



## Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 01:25 pm GMT

PDB ID : 6ZLM  
EMDB ID : EMD-11268  
Title : Dihydrolipoyllysine-residue acetyltransferase component of fungal pyruvate dehydrogenase complex with protein X bound  
Authors : Forsberg, B.O.; Aibara, S.; Howard, R.J.; Mortezaei, N.; Lindahl, E.  
Deposited on : 2020-06-30  
Resolution : 4.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

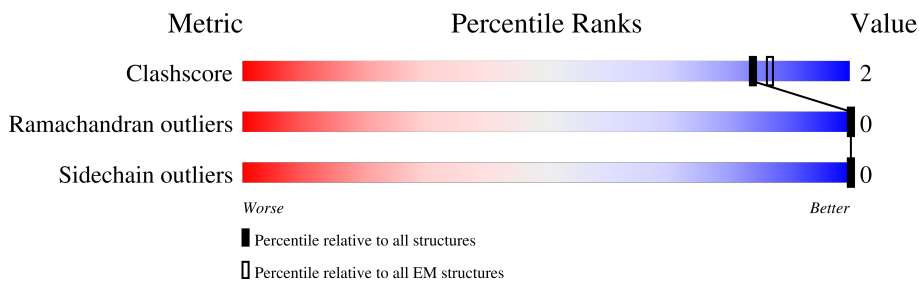
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.










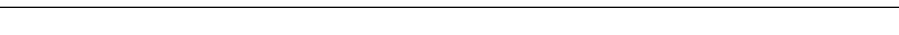
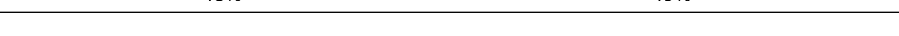
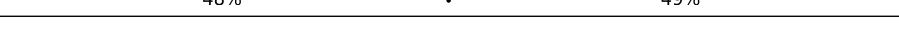
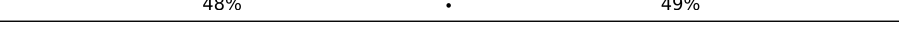
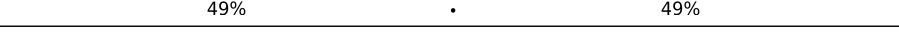











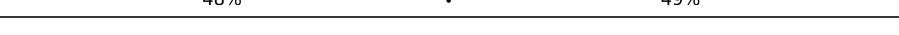
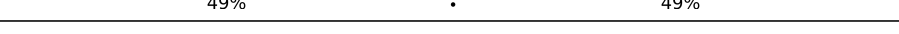
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	458	48% 49%
1	AA	458	48% 49%
1	AB	458	49% 49%
1	B	458	48% 49%
1	BA	458	48% 49%
1	C	458	48% 49%
1	CA	458	49% 49%
1	CB	458	48% 49%

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Mol	Chain	Length	Quality of chain	
1	D	458		49%
1	DB	458		49%
1	E	458		49%
1	EA	458		49%
1	EB	458		49%
1	F	458		49%
1	FA	458		49%
1	FB	458		49%
1	G	458		49%
1	GA	458		49%
1	GB	458		49%
1	H	458		49%
1	HA	458		49%
1	I	458		49%
1	IA	458		49%
1	IB	458		49%
1	J	458		49%
1	JB	458		49%
1	KA	458		49%
1	KB	458		49%
1	L	458		49%
1	LA	458		49%
1	LB	458		49%
1	M	458		49%
1	MA	458		49%

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Mol	Chain	Length	Quality of chain	
1	MB	458	49%	49%
1	N	458	48%	49%
1	NA	458	48%	49%
1	O	458	48%	49%
1	OA	458	49%	49%
1	OB	458	49%	49%
1	P	458	49%	49%
1	PB	458	48%	49%
1	QA	458	48%	49%
1	QB	458	48%	49%
1	R	458	48%	49%
1	RA	458	48%	49%
1	RB	458	47%	49%
1	S	458	48%	49%
1	SA	458	47%	49%
1	SB	458	48%	49%
1	T	458	47%	49%
1	TA	458	47%	49%
1	UA	458	48%	49%
1	V	458	47%	49%
1	W	458	49%	49%
1	WA	458	48%	49%
1	XA	458	48%	49%
1	Y	458	47%	49%
1	YA	458	48%	49%

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Mol	Chain	Length	Quality of chain
1	Z	458	 48% . 49%
1	ZA	458	 48% . 49%
2	BB	13	 100%
2	DA	13	 100%
2	HB	13	 100%
2	JA	13	 100%
2	K	13	 100%
2	NB	13	 100%
2	PA	13	 100%
2	Q	13	 100%
2	TB	13	 100%
2	VA	13	 100%
2	X	13	 100%
2	XC	13	 100%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 214080 atoms, of which 108240 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
			Total	C	H	N	O	S		
1	A	232	3555	1110	1804	302	335	4	0	0
1	B	232	3555	1110	1804	302	335	4	0	0
1	C	232	3555	1110	1804	302	335	4	0	0
1	D	232	3555	1110	1804	302	335	4	0	0
1	E	232	3555	1110	1804	302	335	4	0	0
1	F	232	3555	1110	1804	302	335	4	0	0
1	G	232	3555	1110	1804	302	335	4	0	0
1	H	232	3555	1110	1804	302	335	4	0	0
1	I	232	3555	1110	1804	302	335	4	0	0
1	J	232	3555	1110	1804	302	335	4	0	0
1	L	232	3555	1110	1804	302	335	4	0	0
1	M	232	3555	1110	1804	302	335	4	0	0
1	N	232	3555	1110	1804	302	335	4	0	0
1	O	232	3555	1110	1804	302	335	4	0	0
1	P	232	3555	1110	1804	302	335	4	0	0
1	R	232	3555	1110	1804	302	335	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	S	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	T	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	V	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	W	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	Y	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	Z	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	AA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	BA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	CA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	EA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	FA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	GA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	HA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	IA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	KA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	LA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	MA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	NA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	OA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	QA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	RA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	SA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	TA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	UA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	WA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	XA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	YA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	ZA	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	AB	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	CB	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	DB	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	EB	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	FB	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	GB	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	IB	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	JB	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	KB	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	LB	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	MB	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	OB	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	PB	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0
1	QB	232	Total 3555	C 1110	H 1804	N 302	O 335	S 4	0	0

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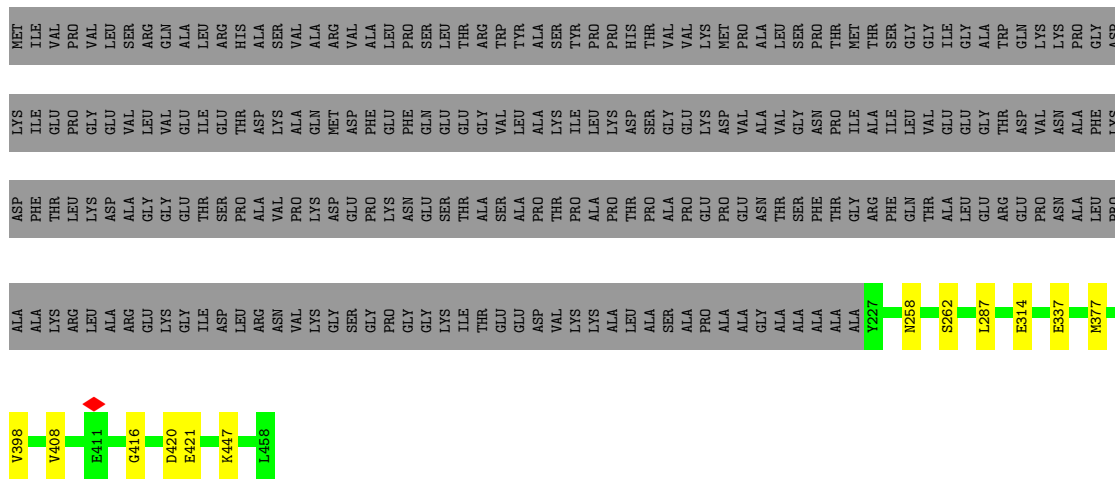
Mol	Chain	Residues	Atoms					AltConf	Trace	
1	RB	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		
1	SB	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		

- Molecule 2 is a protein called Pyruvate dehydrogenase X component.

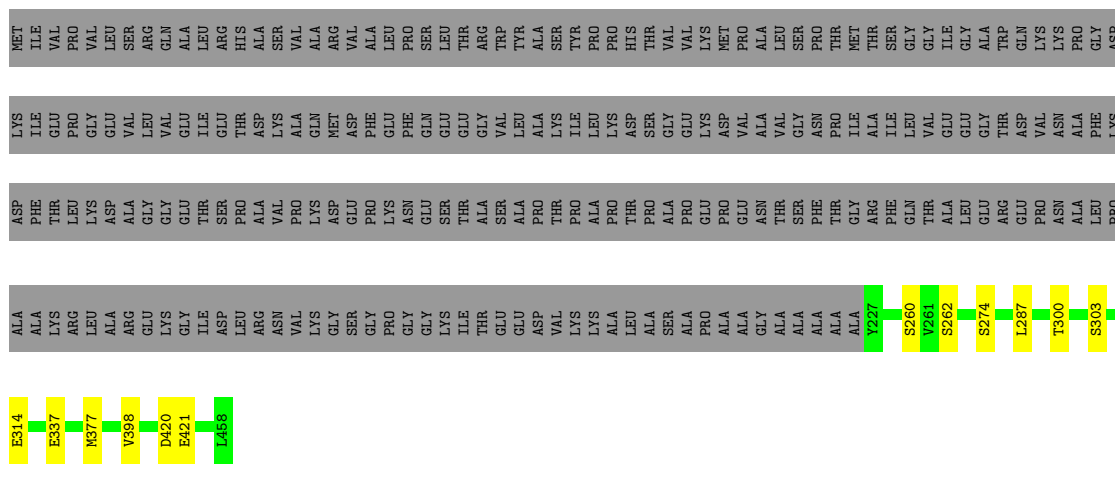
Mol	Chain	Residues	Atoms				AltConf	Trace
2	XC	13	Total	C	N	O	0	0
			65	39	13	13		
2	K	13	Total	C	N	O	0	0
			65	39	13	13		
2	Q	13	Total	C	N	O	0	0
			65	39	13	13		
2	X	13	Total	C	N	O	0	0
			65	39	13	13		
2	DA	13	Total	C	N	O	0	0
			65	39	13	13		
2	JA	13	Total	C	N	O	0	0
			65	39	13	13		
2	PA	13	Total	C	N	O	0	0
			65	39	13	13		
2	VA	13	Total	C	N	O	0	0
			65	39	13	13		
2	BB	13	Total	C	N	O	0	0
			65	39	13	13		
2	HB	13	Total	C	N	O	0	0
			65	39	13	13		
2	NB	13	Total	C	N	O	0	0
			65	39	13	13		
2	TB	13	Total	C	N	O	0	0
			65	39	13	13		



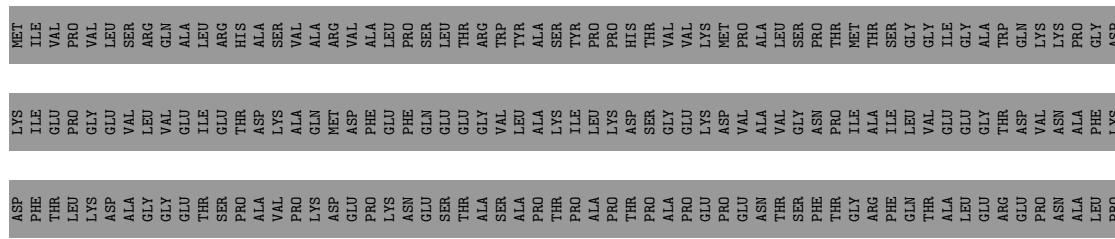
• Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

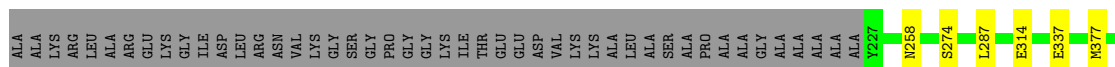


• Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

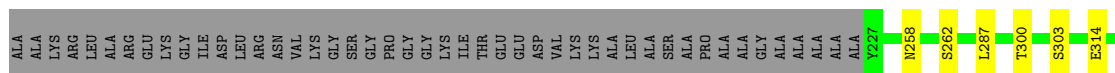
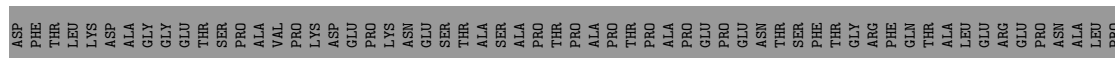
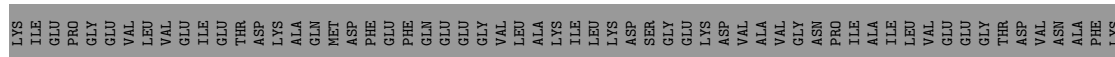
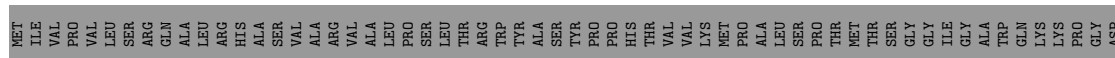


• Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

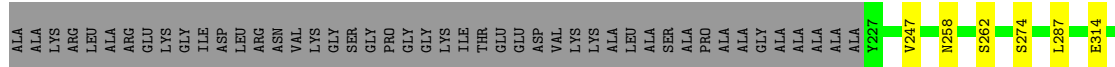
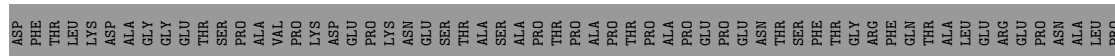
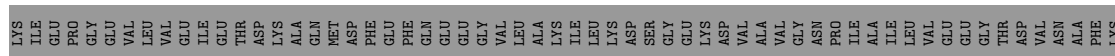
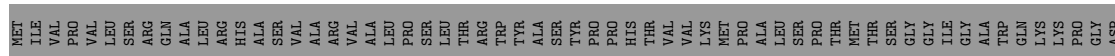




• Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



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



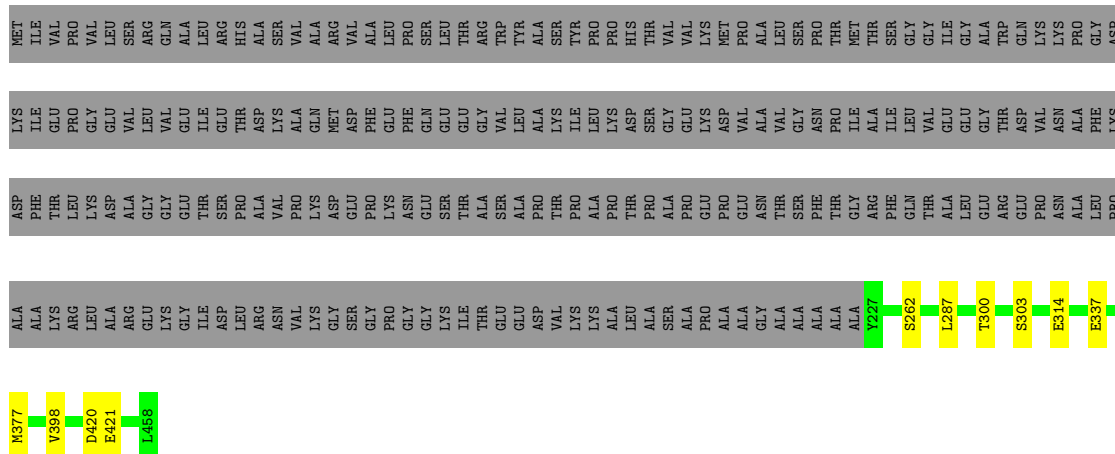
• Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial





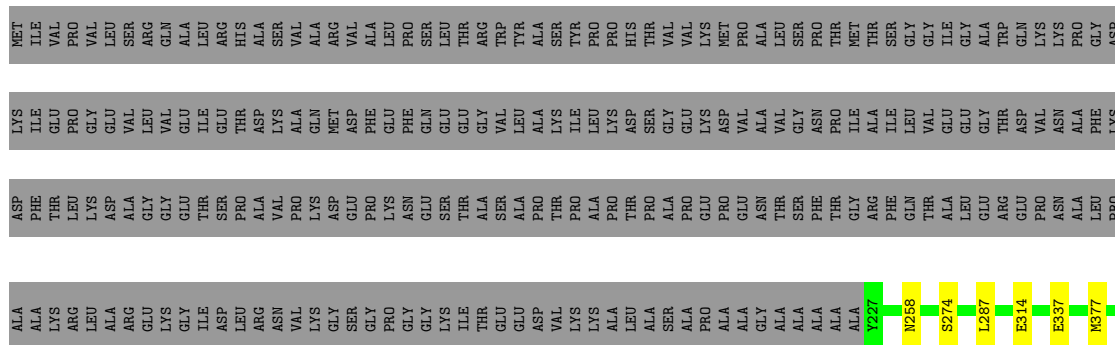
• Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain I:



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

Chain J:

