



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 01:48 AM UTC

PDB ID : 6ZLM / pdb_00006zlm
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

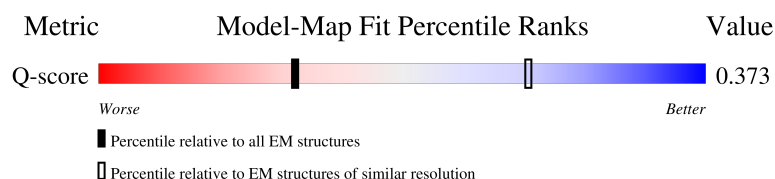
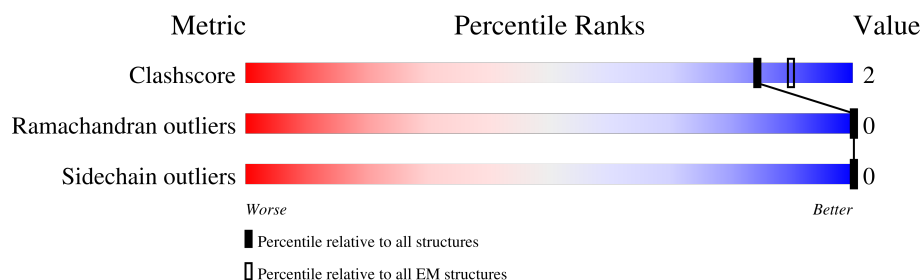
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 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.



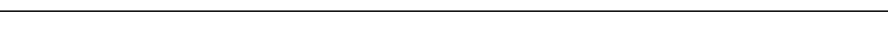
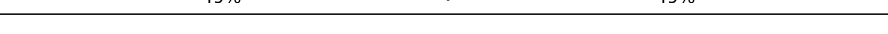
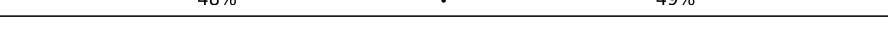
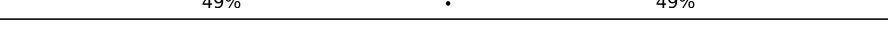
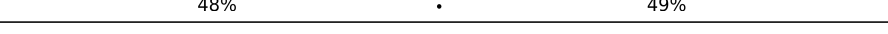
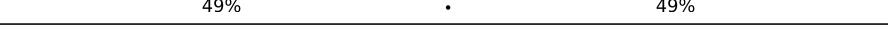
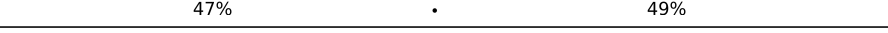
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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	458	
1	AA	458	
1	AB	458	
1	B	458	

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Mol	Chain	Length	Quality of chain
1	BA	458	
1	C	458	
1	CA	458	
1	CB	458	
1	D	458	
1	DB	458	
1	E	458	
1	EA	458	
1	EB	458	
1	F	458	
1	FA	458	
1	FB	458	
1	G	458	
1	GA	458	
1	GB	458	
1	H	458	
1	HA	458	
1	I	458	
1	IA	458	
1	IB	458	
1	J	458	
1	JB	458	
1	KA	458	
1	KB	458	
1	L	458	

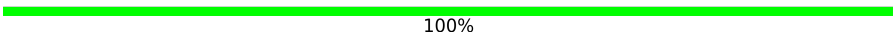
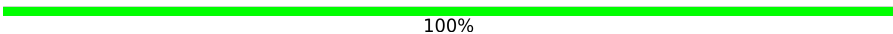
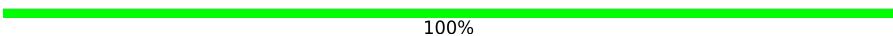
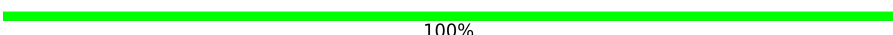
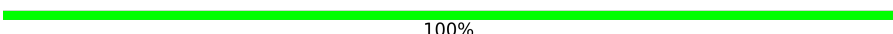
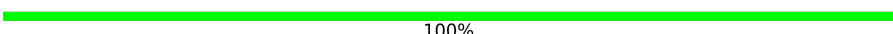
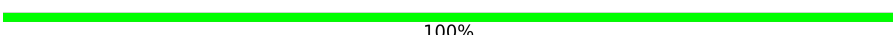
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Mol	Chain	Length	Quality of chain
1	LA	458	 48% . 49%
1	LB	458	 49% . 49%
1	M	458	 48% . 49%
1	MA	458	 48% . 49%
1	MB	458	 48% . 49%
1	N	458	 48% . 49%
1	NA	458	 48% . 49%
1	O	458	 49% . 49%
1	OA	458	 49% . 49%
1	OB	458	 49% . 49%
1	P	458	 49% . 49%
1	PB	458	 48% . 49%
1	QA	458	 48% . 49%
1	QB	458	 48% . 49%
1	R	458	 49% . 49%
1	RA	458	 48% . 49%
1	RB	458	 47% . 49%
1	S	458	 48% . 49%
1	SA	458	 47% . 49%
1	SB	458	 49% . 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%

