760
GA	 0.8380	 0.5760
GB	 0.8430	 0.5750
H	 0.8430	 0.5720
HA	 0.8430	 0.5760
HB	 0.8370	 0.5720
I	 0.8370	 0.5750
IA	 0.8370	 0.5750
IB	 0.8360	 0.5740
J	 0.8360	 0.5750
JA	 0.8360	 0.5720
K	 0.8380	 0.5760
KA	 0.8390	 0.5740
L	 0.8390	 0.5740
LA	 0.8390	 0.5740
M	 0.8430	 0.5740



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Chain	Atom inclusion	Q-score
MA	 0.8430	 0.5730
N	 0.8370	 0.5770
NA	 0.8370	 0.5730
O	 0.8360	 0.5740
OA	 0.8360	 0.5700
P	 0.8370	 0.5740
PA	 0.8390	 0.5720
Q	 0.8380	 0.5750
QA	 0.8380	 0.5750
R	 0.8430	 0.5740
RA	 0.8430	 0.5750
S	 0.8370	 0.5750
SA	 0.8370	 0.5730
T	 0.8360	 0.5750
TA	 0.8360	 0.5740
UA	 0.8380	 0.5720
V	 0.8380	 0.5740
VA	 0.8380	 0.5750
W	 0.8380	 0.5740
WA	 0.8430	 0.5740
X	 0.8430	 0.5740
XA	 0.8370	 0.5740
Y	 0.8370	 0.5750
YA	 0.8360	 0.5740
Z	 0.8360	 0.5710
ZA	 0.8380	 0.5740