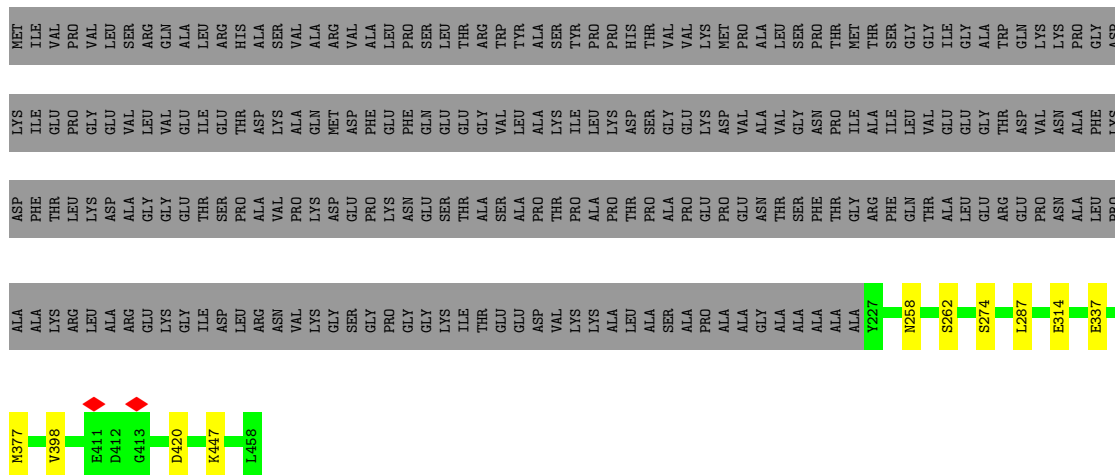






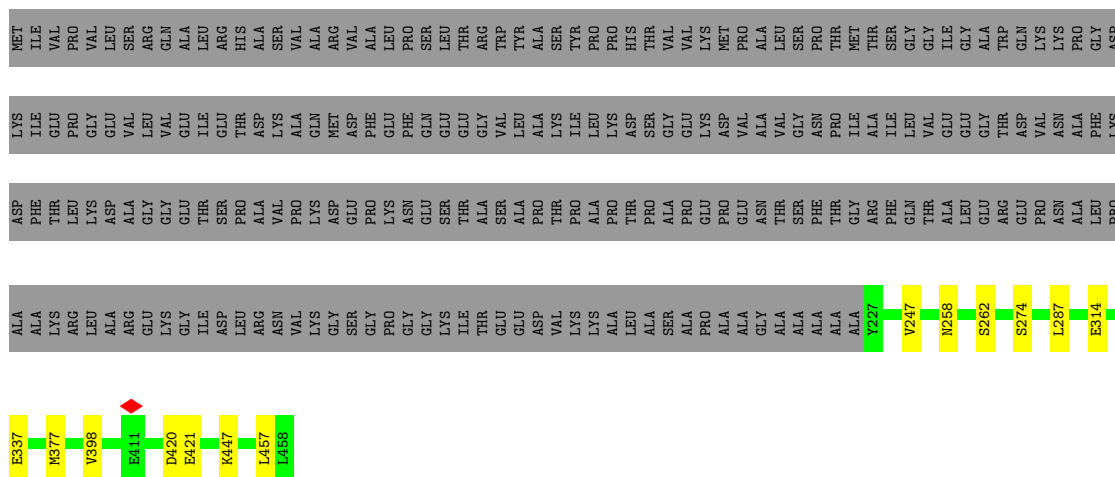
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain R: 48% 49%



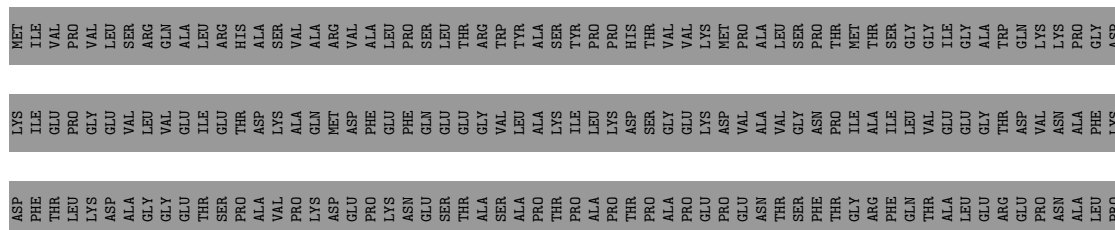
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain S: 48% 49%



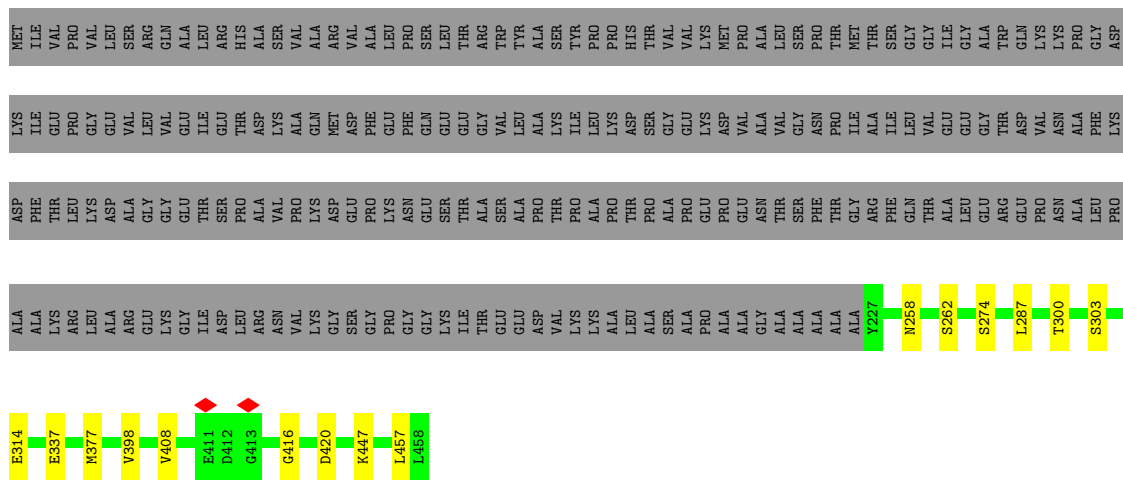
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain T: 47% 49%

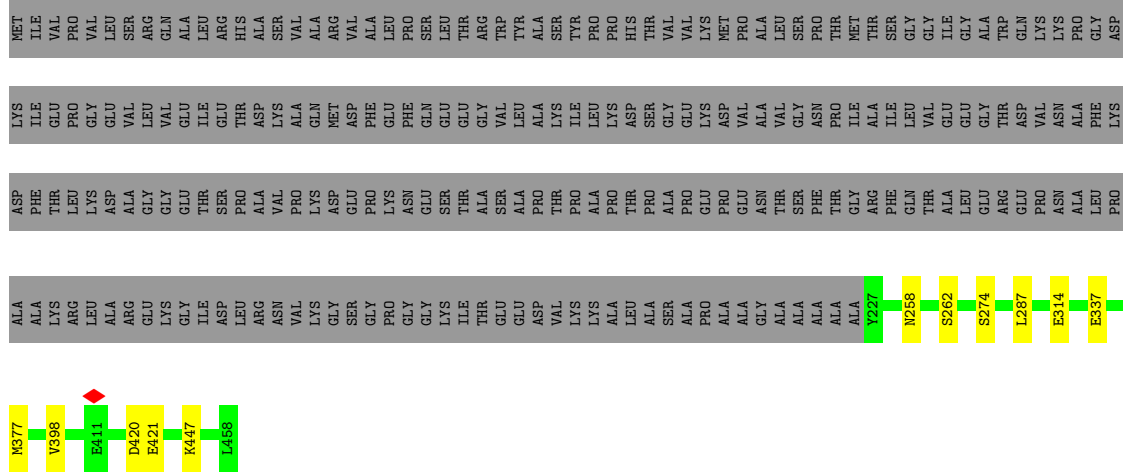




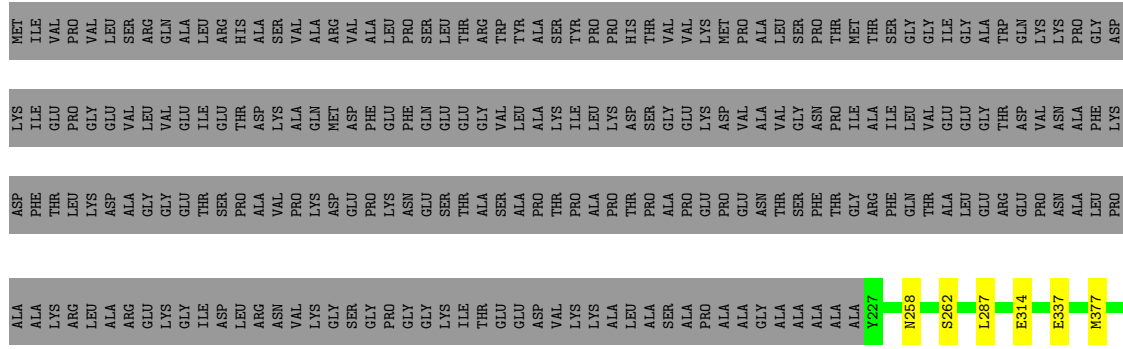




• Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



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

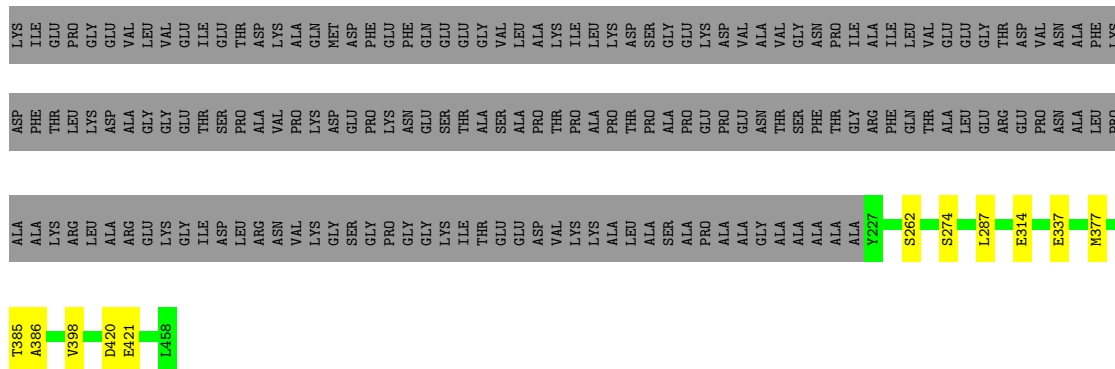




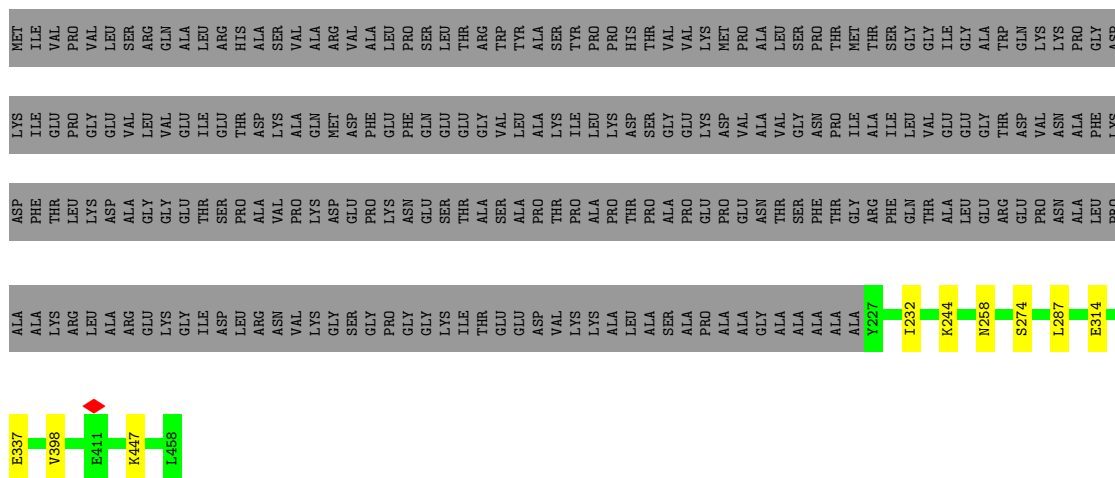




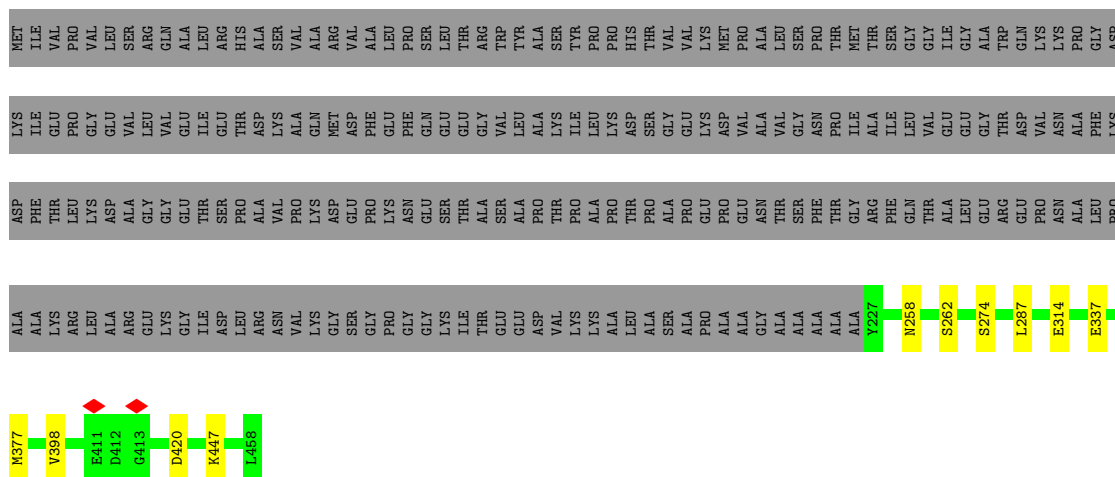




● Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

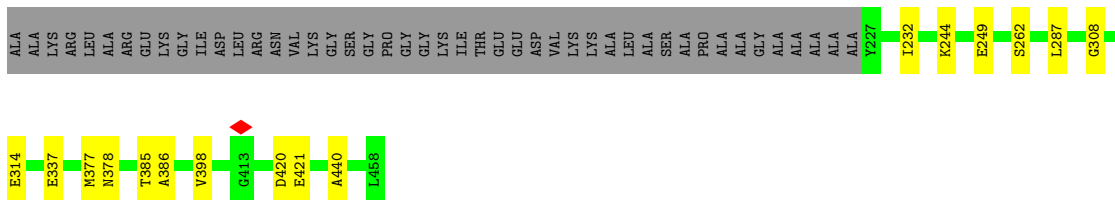


● Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



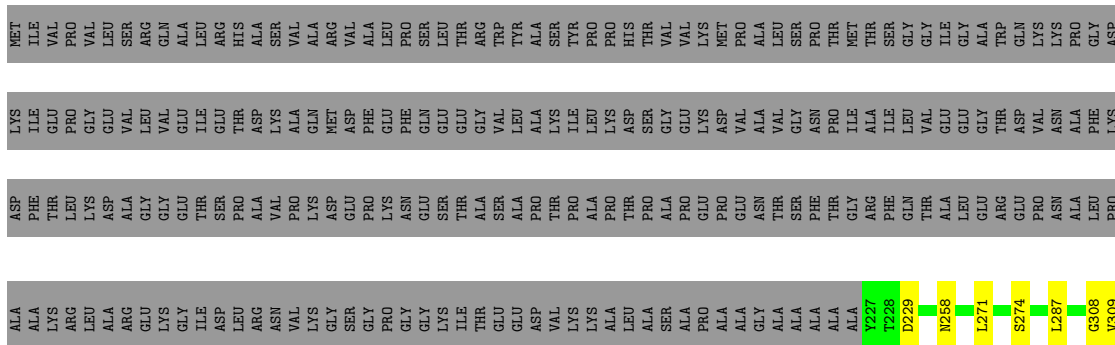






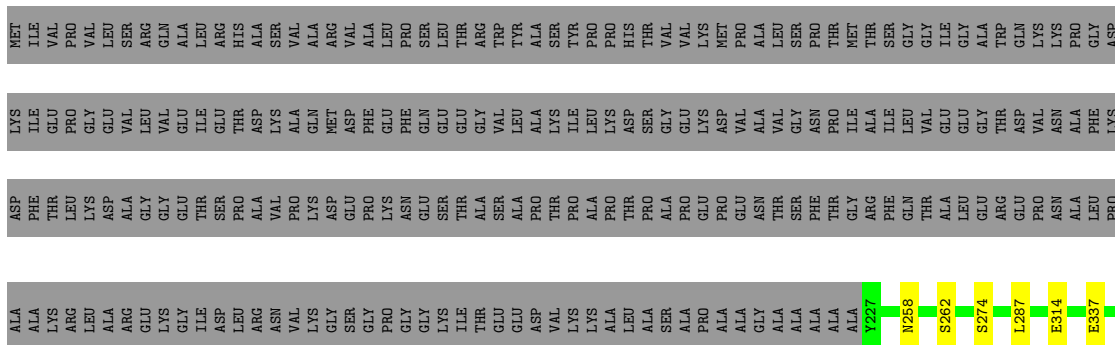
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain UA:  48%  49%



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

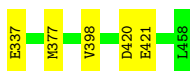
Chain WA:  48%  49%



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

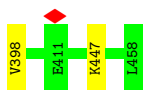
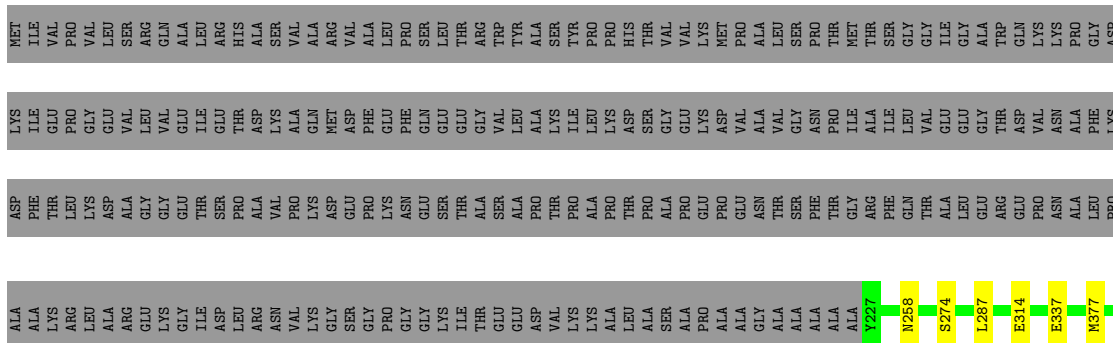
Chain XA:  48%  49%