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Mol	Chain	Length	Quality of chain
1	WA	458	 48% . 49%
1	XA	458	 48% . 49%
1	Y	458	 48% . 49%
1	YA	458	 48% . 49%
1	Z	458	 48% . 49%
1	ZA	458	 49% . 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

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
1	A	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		
1	B	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		
1	C	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		
1	D	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		
1	E	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		
1	F	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		
1	G	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		
1	H	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		
1	I	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		
1	J	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		
1	L	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		
1	M	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		
1	N	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		
1	O	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		
1	P	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		
1	R	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
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
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

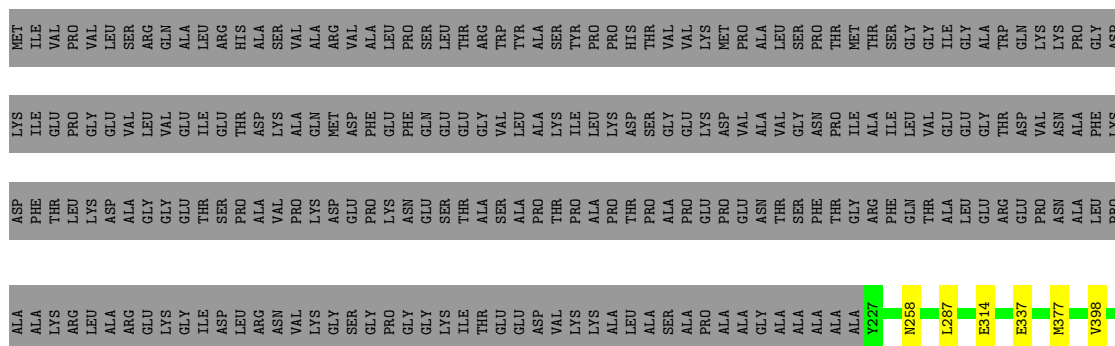
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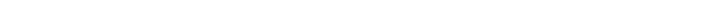
Mol	Chain	Residues	Atoms						AltConf	Trace
1	RB	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		
1	SB	232	Total	C	H	N	O	S	0	0
			3555	1110	1804	302	335	4		

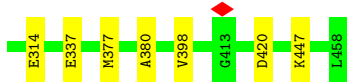
- Molecule 2 is a protein called Pyruvate dehydrogenase X component.

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		

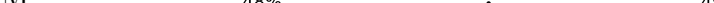


- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

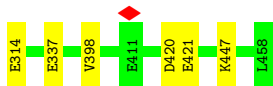
Chain L:  48% 1% 49%

[illegible]

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

Chain M:  48% . 49%

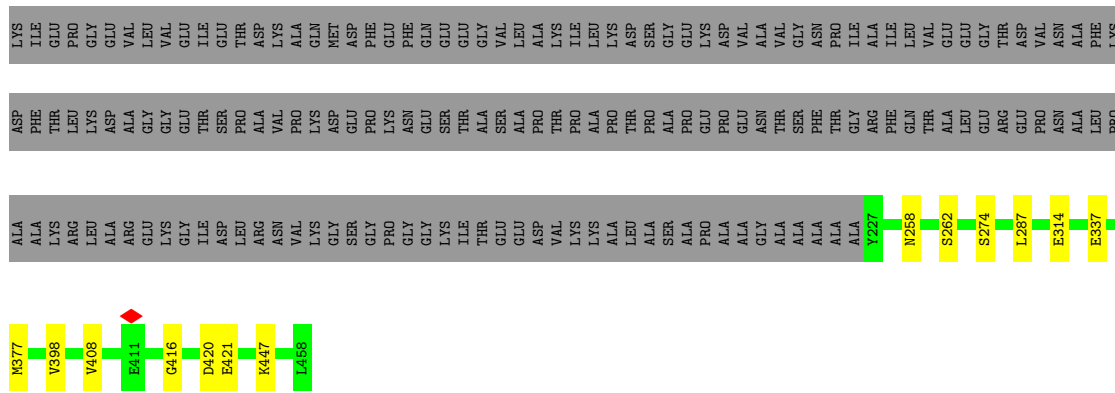
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LYS	LYS	PHE	ILE	ILE
ARG	ARG	THR	GLU	VAL
LEU	LEU	LEU	PRO	VAL
ALA	ALA	LYS	GLY	LEU
ARG	ARG	ASP	GLU	SER
GLU	GLU	GLY	VAL	ARG
LYS	LYS	GLY	VAL	GLN
GLY	GLY	GLU	GLU	ALA
ILE	ILE	THR	ILE	LEU
ASP	ASP	SER	GLU	ARG
LEU	LEU	PRO	THR	HIS
ARG	ARG	ALA	ASP	ALA
ASN	ASN	VAL	LYS	SER
VAL	VAL	PRO	ALA	VAL
LYS	LYS	LYS	GLN	ALA
GLY	GLY	ASP	MET	ARG
SER	SER	GLU	ASP	VAL
GLY	GLY	PRO	PHE	ALA
PRO	PRO	LYS	GLU	LEU
GLY	GLY	ASN	PHE	PRO
LYS	LYS	GLU	GLN	SER
ILE	ILE	SER	GLU	LEU
THR	THR	ALA	GLU	THR
GLU	GLU	SER	GLY	ARG
GLU	GLU	ALA	VAL	THR
GLU	GLU	ALA	LEU	TYR
ASP	ASP	PRO	ALA	ALA
VAL	VAL	THR	LYS	SER
LYS	LYS	PRO	ILE	TYR
LYS	LYS	ALA	LEU	PRO
ALA	ALA	PRO	LYS	PRO
LEU	LEU	THR	ASP	HIS
ALA	ALA	PRO	SER	THR
SER	SER	ALA	GLY	VAL
ALA	ALA	PRO	GLU	VAL
PRO	PRO	GLU	LYS	LYS
ALA	ALA	PRO	ASP	MET
ALA	ALA	GLU	VAL	PRO
GLY	GLY	ASN	ALA	ALA
ALA	ALA	THR	VAL	LEU
ALA	ALA	GLY	ILE	SER
ALA	ALA	ARG	ILE	GLY
Y227	Y227	GLN	LEU	ILE
E249	E249	THR	VAL	GLY
N258	N258	ALA	GLU	ILE
S262	S262	LEU	GLU	GLY
S274	S274	ARG	GLY	ALA
L287	L287	GLU	THR	TRP
L287	L287	GLU	ASP	GLN
G308	G308	PRO	VAL	LYS
		ALA	ASN	LYS
		ALA	ALA	PRO
		LEU	PHE	GLY
		PRO	TYR	ASP