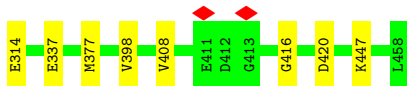
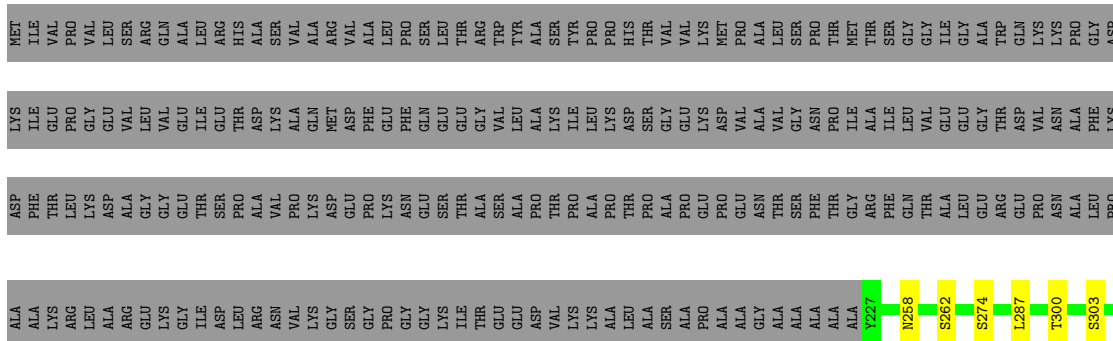
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain AB: 49%



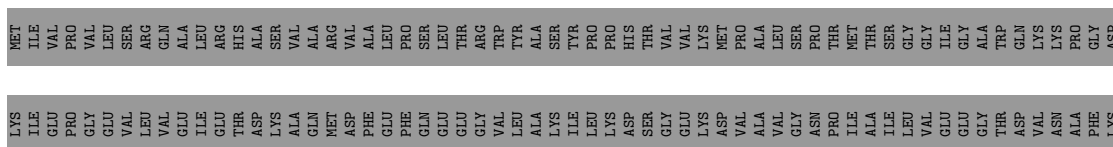
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain CB: 48%



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

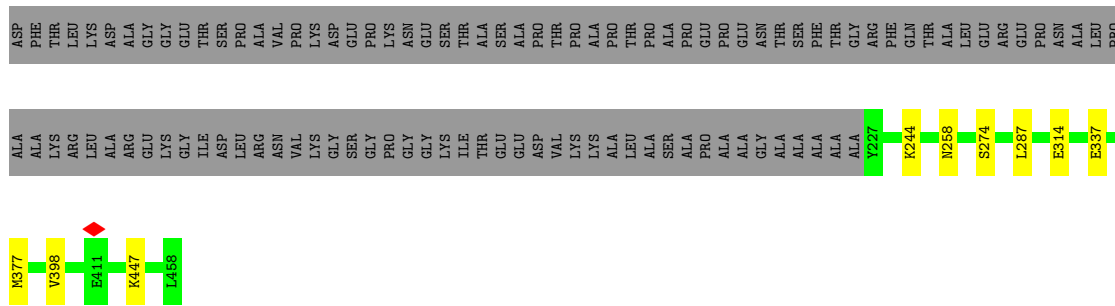
Chain DB: 48%











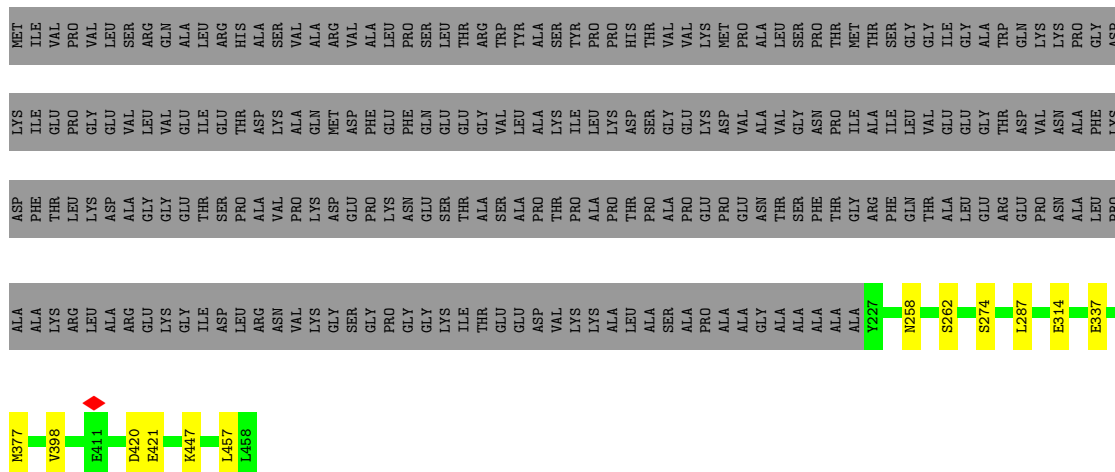
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain OB:  49%  49%



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

Chain PB:  48%  49%



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

Chain QB:  48% . 49%

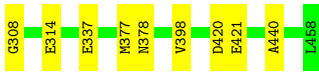
MET ILE VAL PHE THR ASP  
ILE VAL PHE THR ASP  
GLU PRO LEU LYS LEU ASP  
VAL LEU LEU ASP  
SER LEU LEU ASP  
ARG ARG ARG  
GLN ALA  
ALA ALA  
LEU LEU  
LEU LEU  
LEU LEU  
LEU LEU  
ARG ARG  
HIS HIS  
ALA ALA  
SER VAL  
LYS VAL  
VAL VAL  
ALA ALA  
GLN ALA  
MET MET  
ASP ARG  
VAL VAL  
ALA ALA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

  
V398 V408 E411 Q416 D420 E421 K447 L458

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

Chain RB:  47% . 49%

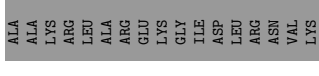
MET ILE VAL PHE THR ASP  
ILE VAL PHE THR ASP  
GLU PRO LEU LYS LEU ASP  
VAL LEU LEU ASP  
SER LEU LEU ASP  
ARG ARG ARG  
GLN ALA  
ALA ALA  
LEU LEU  
LEU LEU  
LEU LEU  
LEU LEU  
ARG ARG  
HIS HIS  
ALA ALA  
SER VAL  
LYS VAL  
VAL VAL  
ALA ALA  
GLN ALA  
MET MET  
ASP ARG  
VAL VAL  
ALA ALA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

  
G308 E314 E337 M377 M378 V398 D420 E421 A440 L458

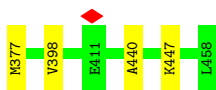
• Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain SB:  48% . 49%

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

  
Y227 M258 S274 L287 G308 E314 E337





- Molecule 2: Pyruvate dehydrogenase X component

Chain XC:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Pyruvate dehydrogenase X component

Chain K:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Pyruvate dehydrogenase X component

Chain Q:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Pyruvate dehydrogenase X component

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Pyruvate dehydrogenase X component

Chain DA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Pyruvate dehydrogenase X component

Chain JA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Pyruvate dehydrogenase X component

Chain PA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Pyruvate dehydrogenase X component

Chain VA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Pyruvate dehydrogenase X component

Chain BB:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Pyruvate dehydrogenase X component

Chain HB:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Pyruvate dehydrogenase X component

Chain NB:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Pyruvate dehydrogenase X component

Chain TB:  100%

There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, T	Depositor
Number of particles used	21129	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.227	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.0325	Depositor
Map size (Å)	400.0, 400.0, 400.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.25, 1.25, 1.25	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	0.31	0/1779	0.49	0/2413
1	AA	0.31	0/1779	0.48	0/2413
1	AB	0.32	0/1779	0.49	0/2413
1	B	0.31	0/1779	0.48	0/2413
1	BA	0.31	0/1779	0.48	0/2413
1	C	0.31	0/1779	0.48	0/2413
1	CA	0.31	0/1779	0.48	0/2413
1	CB	0.31	0/1779	0.49	0/2413
1	D	0.31	0/1779	0.48	0/2413
1	DB	0.31	0/1779	0.49	0/2413
1	E	0.31	0/1779	0.49	0/2413
1	EA	0.31	0/1779	0.49	0/2413
1	EB	0.31	0/1779	0.48	0/2413
1	F	0.31	0/1779	0.49	0/2413
1	FA	0.31	0/1779	0.48	0/2413
1	FB	0.31	0/1779	0.48	0/2413
1	G	0.31	0/1779	0.49	0/2413
1	GA	0.31	0/1779	0.48	0/2413
1	GB	0.31	0/1779	0.49	0/2413
1	H	0.31	0/1779	0.48	0/2413
1	HA	0.31	0/1779	0.48	0/2413
1	I	0.31	0/1779	0.48	0/2413
1	IA	0.31	0/1779	0.49	0/2413
1	IB	0.31	0/1779	0.49	0/2413
1	J	0.31	0/1779	0.49	0/2413
1	JB	0.31	0/1779	0.48	0/2413
1	KA	0.31	0/1779	0.49	0/2413
1	KB	0.31	0/1779	0.48	0/2413
1	L	0.31	0/1779	0.49	0/2413
1	LA	0.31	0/1779	0.48	0/2413
1	LB	0.31	0/1779	0.48	0/2413
1	M	0.31	0/1779	0.48	0/2413
1	MA	0.31	0/1779	0.48	0/2413
1	MB	0.31	0/1779	0.49	0/2413

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	N	0.31	0/1779	0.48	0/2413
1	NA	0.31	0/1779	0.48	0/2413
1	O	0.31	0/1779	0.48	0/2413
1	OA	0.31	0/1779	0.49	0/2413
1	OB	0.31	0/1779	0.49	0/2413
1	P	0.31	0/1779	0.49	0/2413
1	PB	0.31	0/1779	0.48	0/2413
1	QA	0.31	0/1779	0.49	0/2413
1	QB	0.31	0/1779	0.48	0/2413
1	R	0.31	0/1779	0.49	0/2413
1	RA	0.31	0/1779	0.48	0/2413
1	RB	0.31	0/1779	0.48	0/2413
1	S	0.31	0/1779	0.48	0/2413
1	SA	0.31	0/1779	0.48	0/2413
1	SB	0.31	0/1779	0.49	0/2413
1	T	0.31	0/1779	0.48	0/2413
1	TA	0.31	0/1779	0.48	0/2413
1	UA	0.31	0/1779	0.48	0/2413
1	V	0.31	0/1779	0.48	0/2413
1	W	0.31	0/1779	0.49	0/2413
1	WA	0.31	0/1779	0.49	0/2413
1	XA	0.31	0/1779	0.48	0/2413
1	Y	0.31	0/1779	0.49	0/2413
1	YA	0.31	0/1779	0.48	0/2413
1	Z	0.31	0/1779	0.49	0/2413
1	ZA	0.31	0/1779	0.48	0/2413
All	All	0.31	0/106740	0.48	0/144780

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1751	1804	1811	9	0
1	AA	1751	1804	1811	9	0
1	AB	1751	1804	1811	6	0
1	B	1751	1804	1811	9	0
1	BA	1751	1804	1811	9	0
1	C	1751	1804	1811	9	0
1	CA	1751	1804	1811	6	0
1	CB	1751	1804	1811	9	0
1	D	1751	1804	1811	9	0
1	DB	1751	1804	1811	11	0
1	E	1751	1804	1811	6	0
1	EA	1751	1804	1811	8	0
1	EB	1751	1804	1811	10	0
1	F	1751	1804	1811	7	0
1	FA	1751	1804	1811	8	0
1	FB	1751	1804	1811	7	0
1	G	1751	1804	1811	9	0
1	GA	1751	1804	1811	10	0
1	GB	1751	1804	1811	6	0
1	H	1751	1804	1811	10	0
1	HA	1751	1804	1811	7	0
1	I	1751	1804	1811	7	0
1	IA	1751	1804	1811	5	0
1	IB	1751	1804	1811	11	0
1	J	1751	1804	1811	6	0
1	JB	1751	1804	1811	9	0
1	KA	1751	1804	1811	12	0
1	KB	1751	1804	1811	10	0
1	L	1751	1804	1811	10	0
1	LA	1751	1804	1811	10	0
1	LB	1751	1804	1811	7	0
1	M	1751	1804	1811	10	0
1	MA	1751	1804	1811	9	0
1	MB	1751	1804	1811	7	0
1	N	1751	1804	1811	10	0
1	NA	1751	1804	1811	8	0
1	O	1751	1804	1811	8	0
1	OA	1751	1804	1811	7	0
1	OB	1751	1804	1811	6	0
1	P	1751	1804	1811	6	0
1	PB	1751	1804	1811	10	0
1	QA	1751	1804	1811	7	0
1	QB	1751	1804	1811	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	1751	1804	1811	7	0
1	RA	1751	1804	1811	11	0
1	RB	1751	1804	1811	13	0
1	S	1751	1804	1811	11	0
1	SA	1751	1804	1811	13	0
1	SB	1751	1804	1811	9	0
1	T	1751	1804	1811	13	0
1	TA	1751	1804	1811	14	0
1	UA	1751	1804	1811	12	0
1	V	1751	1804	1811	15	0
1	W	1751	1804	1811	8	0
1	WA	1751	1804	1811	8	0
1	XA	1751	1804	1811	9	0
1	Y	1751	1804	1811	10	0
1	YA	1751	1804	1811	9	0
1	Z	1751	1804	1811	8	0
1	ZA	1751	1804	1811	8	0
2	BB	65	0	17	0	0
2	DA	65	0	17	0	0
2	HB	65	0	17	0	0
2	JA	65	0	17	0	0
2	K	65	0	17	0	0
2	NB	65	0	17	0	0
2	PA	65	0	17	0	0
2	Q	65	0	17	0	0
2	TB	65	0	17	0	0
2	VA	65	0	17	0	0
2	X	65	0	17	0	0
2	XC	65	0	17	0	0
All	All	105840	108240	108864	501	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 (501) 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:FA:262:SER:OG	1:FA:420:ASP:OD1	2.09	0.70
1:Z:262:SER:OG	1:Z:420:ASP:OD1	2.09	0.70
1:PB:262:SER:OG	1:PB:420:ASP:OD1	2.09	0.70
1:M:262:SER:OG	1:M:420:ASP:OD1	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:262:SER:OG	1:RA:420:ASP:OD1	2.09	0.69
1:LA:262:SER:OG	1:LA:420:ASP:OD1	2.09	0.69
1:B:262:SER:OG	1:B:420:ASP:OD1	2.09	0.69
1:JB:262:SER:OG	1:JB:420:ASP:OD1	2.09	0.69
1:G:262:SER:OG	1:G:420:ASP:OD1	2.09	0.68
1:DB:262:SER:OG	1:DB:420:ASP:OD1	2.09	0.68
1:XA:262:SER:OG	1:XA:420:ASP:OD1	2.09	0.68
1:L:244:LYS:NZ	1:KA:249:GLU:OE1	2.26	0.66
1:S:262:SER:OG	1:S:420:ASP:OD1	2.09	0.66
1:H:287:LEU:HD13	1:H:398:VAL:HG21	1.79	0.65
1:KB:287:LEU:HD13	1:KB:398:VAL:HG21	1.79	0.65
1:SA:287:LEU:HD13	1:SA:398:VAL:HG21	1.79	0.65
1:W:287:LEU:HD13	1:W:398:VAL:HG21	1.80	0.64
1:C:287:LEU:HD13	1:C:398:VAL:HG21	1.79	0.64
1:E:287:LEU:HD13	1:E:398:VAL:HG21	1.80	0.64
1:YA:287:LEU:HD13	1:YA:398:VAL:HG21	1.79	0.64
1:CA:287:LEU:HD13	1:CA:398:VAL:HG21	1.80	0.64
1:OA:287:LEU:HD13	1:OA:398:VAL:HG21	1.80	0.64
1:GA:287:LEU:HD13	1:GA:398:VAL:HG21	1.79	0.64
1:T:287:LEU:HD13	1:T:398:VAL:HG21	1.79	0.64
1:EB:287:LEU:HD13	1:EB:398:VAL:HG21	1.79	0.64
1:J:287:LEU:HD13	1:J:398:VAL:HG21	1.80	0.64
1:P:287:LEU:HD13	1:P:398:VAL:HG21	1.80	0.64
1:N:287:LEU:HD13	1:N:398:VAL:HG21	1.79	0.63
1:AA:287:LEU:HD13	1:AA:398:VAL:HG21	1.79	0.63
1:MA:287:LEU:HD13	1:MA:398:VAL:HG21	1.79	0.63
1:GB:287:LEU:HD13	1:GB:398:VAL:HG21	1.80	0.63
1:MB:287:LEU:HD13	1:MB:398:VAL:HG21	1.80	0.63
1:AB:287:LEU:HD13	1:AB:398:VAL:HG21	1.80	0.63
1:QB:287:LEU:HD13	1:QB:398:VAL:HG21	1.79	0.63
1:UA:287:LEU:HD13	1:UA:398:VAL:HG21	1.80	0.62
1:IA:287:LEU:HD13	1:IA:398:VAL:HG21	1.80	0.62
1:SB:287:LEU:HD13	1:SB:398:VAL:HG21	1.80	0.62
1:EB:262:SER:OG	1:EB:420:ASP:OD1	2.17	0.61
1:QB:262:SER:OG	1:QB:420:ASP:OD1	2.17	0.61
1:PB:287:LEU:HD13	1:PB:398:VAL:HG21	1.83	0.61
1:RA:287:LEU:HD13	1:RA:398:VAL:HG21	1.83	0.61
1:Z:287:LEU:HD13	1:Z:398:VAL:HG21	1.83	0.61
1:SA:262:SER:OG	1:SA:420:ASP:OD1	2.17	0.60
1:YA:262:SER:OG	1:YA:420:ASP:OD1	2.17	0.60
1:DB:287:LEU:HD13	1:DB:398:VAL:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:287:LEU:HD13	1:G:398:VAL:HG21	1.83	0.60
1:M:287:LEU:HD13	1:M:398:VAL:HG21	1.83	0.60
1:LA:287:LEU:HD13	1:LA:398:VAL:HG21	1.83	0.60
1:B:287:LEU:HD13	1:B:398:VAL:HG21	1.83	0.60
1:S:287:LEU:HD13	1:S:398:VAL:HG21	1.83	0.60
1:D:337:GLU:N	1:D:337:GLU:OE1	2.36	0.59
1:I:337:GLU:N	1:I:337:GLU:OE1	2.36	0.59
1:C:262:SER:OG	1:C:420:ASP:OD1	2.17	0.59
1:FA:287:LEU:HD13	1:FA:398:VAL:HG21	1.83	0.59
1:O:337:GLU:OE1	1:O:337:GLU:N	2.36	0.59
1:KA:244:LYS:NZ	1:IB:249:GLU:OE1	2.34	0.59
1:NA:337:GLU:N	1:NA:337:GLU:OE1	2.36	0.59
1:XA:287:LEU:HD13	1:XA:398:VAL:HG21	1.83	0.59
1:JB:287:LEU:HD13	1:JB:398:VAL:HG21	1.83	0.59
1:RB:337:GLU:N	1:RB:337:GLU:OE1	2.36	0.58
1:R:287:LEU:HD13	1:R:398:VAL:HG21	1.86	0.58
1:BA:337:GLU:OE1	1:BA:337:GLU:N	2.36	0.58
1:QA:287:LEU:HD13	1:QA:398:VAL:HG21	1.86	0.58
1:F:287:LEU:HD13	1:F:398:VAL:HG21	1.86	0.58
1:T:262:SER:OG	1:T:420:ASP:OD1	2.16	0.58
1:F:262:SER:OG	1:F:420:ASP:OD1	2.21	0.58
1:OB:287:LEU:HD13	1:OB:398:VAL:HG21	1.86	0.58
1:KA:287:LEU:HD13	1:KA:398:VAL:HG21	1.86	0.58
1:LB:337:GLU:N	1:LB:337:GLU:OE1	2.36	0.57
1:A:287:LEU:HD13	1:A:398:VAL:HG21	1.86	0.57
1:V:337:GLU:OE1	1:V:337:GLU:N	2.36	0.57
1:Y:287:LEU:HD13	1:Y:398:VAL:HG21	1.86	0.57
1:HA:337:GLU:N	1:HA:337:GLU:OE1	2.36	0.57
1:ZA:337:GLU:N	1:ZA:337:GLU:OE1	2.36	0.57
1:H:262:SER:OG	1:H:420:ASP:OD1	2.17	0.57
1:W:337:GLU:N	1:W:337:GLU:OE1	2.38	0.57
1:WA:287:LEU:HD13	1:WA:398:VAL:HG21	1.86	0.57
1:J:337:GLU:OE1	1:J:337:GLU:N	2.38	0.57
1:AB:337:GLU:N	1:AB:337:GLU:OE1	2.38	0.57
1:G:337:GLU:N	1:G:337:GLU:OE1	2.38	0.57
1:R:337:GLU:N	1:R:337:GLU:OE1	2.38	0.57
1:EA:287:LEU:HD13	1:EA:398:VAL:HG21	1.86	0.57
1:Y:337:GLU:OE1	1:Y:337:GLU:N	2.38	0.57
1:IA:337:GLU:N	1:IA:337:GLU:OE1	2.38	0.57
1:TA:337:GLU:N	1:TA:337:GLU:OE1	2.36	0.57
1:FB:337:GLU:N	1:FB:337:GLU:OE1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:262:SER:OG	1:Y:420:ASP:OD1	2.21	0.57
1:EA:337:GLU:OE1	1:EA:337:GLU:N	2.38	0.57
1:MA:262:SER:OG	1:MA:420:ASP:OD1	2.16	0.57
1:PB:337:GLU:OE1	1:PB:337:GLU:N	2.38	0.57
1:L:337:GLU:N	1:L:337:GLU:OE1	2.38	0.57
1:IB:287:LEU:HD13	1:IB:398:VAL:HG21	1.86	0.57
1:JB:337:GLU:N	1:JB:337:GLU:OE1	2.38	0.57
1:B:337:GLU:N	1:B:337:GLU:OE1	2.38	0.57
1:L:287:LEU:HD13	1:L:398:VAL:HG21	1.86	0.57
1:T:337:GLU:OE1	1:T:337:GLU:N	2.38	0.57
1:OB:262:SER:OG	1:OB:420:ASP:OD1	2.21	0.57
1:F:337:GLU:N	1:F:337:GLU:OE1	2.38	0.56
1:KB:337:GLU:N	1:KB:337:GLU:OE1	2.38	0.56
1:N:262:SER:OG	1:N:420:ASP:OD1	2.17	0.56
1:OB:337:GLU:N	1:OB:337:GLU:OE1	2.38	0.56
1:A:262:SER:OG	1:A:420:ASP:OD1	2.21	0.56
1:A:337:GLU:N	1:A:337:GLU:OE1	2.38	0.56
1:M:337:GLU:OE1	1:M:337:GLU:N	2.38	0.56
1:EB:337:GLU:N	1:EB:337:GLU:OE1	2.38	0.56
1:N:337:GLU:N	1:N:337:GLU:OE1	2.38	0.56
1:UA:337:GLU:N	1:UA:337:GLU:OE1	2.38	0.56
1:KB:262:SER:OG	1:KB:420:ASP:OD1	2.17	0.56
1:P:337:GLU:N	1:P:337:GLU:OE1	2.38	0.56
1:MA:337:GLU:N	1:MA:337:GLU:OE1	2.38	0.56
1:CB:287:LEU:HD13	1:CB:398:VAL:HG21	1.86	0.56
1:MB:337:GLU:N	1:MB:337:GLU:OE1	2.38	0.56
1:L:262:SER:OG	1:L:420:ASP:OD1	2.21	0.56
1:AA:337:GLU:N	1:AA:337:GLU:OE1	2.38	0.56
1:GA:262:SER:OG	1:GA:420:ASP:OD1	2.17	0.56
1:GA:337:GLU:OE1	1:GA:337:GLU:N	2.38	0.56
1:SB:337:GLU:OE1	1:SB:337:GLU:N	2.38	0.56
1:QA:337:GLU:OE1	1:QA:337:GLU:N	2.38	0.56
1:CB:262:SER:OG	1:CB:420:ASP:OD1	2.21	0.56
1:CB:337:GLU:N	1:CB:337:GLU:OE1	2.38	0.56
1:KA:262:SER:OG	1:KA:420:ASP:OD1	2.21	0.56
1:FA:337:GLU:N	1:FA:337:GLU:OE1	2.38	0.56
1:WA:262:SER:OG	1:WA:420:ASP:OD1	2.21	0.56
1:QA:262:SER:OG	1:QA:420:ASP:OD1	2.21	0.55
1:RA:337:GLU:N	1:RA:337:GLU:OE1	2.38	0.55
1:E:337:GLU:OE1	1:E:337:GLU:N	2.38	0.55
1:IB:262:SER:OG	1:IB:420:ASP:OD1	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IB:337:GLU:OE1	1:IB:337:GLU:N	2.38	0.55
1:CA:337:GLU:N	1:CA:337:GLU:OE1	2.38	0.55
1:C:337:GLU:OE1	1:C:337:GLU:N	2.38	0.55
1:R:262:SER:OG	1:R:420:ASP:OD1	2.21	0.55
1:KA:337:GLU:N	1:KA:337:GLU:OE1	2.38	0.55
1:RB:262:SER:OG	1:RB:420:ASP:OD1	2.23	0.55
1:Z:337:GLU:N	1:Z:337:GLU:OE1	2.38	0.55
1:LA:337:GLU:OE1	1:LA:337:GLU:N	2.38	0.55
1:XA:337:GLU:OE1	1:XA:337:GLU:N	2.38	0.55
1:HA:262:SER:OG	1:HA:420:ASP:OD1	2.23	0.55
1:WA:337:GLU:N	1:WA:337:GLU:OE1	2.38	0.55
1:NA:262:SER:OG	1:NA:420:ASP:OD1	2.23	0.55
1:SA:337:GLU:N	1:SA:337:GLU:OE1	2.38	0.55
1:GB:337:GLU:OE1	1:GB:337:GLU:N	2.38	0.55
1:QB:337:GLU:N	1:QB:337:GLU:OE1	2.38	0.55
1:YA:337:GLU:N	1:YA:337:GLU:OE1	2.38	0.54
1:H:337:GLU:OE1	1:H:337:GLU:N	2.38	0.54
1:OA:337:GLU:OE1	1:OA:337:GLU:N	2.38	0.54
1:DB:337:GLU:OE1	1:DB:337:GLU:N	2.38	0.54
1:AA:262:SER:OG	1:AA:420:ASP:OD1	2.17	0.54
1:EA:262:SER:OG	1:EA:420:ASP:OD1	2.21	0.54
1:TA:262:SER:OG	1:TA:420:ASP:OD1	2.23	0.54
1:S:337:GLU:N	1:S:337:GLU:OE1	2.38	0.54
1:FB:262:SER:OG	1:FB:420:ASP:OD1	2.23	0.53
1:FA:274:SER:O	1:FA:274:SER:OG	2.27	0.53
1:D:287:LEU:HD13	1:D:398:VAL:HG21	1.91	0.53
1:I:262:SER:OG	1:I:420:ASP:OD1	2.23	0.53
1:L:380:ALA:O	1:KA:257:THR:OG1	2.17	0.53
1:BA:287:LEU:HD13	1:BA:398:VAL:HG21	1.91	0.53
1:NA:287:LEU:HD13	1:NA:398:VAL:HG21	1.91	0.53
1:LB:262:SER:OG	1:LB:420:ASP:OD1	2.23	0.53
1:V:287:LEU:HD13	1:V:398:VAL:HG21	1.91	0.52
1:V:262:SER:OG	1:V:420:ASP:OD1	2.23	0.52
1:RA:274:SER:O	1:RA:274:SER:OG	2.27	0.52
1:T:378:ASN:ND2	1:UA:440:ALA:HB1	2.25	0.52
1:D:262:SER:OG	1:D:420:ASP:OD1	2.23	0.52
1:T:232:ILE:HD12	1:UA:308:GLY:HA2	1.91	0.52
1:H:251:PRO:HB3	1:RA:247:VAL:HG11	1.92	0.52
1:Z:274:SER:O	1:Z:274:SER:OG	2.27	0.52
1:FB:287:LEU:HD13	1:FB:398:VAL:HG21	1.91	0.52
1:HA:287:LEU:HD13	1:HA:398:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZA:287:LEU:HD13	1:ZA:398:VAL:HG21	1.91	0.52
1:O:262:SER:OG	1:O:420:ASP:OD1	2.23	0.52
1:TA:287:LEU:HD13	1:TA:398:VAL:HG21	1.91	0.52
1:LB:287:LEU:HD13	1:LB:398:VAL:HG21	1.91	0.51
1:O:287:LEU:HD13	1:O:398:VAL:HG21	1.91	0.51
1:BA:274:SER:O	1:BA:274:SER:OG	2.28	0.51
1:I:287:LEU:HD13	1:I:398:VAL:HG21	1.91	0.51
1:RB:287:LEU:HD13	1:RB:398:VAL:HG21	1.91	0.51
1:ZA:262:SER:OG	1:ZA:420:ASP:OD1	2.23	0.51
1:T:378:ASN:HD22	1:UA:440:ALA:HB1	1.76	0.50
1:BA:262:SER:OG	1:BA:420:ASP:OD1	2.23	0.50
1:PB:274:SER:O	1:PB:274:SER:OG	2.27	0.50
1:M:249:GLU:OE1	1:OA:244:LYS:NZ	2.41	0.50
1:LA:274:SER:O	1:LA:274:SER:OG	2.27	0.50
1:S:274:SER:O	1:S:274:SER:OG	2.27	0.49
1:ZA:274:SER:O	1:ZA:274:SER:OG	2.28	0.49
1:V:378:ASN:ND2	1:RB:440:ALA:HB1	2.28	0.49
1:C:314:GLU:OE1	1:C:314:GLU:N	2.47	0.48
1:WA:314:GLU:N	1:WA:314:GLU:OE1	2.47	0.48
1:F:314:GLU:N	1:F:314:GLU:OE1	2.47	0.48
1:GA:314:GLU:OE1	1:GA:314:GLU:N	2.47	0.48
1:L:314:GLU:OE1	1:L:314:GLU:N	2.46	0.48
1:EA:314:GLU:OE1	1:EA:314:GLU:N	2.47	0.48
1:OB:314:GLU:N	1:OB:314:GLU:OE1	2.47	0.48
1:KA:314:GLU:N	1:KA:314:GLU:OE1	2.46	0.48
1:QA:314:GLU:OE1	1:QA:314:GLU:N	2.47	0.48
1:SA:314:GLU:OE1	1:SA:314:GLU:N	2.47	0.48
1:IB:314:GLU:OE1	1:IB:314:GLU:N	2.47	0.48
1:LB:274:SER:O	1:LB:274:SER:OG	2.28	0.48
1:L:249:GLU:OE1	1:IB:244:LYS:NZ	2.41	0.48
1:T:314:GLU:OE1	1:T:314:GLU:N	2.47	0.48
1:O:314:GLU:OE1	1:O:314:GLU:N	2.47	0.48
1:AA:314:GLU:N	1:AA:314:GLU:OE1	2.47	0.48
1:AB:274:SER:O	1:AB:274:SER:OG	2.32	0.48
1:GB:274:SER:O	1:GB:274:SER:OG	2.32	0.48
1:R:314:GLU:N	1:R:314:GLU:OE1	2.47	0.48
1:EA:274:SER:O	1:EA:274:SER:OG	2.32	0.48
1:MA:314:GLU:N	1:MA:314:GLU:OE1	2.47	0.48
1:ZA:314:GLU:N	1:ZA:314:GLU:OE1	2.47	0.48
1:CB:314:GLU:N	1:CB:314:GLU:OE1	2.47	0.48
1:KB:314:GLU:OE1	1:KB:314:GLU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:314:GLU:N	1:FB:314:GLU:OE1	2.47	0.48
1:Y:314:GLU:N	1:Y:314:GLU:OE1	2.46	0.48
1:BA:314:GLU:OE1	1:BA:314:GLU:N	2.47	0.48
1:A:314:GLU:N	1:A:314:GLU:OE1	2.47	0.47
1:H:314:GLU:N	1:H:314:GLU:OE1	2.47	0.47
1:I:314:GLU:N	1:I:314:GLU:OE1	2.47	0.47
1:N:314:GLU:N	1:N:314:GLU:OE1	2.47	0.47
1:TA:308:GLY:HA2	1:RB:232:ILE:HD12	1.95	0.47
1:TA:314:GLU:N	1:TA:314:GLU:OE1	2.47	0.47
1:EB:314:GLU:N	1:EB:314:GLU:OE1	2.47	0.47
1:J:274:SER:O	1:J:274:SER:OG	2.32	0.47
1:KA:274:SER:O	1:KA:274:SER:OG	2.32	0.47
1:NA:314:GLU:OE1	1:NA:314:GLU:N	2.47	0.47
1:XA:274:SER:O	1:XA:274:SER:OG	2.27	0.47
1:QB:314:GLU:N	1:QB:314:GLU:OE1	2.47	0.47
1:V:314:GLU:OE1	1:V:314:GLU:N	2.47	0.47
1:D:314:GLU:N	1:D:314:GLU:OE1	2.47	0.47
1:W:440:ALA:HB1	1:QB:378:ASN:ND2	2.29	0.47
1:HA:314:GLU:N	1:HA:314:GLU:OE1	2.47	0.47
1:YA:314:GLU:N	1:YA:314:GLU:OE1	2.47	0.47
1:RB:314:GLU:N	1:RB:314:GLU:OE1	2.47	0.47
1:V:454:LEU:HB3	1:UA:271:LEU:HD21	1.95	0.47
1:CA:274:SER:O	1:CA:274:SER:OG	2.32	0.47
1:V:249:GLU:OE1	1:TA:244:LYS:NZ	2.46	0.47
1:CB:274:SER:O	1:CB:274:SER:OG	2.32	0.47
1:C:408:VAL:O	1:C:416:GLY:N	2.48	0.46
1:MA:408:VAL:O	1:MA:416:GLY:N	2.48	0.46
1:I:300:THR:O	1:I:303:SER:OG	2.30	0.46
1:LB:314:GLU:N	1:LB:314:GLU:OE1	2.47	0.46
1:RA:314:GLU:N	1:RA:314:GLU:OE1	2.49	0.46
1:D:274:SER:O	1:D:274:SER:OG	2.28	0.46
1:UA:274:SER:O	1:UA:274:SER:OG	2.32	0.46
1:A:274:SER:O	1:A:274:SER:OG	2.32	0.46
1:P:274:SER:O	1:P:274:SER:OG	2.32	0.46
1:EB:258:ASN:O	1:EB:447:LYS:NZ	2.49	0.46
1:C:258:ASN:O	1:C:447:LYS:NZ	2.49	0.46
1:DB:314:GLU:OE1	1:DB:314:GLU:N	2.49	0.46
1:F:300:THR:O	1:F:303:SER:OG	2.30	0.46
1:H:258:ASN:O	1:H:447:LYS:NZ	2.49	0.46
1:N:408:VAL:O	1:N:416:GLY:N	2.48	0.46
1:V:377:MET:SD	1:V:377:MET:N	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:258:ASN:O	1:SA:447:LYS:NZ	2.49	0.46
1:JB:314:GLU:N	1:JB:314:GLU:OE1	2.49	0.46
1:KB:258:ASN:O	1:KB:447:LYS:NZ	2.49	0.46
1:D:377:MET:SD	1:D:377:MET:N	2.89	0.46
1:G:314:GLU:N	1:G:314:GLU:OE1	2.49	0.46
1:I:377:MET:SD	1:I:377:MET:N	2.89	0.46
1:BA:300:THR:O	1:BA:303:SER:OG	2.30	0.46
1:PB:314:GLU:OE1	1:PB:314:GLU:N	2.49	0.46
1:B:314:GLU:N	1:B:314:GLU:OE1	2.49	0.46
1:T:258:ASN:O	1:T:447:LYS:NZ	2.49	0.46
1:LA:314:GLU:OE1	1:LA:314:GLU:N	2.49	0.46
1:SA:408:VAL:O	1:SA:416:GLY:N	2.48	0.46
1:ZA:377:MET:SD	1:ZA:377:MET:N	2.89	0.46
1:DB:274:SER:O	1:DB:274:SER:OG	2.27	0.46
1:LB:377:MET:N	1:LB:377:MET:SD	2.89	0.46
1:O:377:MET:SD	1:O:377:MET:N	2.89	0.45
1:S:314:GLU:N	1:S:314:GLU:OE1	2.49	0.45
1:Z:314:GLU:N	1:Z:314:GLU:OE1	2.49	0.45
1:BA:377:MET:SD	1:BA:377:MET:N	2.89	0.45
1:GA:258:ASN:O	1:GA:447:LYS:NZ	2.49	0.45
1:H:408:VAL:O	1:H:416:GLY:N	2.48	0.45
1:O:260:SER:OG	1:O:420:ASP:OD2	2.31	0.45
1:HA:377:MET:SD	1:HA:377:MET:N	2.89	0.45
1:YA:408:VAL:O	1:YA:416:GLY:N	2.48	0.45
1:JB:274:SER:O	1:JB:274:SER:OG	2.27	0.45
1:FA:314:GLU:N	1:FA:314:GLU:OE1	2.49	0.45
1:XA:314:GLU:OE1	1:XA:314:GLU:N	2.49	0.45
1:AA:258:ASN:O	1:AA:447:LYS:NZ	2.49	0.45
1:MA:258:ASN:O	1:MA:447:LYS:NZ	2.49	0.45
1:N:258:ASN:O	1:N:447:LYS:NZ	2.49	0.45
1:NA:377:MET:SD	1:NA:377:MET:N	2.89	0.45
1:KB:408:VAL:O	1:KB:416:GLY:N	2.48	0.45
1:QB:258:ASN:O	1:QB:447:LYS:NZ	2.49	0.45
1:M:314:GLU:N	1:M:314:GLU:OE1	2.49	0.45
1:WA:274:SER:O	1:WA:274:SER:OG	2.32	0.45
1:EB:408:VAL:O	1:EB:416:GLY:N	2.48	0.45
1:AA:408:VAL:O	1:AA:416:GLY:N	2.48	0.45
1:YA:258:ASN:O	1:YA:447:LYS:NZ	2.49	0.45
1:FB:377:MET:SD	1:FB:377:MET:N	2.89	0.45
1:G:274:SER:O	1:G:274:SER:OG	2.27	0.45
1:V:232:ILE:HD12	1:RB:308:GLY:HA2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:300:THR:O	1:EA:303:SER:OG	2.30	0.45
1:HA:274:SER:O	1:HA:274:SER:OG	2.28	0.45
1:QA:274:SER:O	1:QA:274:SER:OG	2.32	0.45
1:CB:300:THR:O	1:CB:303:SER:OG	2.30	0.45
1:O:300:THR:O	1:O:303:SER:OG	2.30	0.44
1:V:378:ASN:HD22	1:RB:440:ALA:HB1	1.82	0.44
1:TA:440:ALA:HB1	1:RB:378:ASN:ND2	2.32	0.44
1:RB:377:MET:SD	1:RB:377:MET:N	2.89	0.44