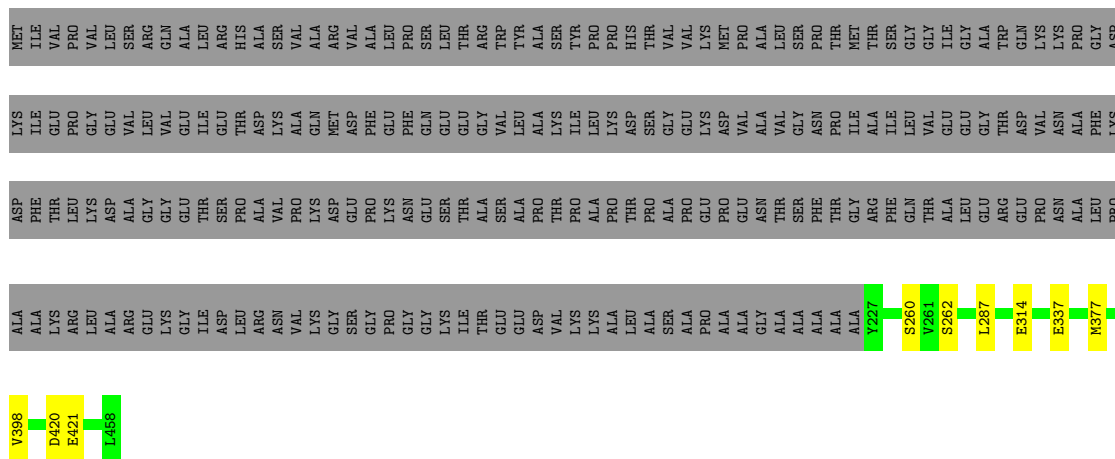
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain N: 48% 0 49%

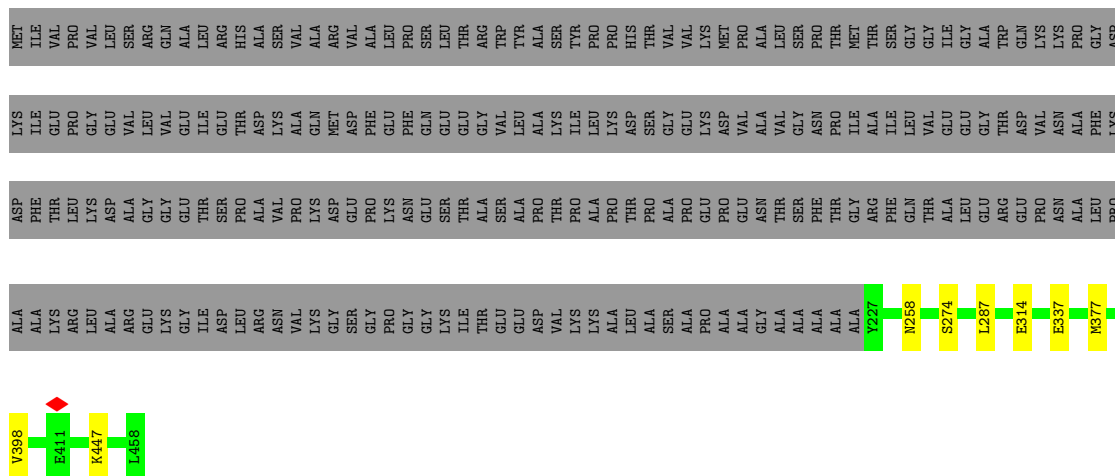
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-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