1:KA:258:ASN:O	1:KA:447:LYS:NZ	2.51	0.44
1:IB:258:ASN:O	1:IB:447:LYS:NZ	2.51	0.44
1:T:408:VAL:O	1:T:416:GLY:N	2.48	0.44
1:Y:258:ASN:O	1:Y:447:LYS:NZ	2.51	0.44
1:NA:274:SER:O	1:NA:274:SER:OG	2.28	0.44
1:QA:258:ASN:O	1:QA:447:LYS:NZ	2.51	0.44
1:TA:377:MET:N	1:TA:377:MET:SD	2.89	0.44
1:OB:258:ASN:O	1:OB:447:LYS:NZ	2.51	0.44
1:SB:274:SER:O	1:SB:274:SER:OG	2.32	0.44
1:A:258:ASN:O	1:A:447:LYS:NZ	2.51	0.44
1:A:457:LEU:HD23	1:S:457:LEU:HD23	1.98	0.44
1:F:258:ASN:O	1:F:447:LYS:NZ	2.51	0.44
1:P:377:MET:SD	1:P:377:MET:N	2.91	0.44
1:SA:232:ILE:HD12	1:SB:308:GLY:HA2	1.98	0.44
1:WA:258:ASN:O	1:WA:447:LYS:NZ	2.51	0.44
1:G:247:VAL:HG11	1:SA:251:PRO:HB3	1.99	0.44
1:L:258:ASN:O	1:L:447:LYS:NZ	2.51	0.44
1:W:274:SER:O	1:W:274:SER:OG	2.32	0.44
1:GA:408:VAL:O	1:GA:416:GLY:N	2.48	0.44
1:CB:258:ASN:O	1:CB:447:LYS:NZ	2.51	0.44
1:RA:377:MET:SD	1:RA:377:MET:N	2.91	0.44
1:SB:377:MET:SD	1:SB:377:MET:N	2.91	0.44
1:W:377:MET:SD	1:W:377:MET:N	2.91	0.44
1:Y:274:SER:O	1:Y:274:SER:OG	2.32	0.44
1:IA:377:MET:SD	1:IA:377:MET:N	2.91	0.44
1:R:258:ASN:O	1:R:447:LYS:NZ	2.51	0.44
1:Y:457:LEU:HD23	1:RA:457:LEU:HD23	2.00	0.44
1:SA:378:ASN:ND2	1:SB:440:ALA:HB1	2.33	0.44
1:XA:377:MET:SD	1:XA:377:MET:N	2.91	0.44
1:SB:258:ASN:O	1:SB:447:LYS:NZ	2.51	0.44
1:MB:258:ASN:O	1:MB:447:LYS:NZ	2.51	0.43
1:MB:274:SER:O	1:MB:274:SER:OG	2.32	0.43
1:M:308:GLY:HA2	1:OA:232:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZA:300:THR:O	1:ZA:303:SER:OG	2.30	0.43
1:JB:377:MET:SD	1:JB:377:MET:N	2.91	0.43
1:EA:258:ASN:O	1:EA:447:LYS:NZ	2.51	0.43
1:OA:258:ASN:O	1:OA:447:LYS:NZ	2.51	0.43
1:J:377:MET:SD	1:J:377:MET:N	2.91	0.43
1:XA:258:ASN:O	1:XA:447:LYS:NZ	2.52	0.43
1:AB:258:ASN:O	1:AB:447:LYS:NZ	2.51	0.43
1:GB:258:ASN:O	1:GB:447:LYS:NZ	2.51	0.43
1:A:300:THR:O	1:A:303:SER:OG	2.30	0.43
1:B:258:ASN:O	1:B:447:LYS:NZ	2.52	0.43
1:N:377:MET:SD	1:N:377:MET:N	2.91	0.43
1:P:258:ASN:O	1:P:447:LYS:NZ	2.51	0.43
1:IA:258:ASN:O	1:IA:447:LYS:NZ	2.51	0.43
1:KB:377:MET:SD	1:KB:377:MET:N	2.91	0.43
1:N:274:SER:O	1:N:274:SER:OG	2.36	0.43
1:S:377:MET:SD	1:S:377:MET:N	2.91	0.43
1:LA:377:MET:SD	1:LA:377:MET:N	2.91	0.43
1:WA:457:LEU:HD23	1:PB:457:LEU:HD23	2.00	0.43
1:DB:260:SER:OG	1:DB:420:ASP:OD2	2.31	0.43
1:QB:377:MET:SD	1:QB:377:MET:N	2.91	0.43
1:D:260:SER:OG	1:D:420:ASP:OD2	2.31	0.43
1:E:377:MET:SD	1:E:377:MET:N	2.91	0.43
1:S:420:ASP:OD1	1:S:421:GLU:N	2.52	0.43
1:W:258:ASN:O	1:W:447:LYS:NZ	2.51	0.43
1:W:440:ALA:HB1	1:QB:378:ASN:HD22	1.83	0.43
1:Z:258:ASN:O	1:Z:447:LYS:NZ	2.52	0.43
1:Z:420:ASP:OD1	1:Z:421:GLU:N	2.52	0.43
1:GA:377:MET:SD	1:GA:377:MET:N	2.91	0.43
1:MA:377:MET:SD	1:MA:377:MET:N	2.91	0.43
1:XA:420:ASP:OD1	1:XA:421:GLU:N	2.52	0.43
1:PB:420:ASP:OD1	1:PB:421:GLU:N	2.52	0.43
1:H:377:MET:SD	1:H:377:MET:N	2.91	0.43
1:LA:258:ASN:O	1:LA:447:LYS:NZ	2.52	0.43
1:UA:229:ASP:HB3	1:DB:309:VAL:HG21	2.01	0.43
1:G:258:ASN:O	1:G:447:LYS:NZ	2.52	0.43
1:G:420:ASP:OD1	1:G:421:GLU:N	2.52	0.43
1:J:258:ASN:O	1:J:447:LYS:NZ	2.51	0.43
1:EB:377:MET:SD	1:EB:377:MET:N	2.91	0.43
1:B:420:ASP:OD1	1:B:421:GLU:N	2.52	0.43
1:E:314:GLU:OE1	1:E:314:GLU:N	2.52	0.43
1:G:377:MET:SD	1:G:377:MET:N	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:377:MET:SD	1:AA:377:MET:N	2.91	0.43
1:CA:377:MET:SD	1:CA:377:MET:N	2.91	0.43
1:FB:300:THR:O	1:FB:303:SER:OG	2.30	0.43
1:JB:260:SER:OG	1:JB:420:ASP:OD2	2.31	0.43
1:QB:408:VAL:O	1:QB:416:GLY:N	2.48	0.43
1:SB:314:GLU:OE1	1:SB:314:GLU:N	2.52	0.43
1:C:377:MET:SD	1:C:377:MET:N	2.91	0.42
1:KA:408:VAL:O	1:KA:416:GLY:N	2.50	0.42
1:RA:258:ASN:O	1:RA:447:LYS:NZ	2.52	0.42
1:JB:258:ASN:O	1:JB:447:LYS:NZ	2.52	0.42
1:B:377:MET:SD	1:B:377:MET:N	2.91	0.42
1:E:258:ASN:O	1:E:447:LYS:NZ	2.51	0.42
1:R:274:SER:O	1:R:274:SER:OG	2.32	0.42
1:S:258:ASN:O	1:S:447:LYS:NZ	2.52	0.42
1:Y:300:THR:O	1:Y:303:SER:OG	2.30	0.42
1:CA:314:GLU:N	1:CA:314:GLU:OE1	2.52	0.42
1:UA:314:GLU:N	1:UA:314:GLU:OE1	2.52	0.42
1:MB:314:GLU:N	1:MB:314:GLU:OE1	2.52	0.42
1:RB:300:THR:O	1:RB:303:SER:OG	2.30	0.42
1:M:258:ASN:O	1:M:447:LYS:NZ	2.52	0.42
1:CA:258:ASN:O	1:CA:447:LYS:NZ	2.51	0.42
1:FA:420:ASP:OD1	1:FA:421:GLU:N	2.52	0.42
1:RA:420:ASP:OD1	1:RA:421:GLU:N	2.52	0.42
1:TA:249:GLU:OE1	1:RB:244:LYS:NZ	2.46	0.42
1:PB:258:ASN:O	1:PB:447:LYS:NZ	2.52	0.42
1:E:274:SER:O	1:E:274:SER:OG	2.32	0.42
1:LA:420:ASP:OD1	1:LA:421:GLU:N	2.52	0.42
1:MA:258:ASN:N	1:MA:258:ASN:OD1	2.53	0.42
1:SA:258:ASN:OD1	1:SA:258:ASN:N	2.53	0.42
1:UA:258:ASN:O	1:UA:447:LYS:NZ	2.51	0.42
1:M:274:SER:O	1:M:274:SER:OG	2.27	0.42
1:FA:258:ASN:O	1:FA:447:LYS:NZ	2.52	0.42
1:GB:314:GLU:N	1:GB:314:GLU:OE1	2.52	0.42
1:T:258:ASN:N	1:T:258:ASN:OD1	2.53	0.42
1:V:440:ALA:HB1	1:TA:378:ASN:HD22	1.85	0.42
1:AB:377:MET:SD	1:AB:377:MET:N	2.91	0.42
1:MB:377:MET:SD	1:MB:377:MET:N	2.91	0.42
1:OB:377:MET:SD	1:OB:377:MET:N	2.93	0.42
1:C:258:ASN:OD1	1:C:258:ASN:N	2.53	0.42
1:W:314:GLU:N	1:W:314:GLU:OE1	2.52	0.42
1:IA:314:GLU:N	1:IA:314:GLU:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:377:MET:SD	1:L:377:MET:N	2.93	0.42
1:LA:271:LEU:HD21	1:IB:454:LEU:HB3	2.02	0.42
1:OA:274:SER:O	1:OA:274:SER:OG	2.32	0.42
1:SA:377:MET:SD	1:SA:377:MET:N	2.91	0.42
1:DB:258:ASN:O	1:DB:447:LYS:NZ	2.52	0.42
1:IB:377:MET:SD	1:IB:377:MET:N	2.93	0.42
1:JB:420:ASP:OD1	1:JB:421:GLU:N	2.52	0.42
1:LB:420:ASP:OD1	1:LB:421:GLU:N	2.53	0.42
1:J:314:GLU:OE1	1:J:314:GLU:N	2.52	0.42
1:Y:377:MET:SD	1:Y:377:MET:N	2.93	0.42
1:AB:314:GLU:N	1:AB:314:GLU:OE1	2.52	0.42
1:DB:420:ASP:OD1	1:DB:421:GLU:N	2.52	0.42
1:EB:258:ASN:OD1	1:EB:258:ASN:N	2.53	0.42
1:RB:420:ASP:OD1	1:RB:421:GLU:N	2.53	0.42
1:Y:408:VAL:O	1:Y:416:GLY:N	2.50	0.42
1:HA:420:ASP:OD1	1:HA:421:GLU:N	2.53	0.42
1:CB:377:MET:SD	1:CB:377:MET:N	2.93	0.42
1:GB:377:MET:SD	1:GB:377:MET:N	2.91	0.42
1:M:420:ASP:OD1	1:M:421:GLU:N	2.52	0.41
1:O:420:ASP:OD1	1:O:421:GLU:N	2.53	0.41
1:T:420:ASP:OD1	1:T:421:GLU:N	2.53	0.41
1:Z:377:MET:SD	1:Z:377:MET:N	2.91	0.41
1:YA:258:ASN:N	1:YA:258:ASN:OD1	2.53	0.41
1:QB:420:ASP:OD1	1:QB:421:GLU:N	2.53	0.41
1:I:420:ASP:OD1	1:I:421:GLU:N	2.53	0.41
1:N:420:ASP:OD1	1:N:421:GLU:N	2.53	0.41
1:R:377:MET:SD	1:R:377:MET:N	2.93	0.41
1:V:420:ASP:OD1	1:V:421:GLU:N	2.53	0.41
1:V:440:ALA:HB1	1:TA:378:ASN:ND2	2.35	0.41
1:GA:258:ASN:OD1	1:GA:258:ASN:N	2.53	0.41
1:YA:377:MET:SD	1:YA:377:MET:N	2.91	0.41
1:QB:258:ASN:OD1	1:QB:258:ASN:N	2.53	0.41
1:N:258:ASN:OD1	1:N:258:ASN:N	2.53	0.41
1:P:314:GLU:N	1:P:314:GLU:OE1	2.52	0.41
1:T:230:VAL:C	1:UA:309:VAL:HG23	2.40	0.41
1:V:300:THR:O	1:V:303:SER:OG	2.30	0.41
1:ZA:420:ASP:OD1	1:ZA:421:GLU:N	2.53	0.41
1:L:308:GLY:HA2	1:IB:232:ILE:HD12	2.01	0.41
1:BA:420:ASP:OD1	1:BA:421:GLU:N	2.53	0.41
1:TA:420:ASP:OD1	1:TA:421:GLU:N	2.53	0.41
1:KB:258:ASN:OD1	1:KB:258:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:377:MET:SD	1:T:377:MET:N	2.91	0.41
1:LA:249:GLU:OE1	1:MB:244:LYS:NZ	2.48	0.41
1:MA:420:ASP:OD1	1:MA:421:GLU:N	2.53	0.41
1:OA:314:GLU:N	1:OA:314:GLU:OE1	2.52	0.41
1:AA:258:ASN:OD1	1:AA:258:ASN:N	2.53	0.41
1:QA:377:MET:SD	1:QA:377:MET:N	2.93	0.41
1:SA:378:ASN:HD22	1:SB:440:ALA:HB1	1.86	0.41
1:UA:377:MET:SD	1:UA:377:MET:N	2.91	0.41
1:D:420:ASP:OD1	1:D:421:GLU:N	2.53	0.41
1:H:420:ASP:OD1	1:H:421:GLU:N	2.53	0.41
1:SA:420:ASP:OD1	1:SA:421:GLU:N	2.53	0.41
1:C:420:ASP:OD1	1:C:421:GLU:N	2.53	0.41
1:H:258:ASN:OD1	1:H:258:ASN:N	2.53	0.41
1:AA:420:ASP:OD1	1:AA:421:GLU:N	2.53	0.41
1:EA:377:MET:SD	1:EA:377:MET:N	2.93	0.41
1:FA:377:MET:SD	1:FA:377:MET:N	2.91	0.41
1:XA:260:SER:OG	1:XA:420:ASP:OD2	2.31	0.41
1:YA:420:ASP:OD1	1:YA:421:GLU:N	2.53	0.41
1:F:377:MET:SD	1:F:377:MET:N	2.93	0.41
1:S:247:VAL:HG11	1:EB:251:PRO:HB3	2.03	0.41
1:GA:420:ASP:OD1	1:GA:421:GLU:N	2.53	0.41
1:NA:420:ASP:OD1	1:NA:421:GLU:N	2.53	0.41
1:CB:408:VAL:O	1:CB:416:GLY:N	2.50	0.41
1:S:258:ASN:OD1	1:S:258:ASN:N	2.54	0.41
1:RA:258:ASN:N	1:RA:258:ASN:OD1	2.54	0.41
1:KB:420:ASP:OD1	1:KB:421:GLU:N	2.53	0.41
1:M:258:ASN:OD1	1:M:258:ASN:N	2.54	0.40
1:KA:232:ILE:HD12	1:IB:308:GLY:HA2	2.03	0.40
1:DB:258:ASN:OD1	1:DB:258:ASN:N	2.54	0.40
1:EB:420:ASP:OD1	1:EB:421:GLU:N	2.53	0.40
1:B:258:ASN:OD1	1:B:258:ASN:N	2.54	0.40
1:FB:420:ASP:OD1	1:FB:421:GLU:N	2.53	0.40
1:PB:377:MET:SD	1:PB:377:MET:N	2.91	0.40
1:A:408:VAL:O	1:A:416:GLY:N	2.50	0.40
1:B:274:SER:O	1:B:274:SER:OG	2.27	0.40
1:D:300:THR:O	1:D:303:SER:OG	2.30	0.40
1:GA:385:THR:HG22	1:GA:386:ALA:N	2.37	0.40
1:PB:258:ASN:OD1	1:PB:258:ASN:N	2.54	0.40
1:V:308:GLY:HA2	1:TA:232:ILE:HD12	2.03	0.40
1:NA:385:THR:HG22	1:NA:386:ALA:N	2.37	0.40
1:TA:385:THR:HG22	1:TA:386:ALA:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:377:MET:SD	1:DB:377:MET:N	2.91	0.40
1:KB:385:THR:HG22	1:KB:386:ALA:N	2.37	0.40
1:BA:385:THR:HG22	1:BA:386:ALA:N	2.37	0.40
1:KA:377:MET:N	1:KA:377:MET:SD	2.93	0.40
1:WA:408:VAL:O	1:WA:416:GLY:N	2.50	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	AA	230/458 (50%)	226 (98%)	4 (2%)	0	100	100
1	AB	230/458 (50%)	224 (97%)	6 (3%)	0	100	100
1	B	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	BA	230/458 (50%)	223 (97%)	7 (3%)	0	100	100
1	C	230/458 (50%)	226 (98%)	4 (2%)	0	100	100
1	CA	230/458 (50%)	224 (97%)	6 (3%)	0	100	100
1	CB	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	D	230/458 (50%)	223 (97%)	7 (3%)	0	100	100
1	DB	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	E	230/458 (50%)	224 (97%)	6 (3%)	0	100	100
1	EA	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	EB	230/458 (50%)	226 (98%)	4 (2%)	0	100	100
1	F	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	FA	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	FB	230/458 (50%)	223 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	GA	230/458 (50%)	226 (98%)	4 (2%)	0	100	100
1	GB	230/458 (50%)	224 (97%)	6 (3%)	0	100	100
1	H	230/458 (50%)	226 (98%)	4 (2%)	0	100	100
1	HA	230/458 (50%)	223 (97%)	7 (3%)	0	100	100
1	I	230/458 (50%)	223 (97%)	7 (3%)	0	100	100
1	IA	230/458 (50%)	224 (97%)	6 (3%)	0	100	100
1	IB	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	J	230/458 (50%)	224 (97%)	6 (3%)	0	100	100
1	JB	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	KA	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	KB	230/458 (50%)	226 (98%)	4 (2%)	0	100	100
1	L	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	LA	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	LB	230/458 (50%)	223 (97%)	7 (3%)	0	100	100
1	M	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	MA	230/458 (50%)	226 (98%)	4 (2%)	0	100	100
1	MB	230/458 (50%)	224 (97%)	6 (3%)	0	100	100
1	N	230/458 (50%)	226 (98%)	4 (2%)	0	100	100
1	NA	230/458 (50%)	223 (97%)	7 (3%)	0	100	100
1	O	230/458 (50%)	223 (97%)	7 (3%)	0	100	100
1	OA	230/458 (50%)	224 (97%)	6 (3%)	0	100	100
1	OB	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	P	230/458 (50%)	224 (97%)	6 (3%)	0	100	100
1	PB	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	QA	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	QB	230/458 (50%)	226 (98%)	4 (2%)	0	100	100
1	R	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	RA	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	RB	230/458 (50%)	223 (97%)	7 (3%)	0	100	100
1	S	230/458 (50%)	225 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	SA	230/458 (50%)	226 (98%)	4 (2%)	0	100	100
1	SB	230/458 (50%)	224 (97%)	6 (3%)	0	100	100
1	T	230/458 (50%)	226 (98%)	4 (2%)	0	100	100
1	TA	230/458 (50%)	223 (97%)	7 (3%)	0	100	100
1	UA	230/458 (50%)	224 (97%)	6 (3%)	0	100	100
1	V	230/458 (50%)	223 (97%)	7 (3%)	0	100	100
1	W	230/458 (50%)	224 (97%)	6 (3%)	0	100	100
1	WA	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	XA	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	Y	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	YA	230/458 (50%)	226 (98%)	4 (2%)	0	100	100
1	Z	230/458 (50%)	225 (98%)	5 (2%)	0	100	100
1	ZA	230/458 (50%)	223 (97%)	7 (3%)	0	100	100
All	All	13800/27480 (50%)	13476 (98%)	324 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	193/368 (52%)	193 (100%)	0	100	100
1	AA	193/368 (52%)	193 (100%)	0	100	100
1	AB	193/368 (52%)	193 (100%)	0	100	100
1	B	193/368 (52%)	193 (100%)	0	100	100
1	BA	193/368 (52%)	193 (100%)	0	100	100
1	C	193/368 (52%)	193 (100%)	0	100	100
1	CA	193/368 (52%)	193 (100%)	0	100	100
1	CB	193/368 (52%)	193 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	193/368 (52%)	193 (100%)	0	100	100
1	DB	193/368 (52%)	193 (100%)	0	100	100
1	E	193/368 (52%)	193 (100%)	0	100	100
1	EA	193/368 (52%)	193 (100%)	0	100	100
1	EB	193/368 (52%)	193 (100%)	0	100	100
1	F	193/368 (52%)	193 (100%)	0	100	100
1	FA	193/368 (52%)	193 (100%)	0	100	100
1	FB	193/368 (52%)	193 (100%)	0	100	100
1	G	193/368 (52%)	193 (100%)	0	100	100
1	GA	193/368 (52%)	193 (100%)	0	100	100
1	GB	193/368 (52%)	193 (100%)	0	100	100
1	H	193/368 (52%)	193 (100%)	0	100	100
1	HA	193/368 (52%)	193 (100%)	0	100	100
1	I	193/368 (52%)	193 (100%)	0	100	100
1	IA	193/368 (52%)	193 (100%)	0	100	100
1	IB	193/368 (52%)	193 (100%)	0	100	100
1	J	193/368 (52%)	193 (100%)	0	100	100
1	JB	193/368 (52%)	193 (100%)	0	100	100
1	KA	193/368 (52%)	193 (100%)	0	100	100
1	KB	193/368 (52%)	193 (100%)	0	100	100
1	L	193/368 (52%)	193 (100%)	0	100	100
1	LA	193/368 (52%)	193 (100%)	0	100	100
1	LB	193/368 (52%)	193 (100%)	0	100	100
1	M	193/368 (52%)	193 (100%)	0	100	100
1	MA	193/368 (52%)	193 (100%)	0	100	100
1	MB	193/368 (52%)	193 (100%)	0	100	100
1	N	193/368 (52%)	193 (100%)	0	100	100
1	NA	193/368 (52%)	193 (100%)	0	100	100
1	O	193/368 (52%)	193 (100%)	0	100	100
1	OA	193/368 (52%)	193 (100%)	0	100	100
1	OB	193/368 (52%)	193 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	193/368 (52%)	193 (100%)	0	100	100
1	PB	193/368 (52%)	193 (100%)	0	100	100
1	QA	193/368 (52%)	193 (100%)	0	100	100
1	QB	193/368 (52%)	193 (100%)	0	100	100
1	R	193/368 (52%)	193 (100%)	0	100	100
1	RA	193/368 (52%)	193 (100%)	0	100	100
1	RB	193/368 (52%)	193 (100%)	0	100	100
1	S	193/368 (52%)	193 (100%)	0	100	100
1	SA	193/368 (52%)	193 (100%)	0	100	100
1	SB	193/368 (52%)	193 (100%)	0	100	100
1	T	193/368 (52%)	193 (100%)	0	100	100
1	TA	193/368 (52%)	193 (100%)	0	100	100
1	UA	193/368 (52%)	193 (100%)	0	100	100
1	V	193/368 (52%)	193 (100%)	0	100	100
1	W	193/368 (52%)	193 (100%)	0	100	100
1	WA	193/368 (52%)	193 (100%)	0	100	100
1	XA	193/368 (52%)	193 (100%)	0	100	100
1	Y	193/368 (52%)	193 (100%)	0	100	100
1	YA	193/368 (52%)	193 (100%)	0	100	100
1	Z	193/368 (52%)	193 (100%)	0	100	100
1	ZA	193/368 (52%)	193 (100%)	0	100	100
All	All	11580/22080 (52%)	11580 (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 (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	382	GLN
1	B	250	ASN
1	B	382	GLN
1	C	382	GLN
1	D	382	GLN
1	D	452	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	382	GLN
1	F	382	GLN
1	G	250	ASN
1	G	402	GLN
1	H	382	GLN
1	I	382	GLN
1	I	452	ASN
1	J	382	GLN
1	L	382	GLN
1	M	250	ASN
1	M	382	GLN
1	N	382	GLN
1	O	382	GLN
1	O	452	ASN
1	P	382	GLN
1	R	382	GLN
1	S	250	ASN
1	S	402	GLN
1	T	382	GLN
1	V	382	GLN
1	V	452	ASN
1	W	382	GLN
1	Y	382	GLN
1	Z	250	ASN
1	Z	402	GLN
1	AA	382	GLN
1	BA	382	GLN
1	BA	452	ASN
1	CA	382	GLN
1	EA	382	GLN
1	FA	250	ASN
1	FA	402	GLN
1	GA	382	GLN
1	HA	382	GLN
1	HA	452	ASN
1	IA	382	GLN
1	KA	382	GLN
1	LA	250	ASN
1	LA	382	GLN
1	MA	382	GLN
1	NA	382	GLN
1	NA	452	ASN