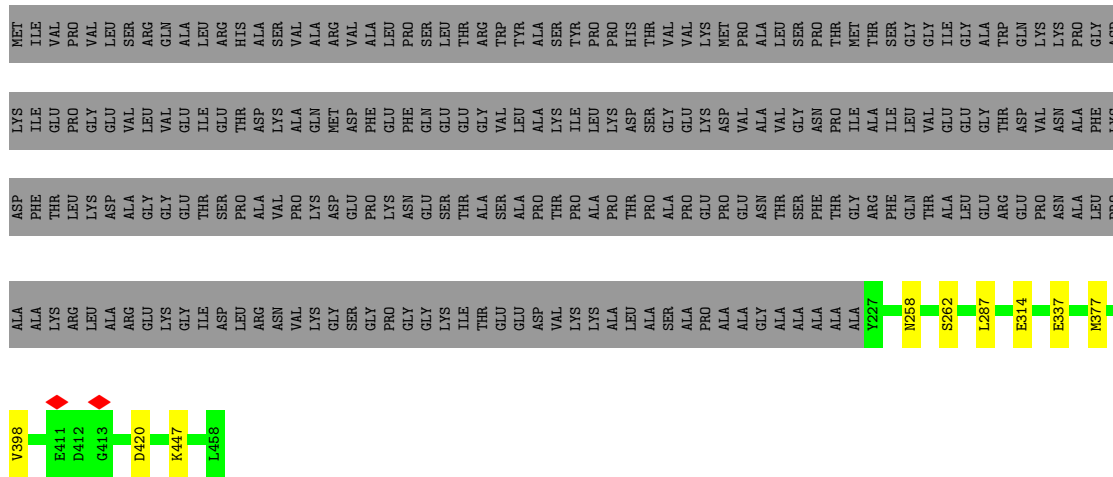
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



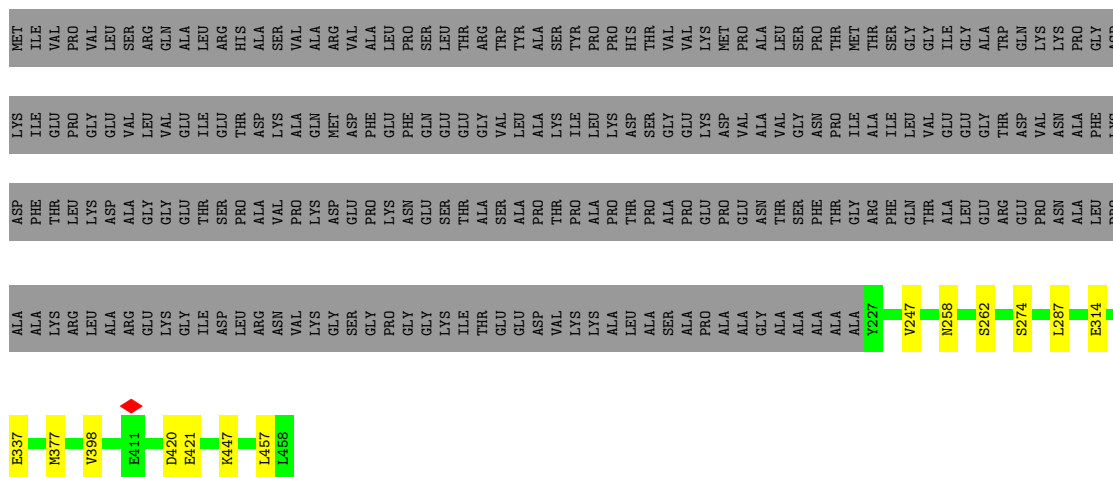
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



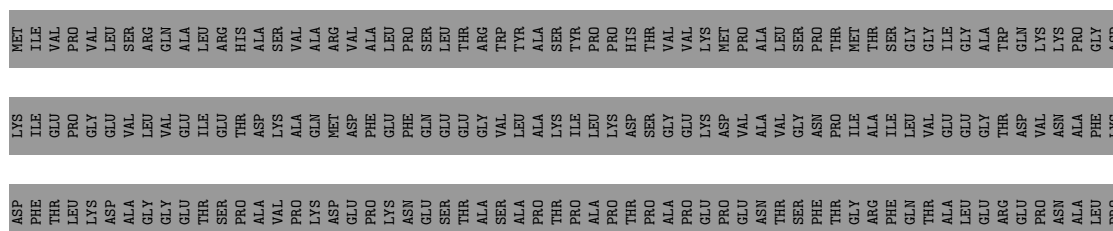
- Molecule 1: Dihydrolipoylysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



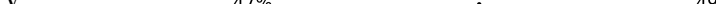
- Molecule 1: Dihydrolipoylysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



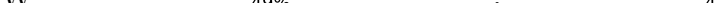
- Molecule 1: Dihydrolipoylysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

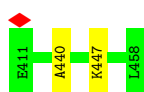


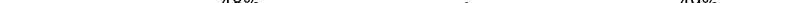


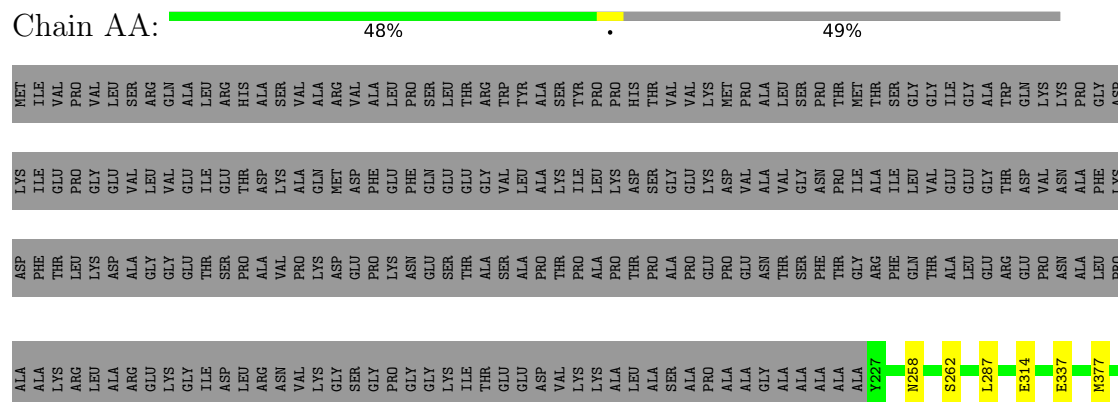
Chain V:  47% . 49%



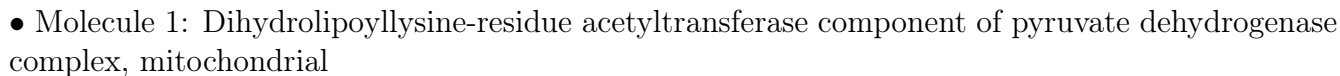
Chain W:  49% . 49%



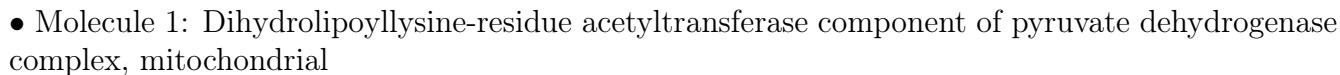
Chain Y:  48% 1% 49%



Frequency	Percentage
At least once a day	49%
Less than once a day	1%
Never	49%

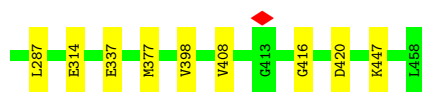


Category	Percentage
Very satisfied	49%
Satisfied	49%
Dissatisfied	2%



Response	Percentage
Yes	47%
No	1%
Don't know	49%

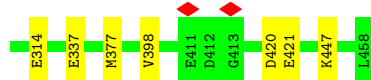




- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain LA: 48% 49%

MET	ILE	VAL	PRO	VAL	LEU	SER	ARG	GLN	LEU	ARG	HIS	ALA	SER	GLN	VAL	ALA	ARG	VAL	ALA	LEU	PRO	SER	GLN	THR	ARG	TRP	TYR	ALA	SER	TYR	PRO	PRO	HIS	THR	THR	VAL	VAL	LYS	MET	PRO	ALA	ALA	LEU	SER	PRO	THR	THR	ILE	GLY	GLY	ILE	GLY	ALA	TRP	GLN	LYS	LYS	PRO	GLY	ASP							
LYS	ILE	GLU	PRO	GLY	GLY	VAL	LEU	VAL	GLU	ILE	THR	ASP	THR	ASP	LYS	ALA	GLN	MET	ASP	PHE	GLU	PHE	ASN	GLY	SER	THR	ALA	GLY	ILE	LEU	PRO	LYS	ASP	THR	THR	ALA	PRO	GLU	LYS	ASP	VAL	VAL	ALA	LEU	GLY	ASN	PRO	THR	ILE	VAL	GLU	GLY	ALA	TRP	ASP	VAL	ASN	ALA	PHE	LYS							
ASP	PHE	THR	LEU	LYS	ASP	ALA	GLY	GLY	GLU	THR	PRO	ALA	VAL	VAL	LYS	LYS	ASP	GLU	PRO	PRO	GLY	ASN	GLY	SER	THR	ALA	THR	ALA	THR	PRO	ALA	ALA	THR	THR	ALA	PRO	GLU	PRO	GLU	ASN	GLY	THR	THR	PHE	THR	GLY	ARG	PHE	ILE	SER	THR	GLY	ILE	GLY	VAL	GLU	GLY	ALA	TRP	ASP	GLN	ASP	VAL	ASN	ALA	PHE	LYS
ALA	ALA	LYS	ARG	LEU	ALA	ARG	GLU	GLY	ILE	ILE	THR	SER	PRO	LEU	ARG	ASN	VAL	VAL	GLY	SER	PRO	GLY	GLY	LYS	THR	ILE	THR	GLU	GLY	ALA	ASP	VAL	LYS	LYS	ALA	PRO	ALA	ALA	PRO	ALA	GLY	ASN	THR	THR	ALA	ALA	ALA	Y227	E249	T257	N258	S262	L271	S274	L287												