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Mol	Chain	Res	Type
1	OA	382	GLN
1	QA	382	GLN
1	RA	250	ASN
1	RA	402	GLN
1	SA	382	GLN
1	TA	382	GLN
1	TA	452	ASN
1	UA	382	GLN
1	WA	382	GLN
1	XA	250	ASN
1	XA	382	GLN
1	YA	382	GLN
1	ZA	382	GLN
1	ZA	452	ASN
1	AB	382	GLN
1	CB	382	GLN
1	DB	250	ASN
1	DB	382	GLN
1	EB	382	GLN
1	FB	382	GLN
1	FB	452	ASN
1	GB	382	GLN
1	IB	382	GLN
1	JB	250	ASN
1	JB	382	GLN
1	KB	382	GLN
1	LB	382	GLN
1	LB	452	ASN
1	MB	382	GLN
1	OB	382	GLN
1	PB	250	ASN
1	PB	402	GLN
1	QB	382	GLN
1	RB	382	GLN
1	RB	452	ASN
1	SB	382	GLN

### 5.3.3 RNA

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 monosaccharides 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.

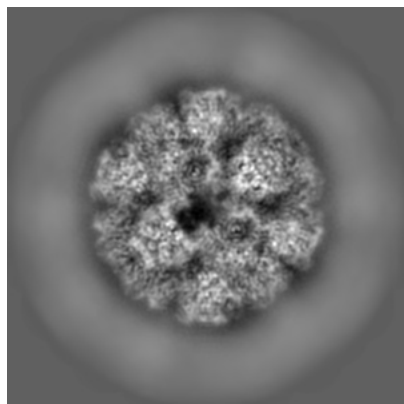
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11268. These allow visual inspection of the internal detail of the map and identification of artifacts.

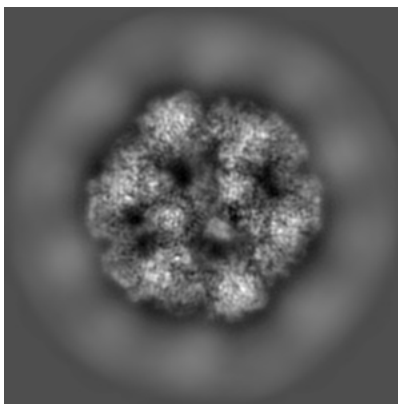
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

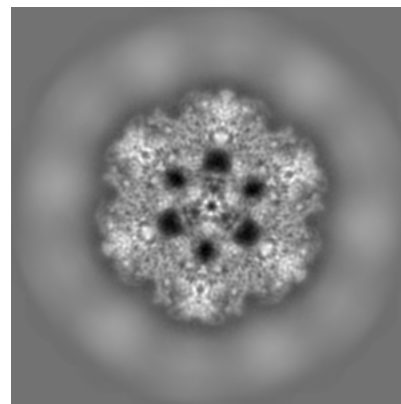
#### 6.1.1 Primary map



X

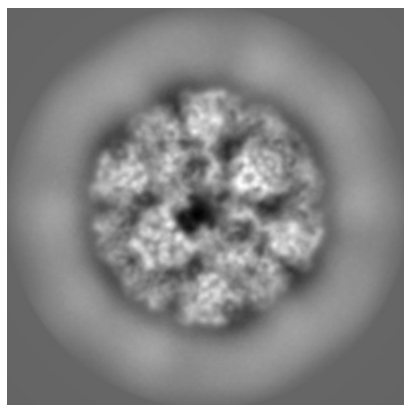


Y

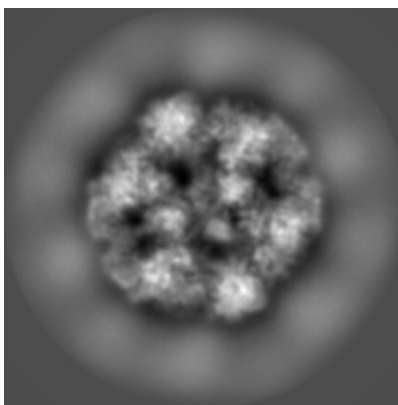


Z

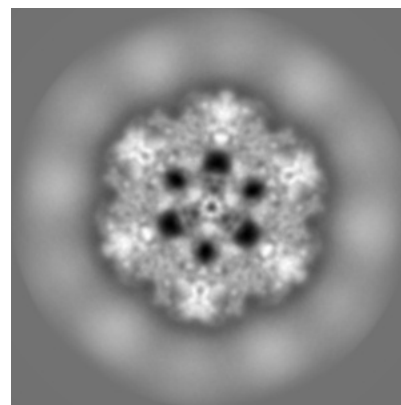
#### 6.1.2 Raw map



X



Y

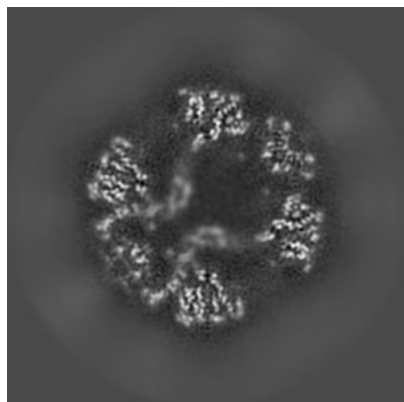


Z

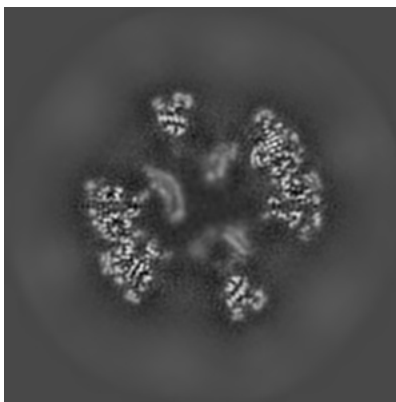
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

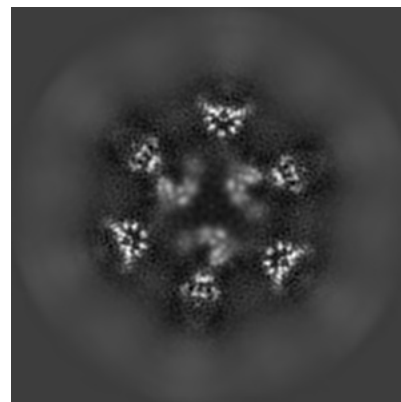
### 6.2.1 Primary map



X Index: 160

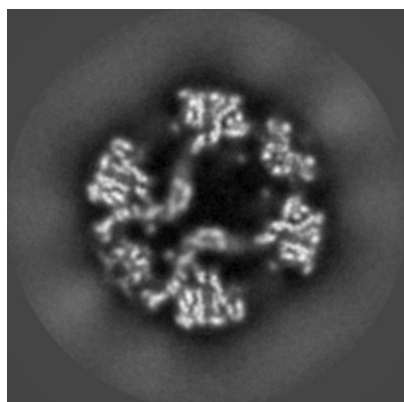


Y Index: 160

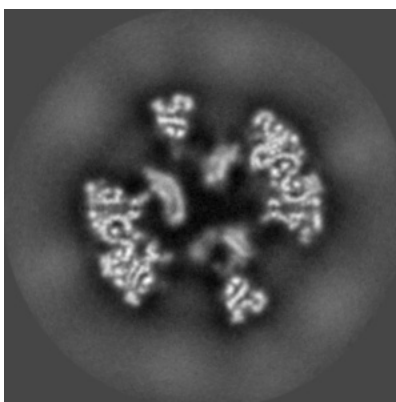


Z Index: 160

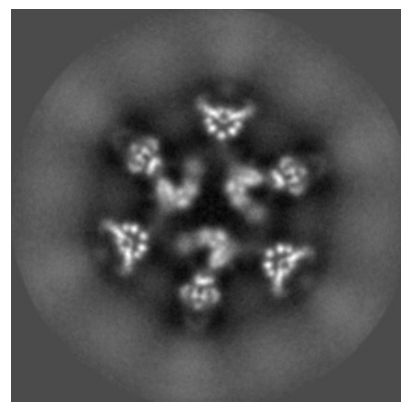
### 6.2.2 Raw map



X Index: 160



Y Index: 160

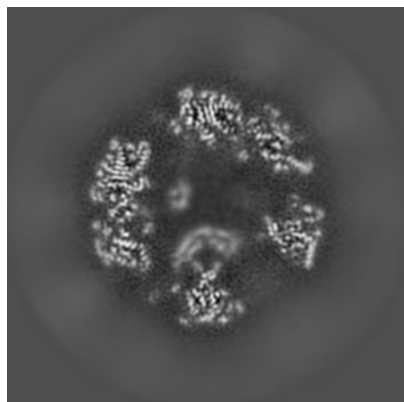


Z Index: 160

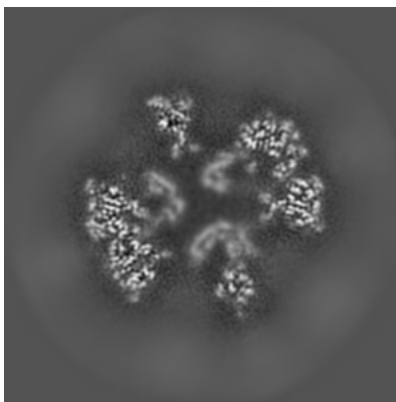
The images above show central slices of the map in three orthogonal directions.