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

Chain MA: 48% 49%

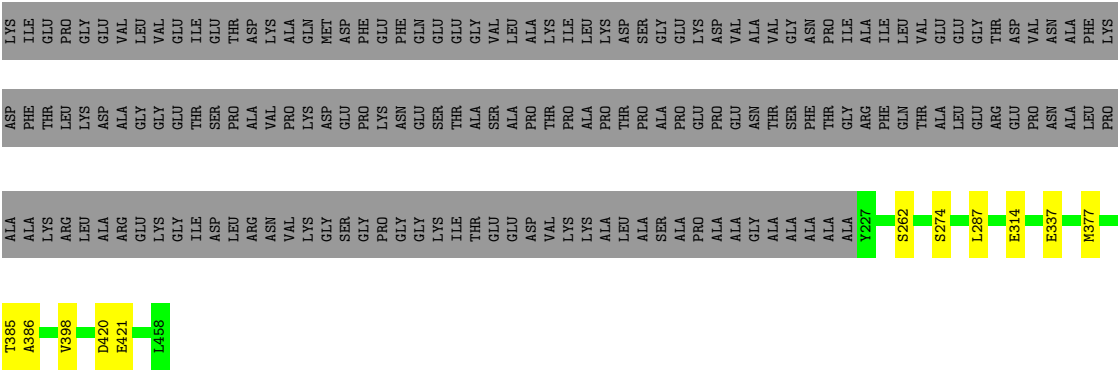
MET	ILE	VAL	PRO	VAL	LEU	SER	ARG	GLN	ALA	LEU	ARG	HIS	SER	VAL	ALA	ARG	VAL	ALA	LEU	PRO	SER	GLN	THR	ARG	TRP	TYR	ALA	SER	TYR	PRO	PRO	HIS	THR	THR	VAL	VAL	LYS	MET	PRO	ALA	ALA	LEU	SER	PRO	THR	THR	ILE	GLY	GLY	ILE	GLY	ALA	TRP	GLN	LYS	LYS	PRO	GLY	ASP																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
LYS	ILE	GLU	PRO	GLY	GLU	VAL	GLU	THR	GLN	MET	ASP	THR	ASP	LYS	ALA	GLN	MET	ASP	PHE	GLU	PHE	ASN	GLU	SER	THR	ALA	THR	ALA	LEU	PRO	LYS	ASP	THR	THR	ALA	GLY	GLU	LYS	ASP	VAL	VAL	VAL	VAL	GLY	ASN	PRO	THR	ILE	VAL	GLU	GLY	ALA	TRP	ASP	VAL	VAL	ASN	ALA	PHE	LYS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
ASP	PHE	THR	LEU	LYS	ASP	ALA	GLY	GLY	THR	THR	PRO	ALA	VAL	VAL	LYS	LYS	ASP	GLU	PRO	PRO	GLY	ASN	GLY	SER	THR	ALA	SER	GLU	GLY	ALA	PRO	LYS	ALA	PRO	THR	THR	ALA	PRO	GLU	PRO	GLU	ASN	THR	THR	ALA	ALA	ALA	ALA	Y227	N258	S262	L287	E314	E337	K377																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
ALA	ALA	LYS	ARG	LEU	ALA	ARG	GLU	GLY	ILE	ILE	THR	ASP	LEU	ARG	ASN	VAL	VAL	GLY	SER	GLY	PRO	GLY	GLY	LYS	THR	GLU	GLY	ASP	VAL	LYS	LYS	ALA	PRO	ALA	ALA	PRO	ALA	ALA	GLY	ASN	THR	THR	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA



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

Chain NA: 48% 49%

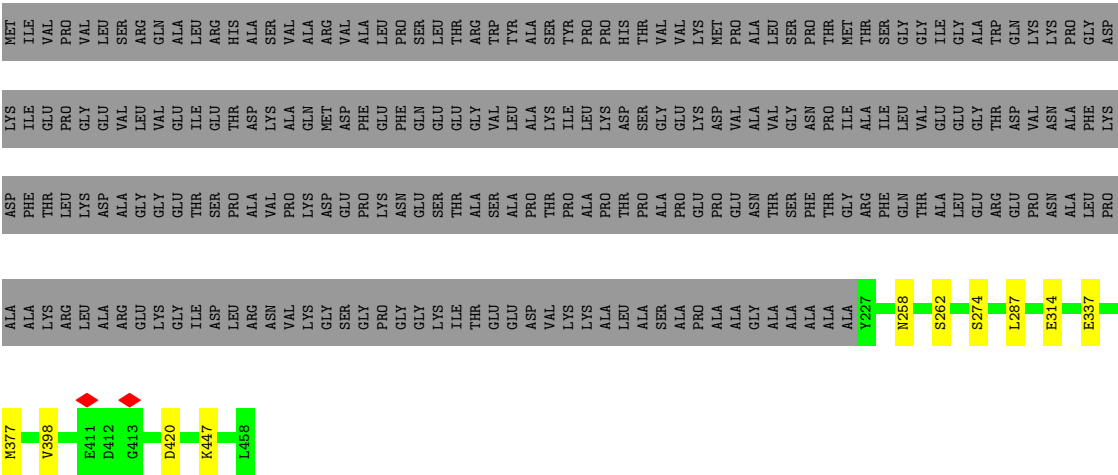
MET	ILE	VAL	PRO	VAL	LEU	SER	ARG	GLN	LEU	ARG	HIS	ALA	SER	GLN	VAL	ALA	ARG	VAL	ALA	LEU	PRO	SER	GLN	THR	ARG	TRP	TYR	ALA	SER	TYR	PRO	PRO	HIS	THR	THR	VAL	VAL	LYS	MET	PRO	ALA	ALA	LEU	SER	PRO	THR	THR	ILE	GLY	GLY	ILE	GLY	ALA	TRP	GLN	LYS	LYS	PRO	GLY	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



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



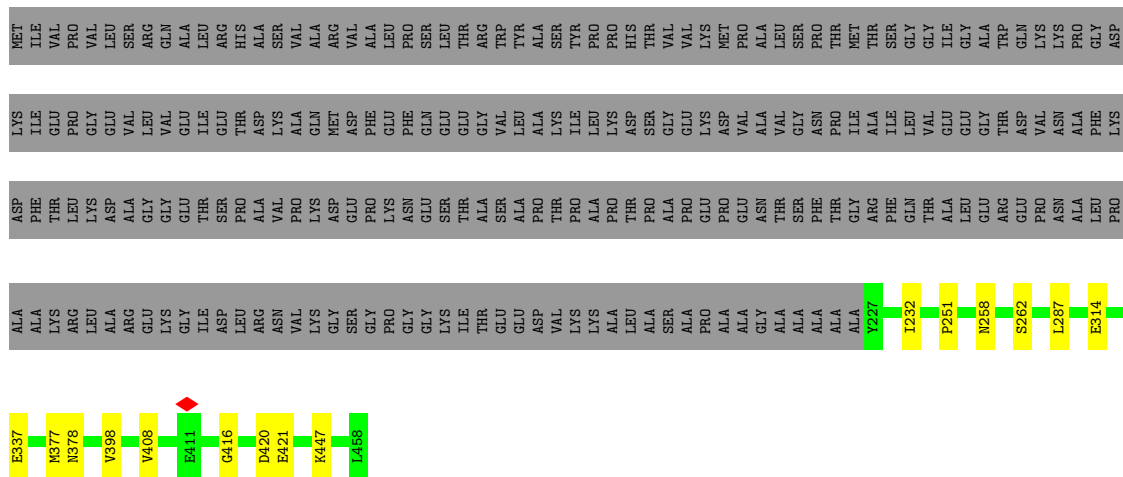
● Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



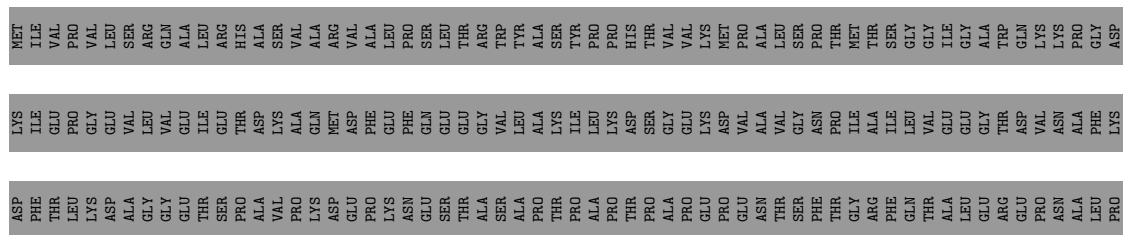
- Molecule 1: Dihydrolipoylysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



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

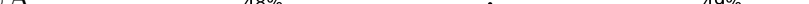


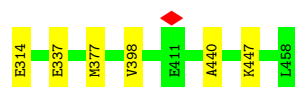
- Molecule 1: Dihydrolipoylysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial





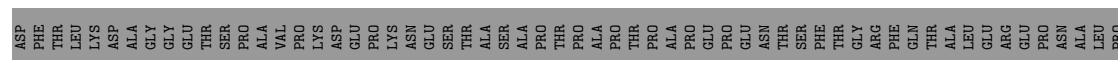
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain UA:  48% . 49%