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

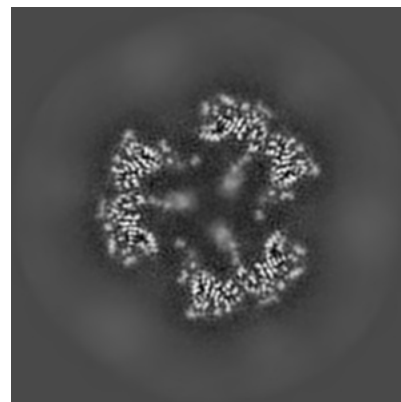
### 6.3.1 Primary map



X Index: 155

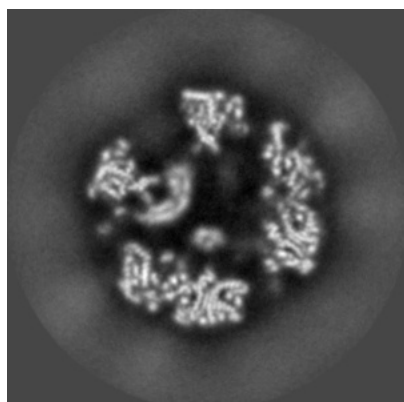


Y Index: 166

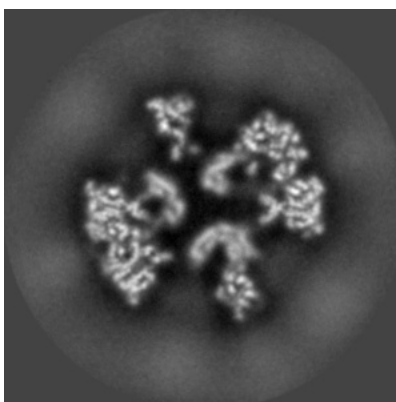


Z Index: 190

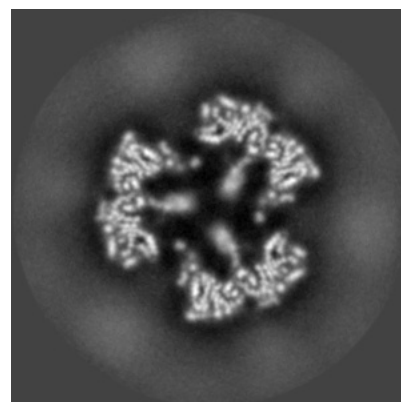
### 6.3.2 Raw map



X Index: 165



Y Index: 165

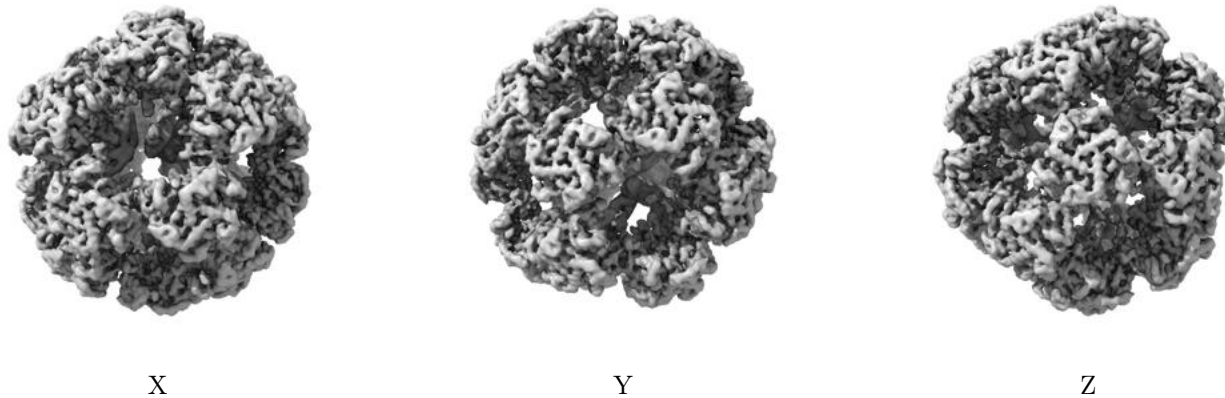


Z Index: 190

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

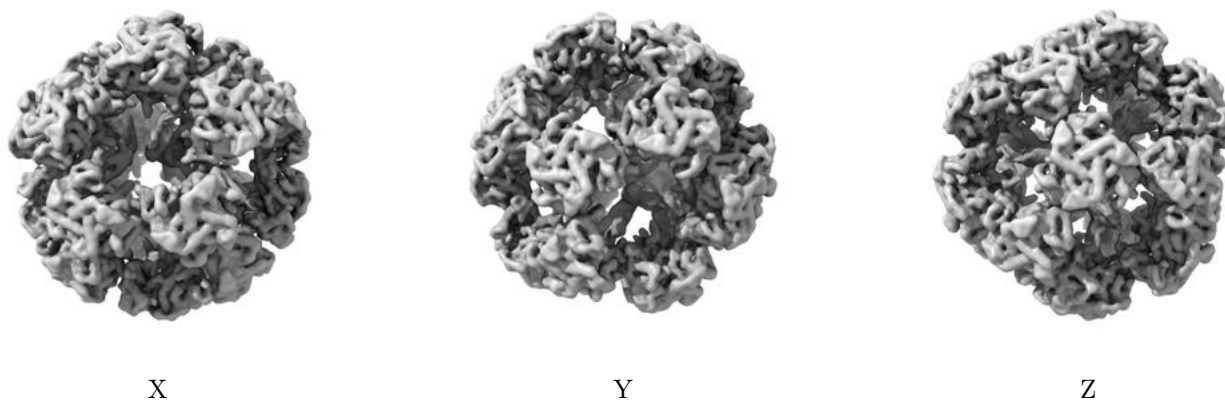
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0325. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

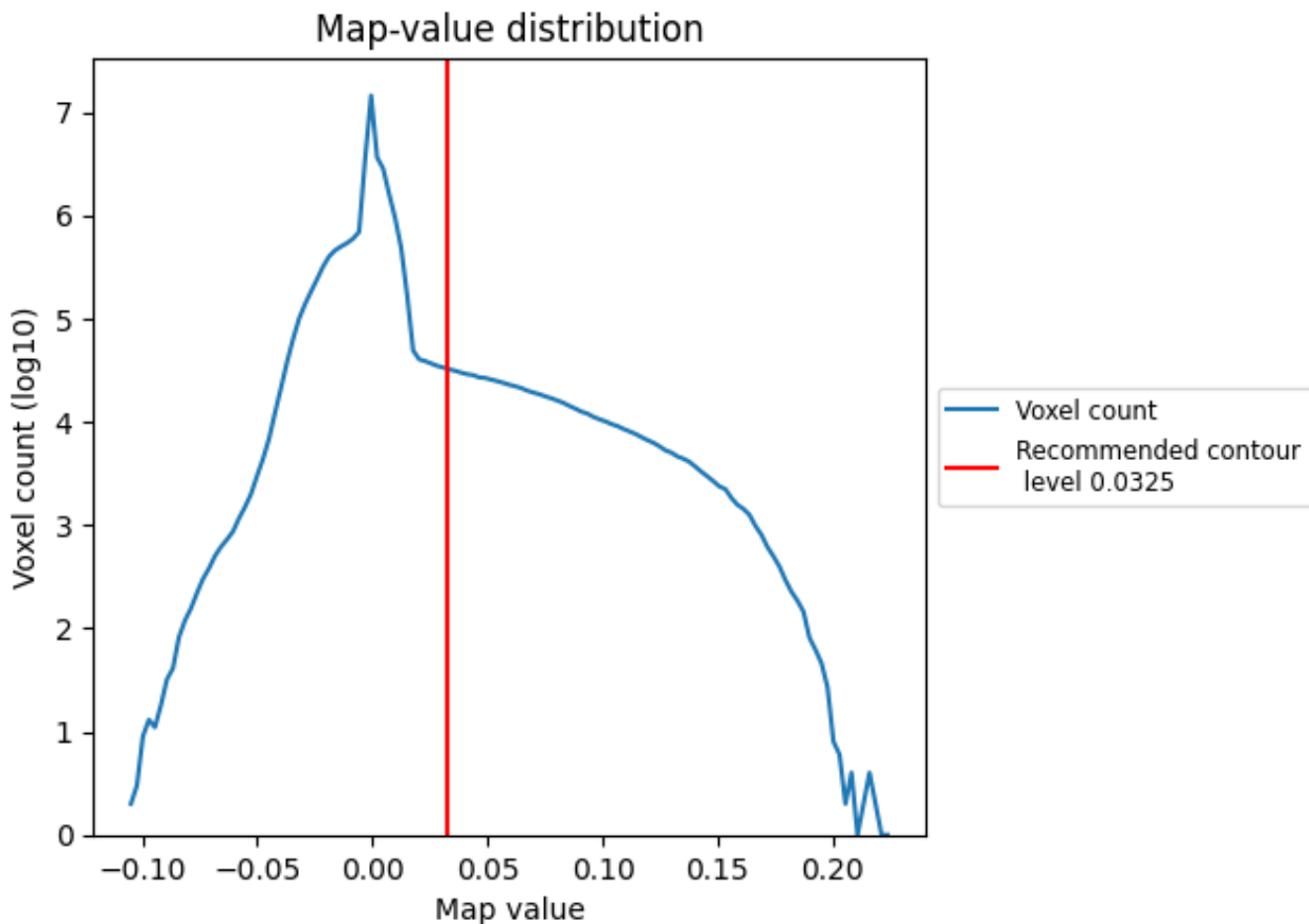
## 6.5 Mask visualisation [i](#)

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.

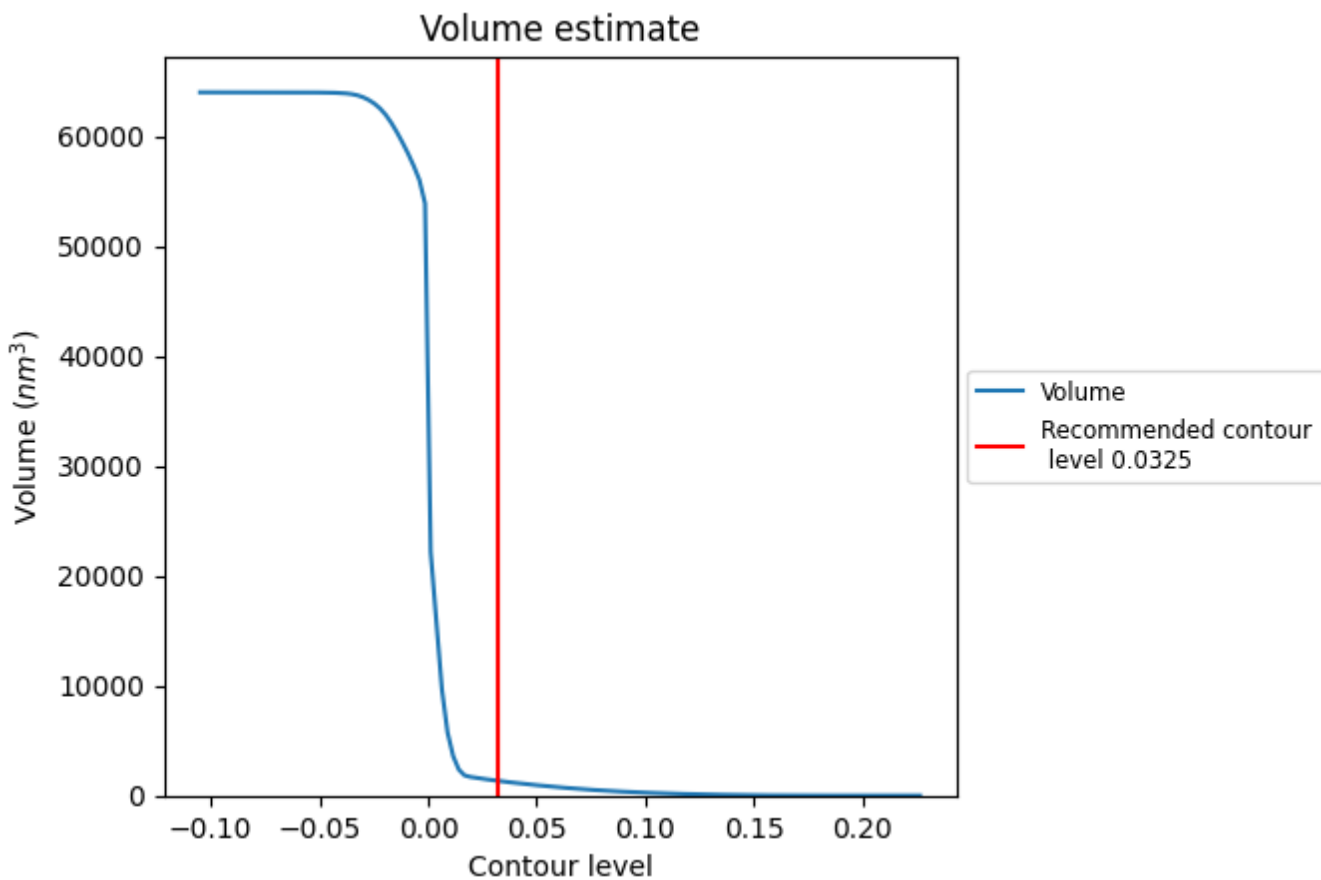
### 7.1 Map-value distribution [i](#)



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.



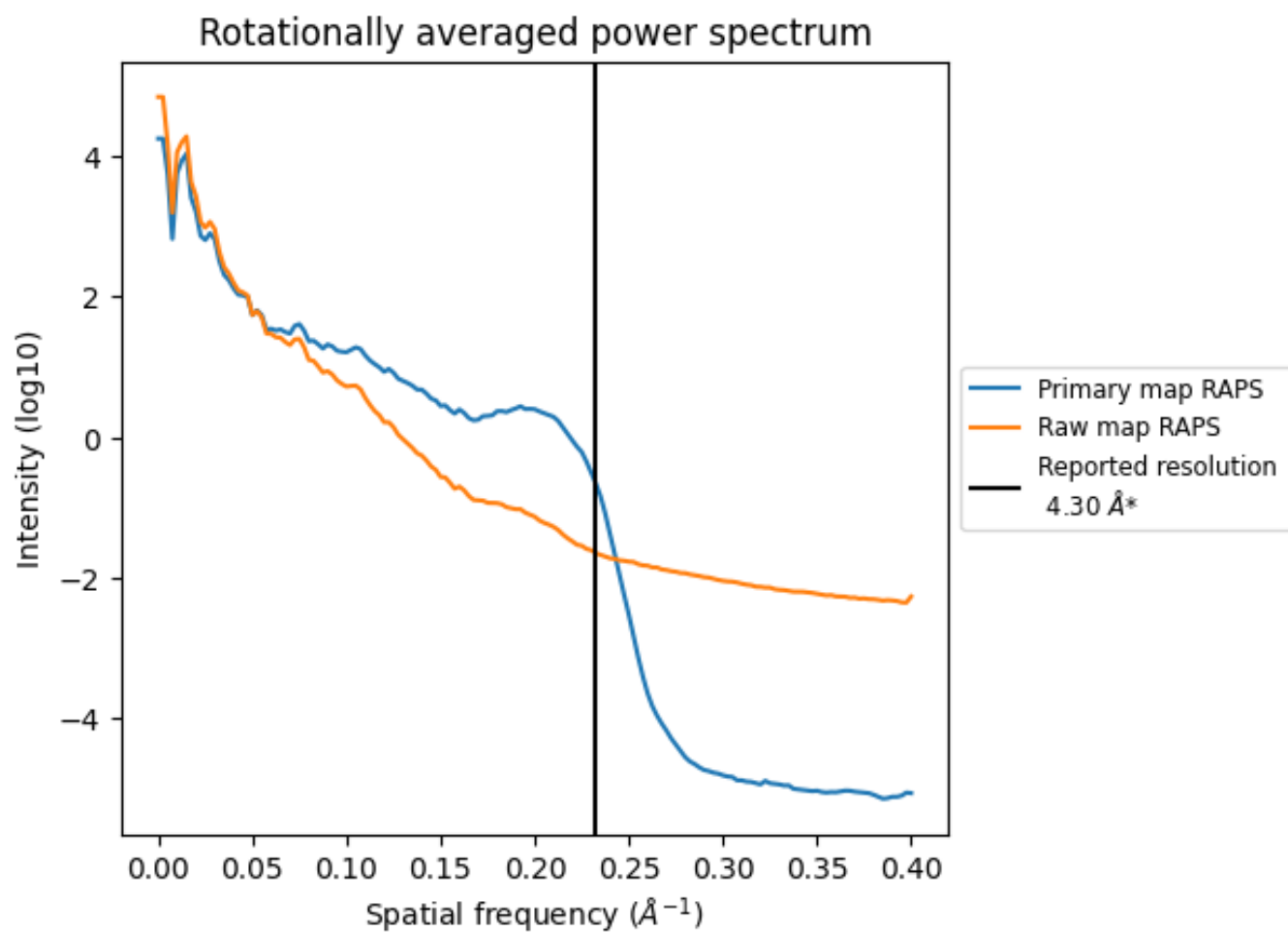
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1333 nm<sup>3</sup>; this corresponds to an approximate mass of 1204 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 i

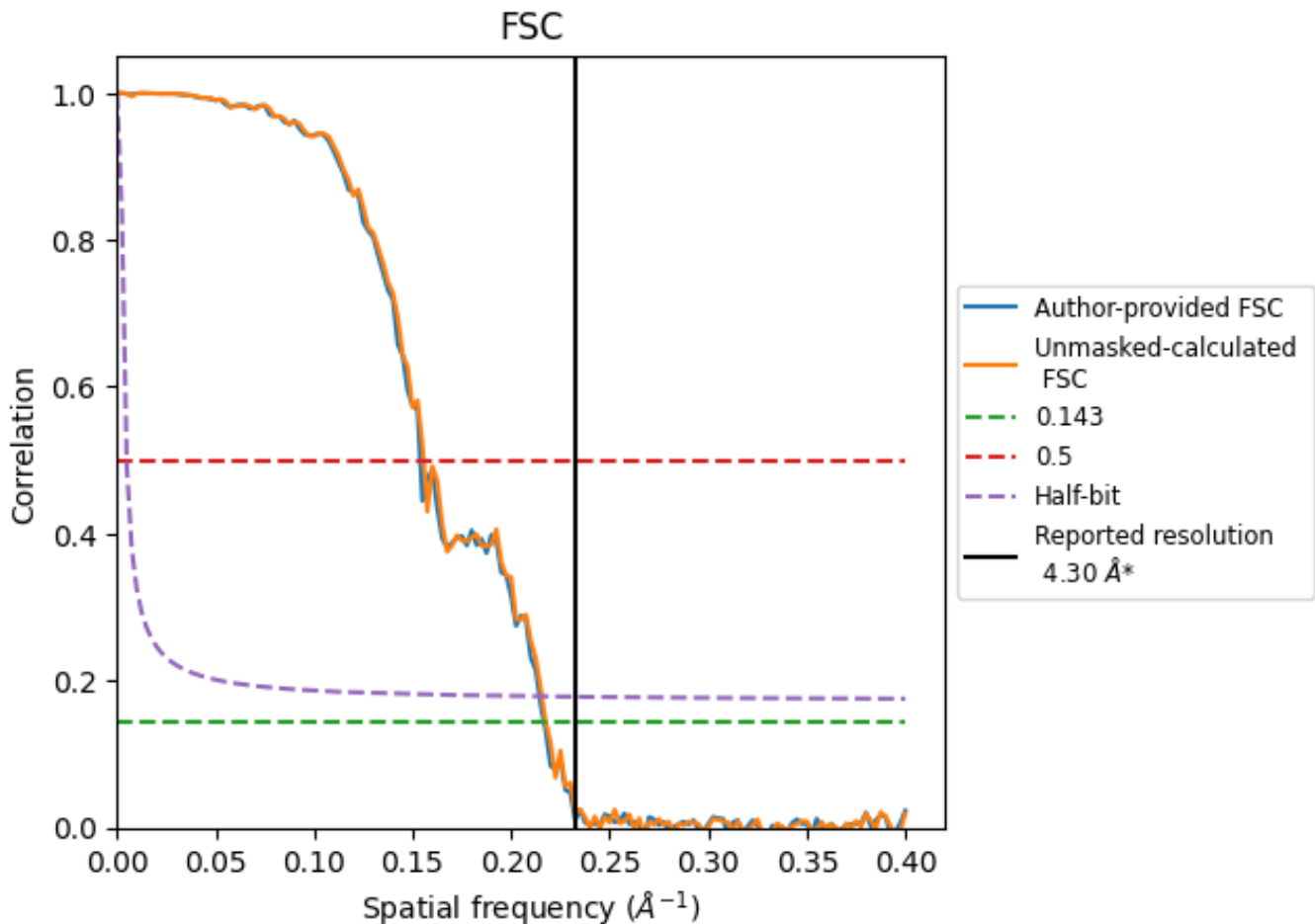


\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

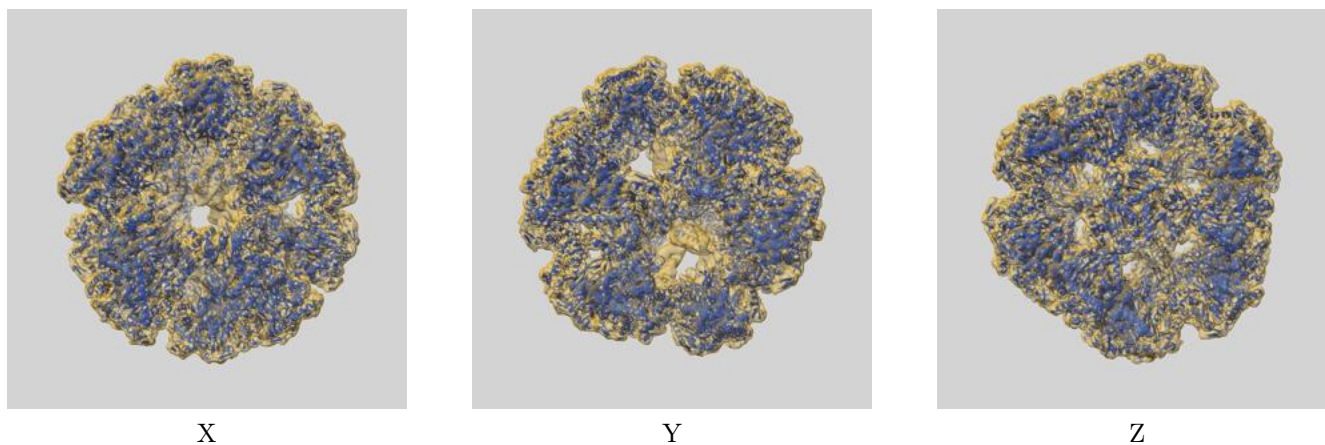
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.61	6.50	4.66
Unmasked-calculated*	4.60	6.43	4.64

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

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

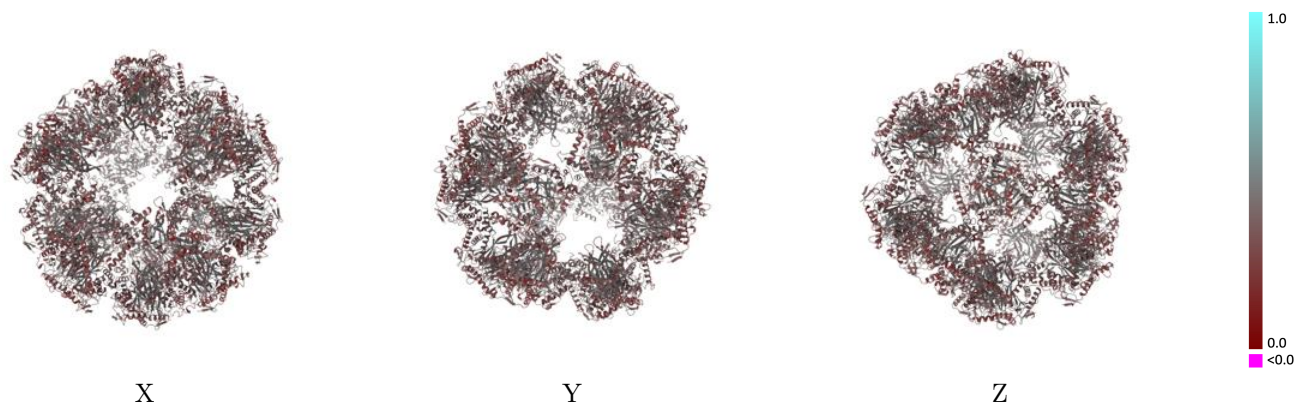
This section contains information regarding the fit between EMDB map EMD-11268 and PDB model 6ZLM. Per-residue inclusion information can be found in section 3 on page 10.

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



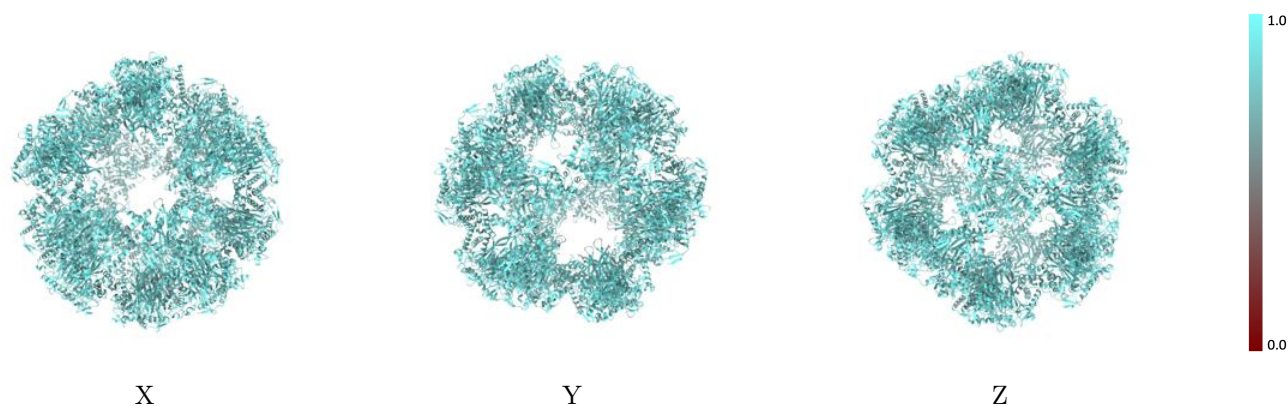
The images above show the 3D surface view of the map at the recommended contour level 0.0325 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



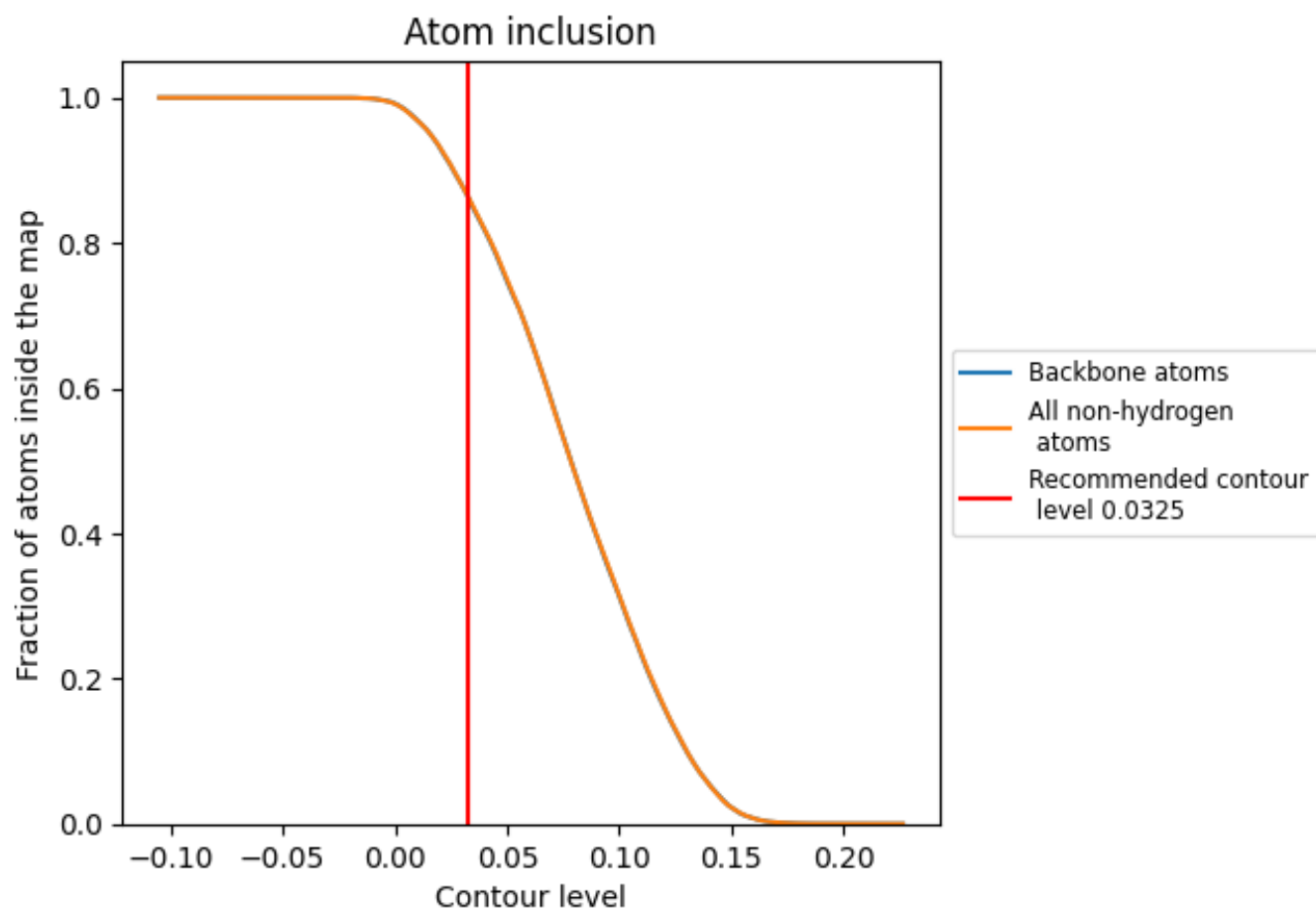
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0325).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.0325) and Q-score for the entire model and for each chain.













































































Chain	Atom inclusion	Q-score
All	 0.8648	 0.3730
A	 0.8720	 0.3790
AA	 0.8657	 0.3680
AB	 0.8709	 0.3740
B	 0.8674	 0.3740
BA	 0.8709	 0.3770
BB	 1.0000	 0.4400
C	 0.8674	 0.3720
CA	 0.8726	 0.3750
CB	 0.8645	 0.3740
D	 0.8691	 0.3760
DA	 1.0000	 0.4390
DB	 0.8720	 0.3730
E	 0.8738	 0.3750
EA	 0.8662	 0.3760
EB	 0.8709	 0.3720
F	 0.8691	 0.3780
FA	 0.8732	 0.3740
FB	 0.8697	 0.3760
G	 0.8703	 0.3730
GA	 0.8680	 0.3700
GB	 0.8691	 0.3740
H	 0.8668	 0.3720
HA	 0.8715	 0.3760
HB	 1.0000	 0.4410
I	 0.8715	 0.3770
IA	 0.8715	 0.3740
IB	 0.8709	 0.3740
J	 0.8738	 0.3730
JA	 1.0000	 0.4440
JB	 0.8761	 0.3760
K	 1.0000	 0.4480
KA	 0.8743	 0.3700
KB	 0.8668	 0.3720
L	 0.8715	 0.3700



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Chain	Atom inclusion	Q-score
LA	 0.8761	 0.3740
LB	 0.8674	 0.3750
M	 0.8772	 0.3770
MA	 0.8628	 0.3690
MB	 0.8668	 0.3710
N	 0.8610	 0.3710
NA	 0.8674	 0.3690
NB	 1.0000	 0.4300
O	 0.8662	 0.3710
OA	 0.8668	 0.3610
OB	 0.8639	 0.3750
P	 0.8691	 0.3650
PA	 1.0000	 0.4370
PB	 0.8691	 0.3720
Q	 1.0000	 0.4370
QA	 0.8616	 0.3710
QB	 0.8668	 0.3690
R	 0.8622	 0.3740
RA	 0.8662	 0.3680
RB	 0.8726	 0.3740
S	 0.8732	 0.3680
SA	 0.8726	 0.3660
SB	 0.8662	 0.3770
T	 0.8738	 0.3660
TA	 0.8674	 0.3680
TB	 1.0000	 0.4450
UA	 0.8668	 0.3730
V	 0.8715	 0.3690
VA	 0.9846	 0.4480
W	 0.8668	 0.3750
WA	 0.8709	 0.3740
X	 0.9846	 0.4430
XA	 0.8761	 0.3780
XC	 1.0000	 0.4470
Y	 0.8686	 0.3740
YA	 0.8674	 0.3730
Z	 0.8732	 0.3770
ZA	 0.8686	 0.3730