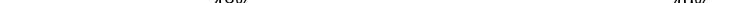


- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain WA: 48% 49%

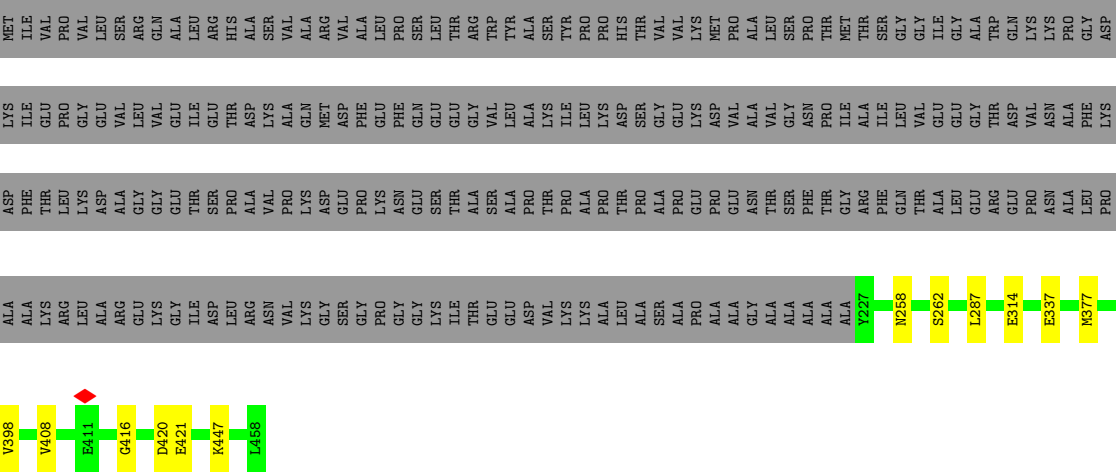


- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

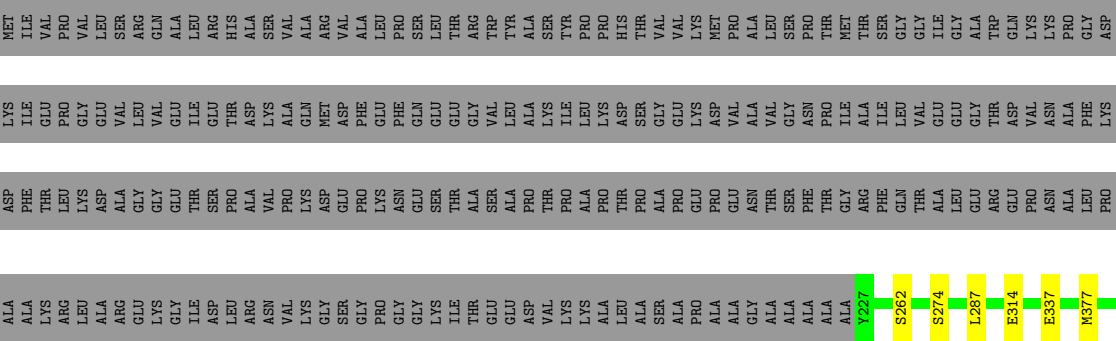
Chain XA: 



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



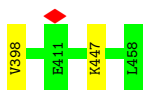
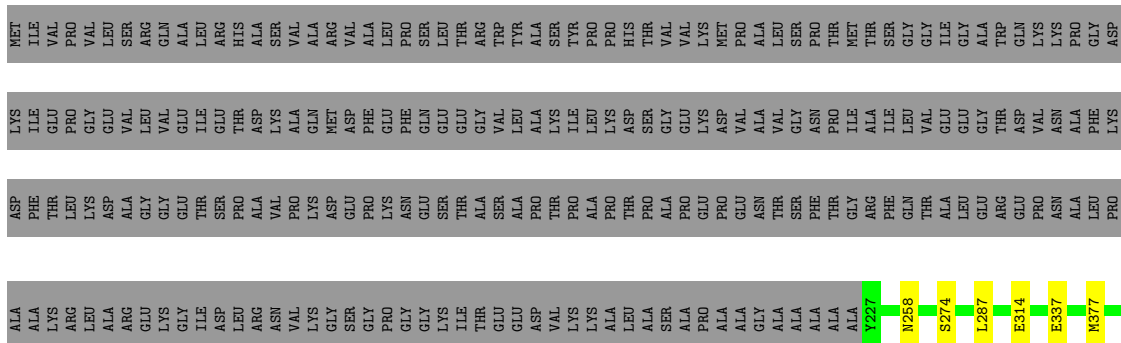
● Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial





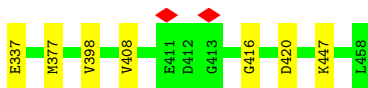
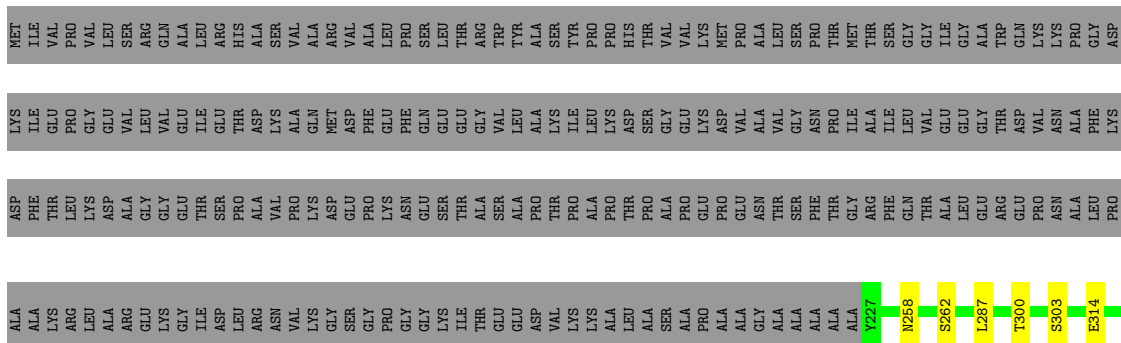
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain AB:

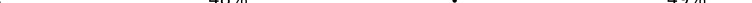


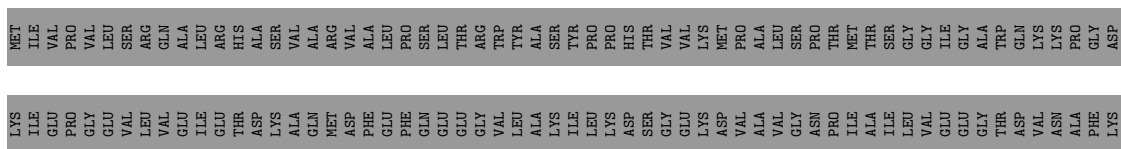
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain CB: 48% . 49%

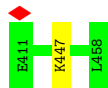


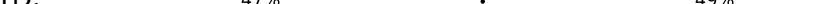
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial

Chain DB:  48% . 49%



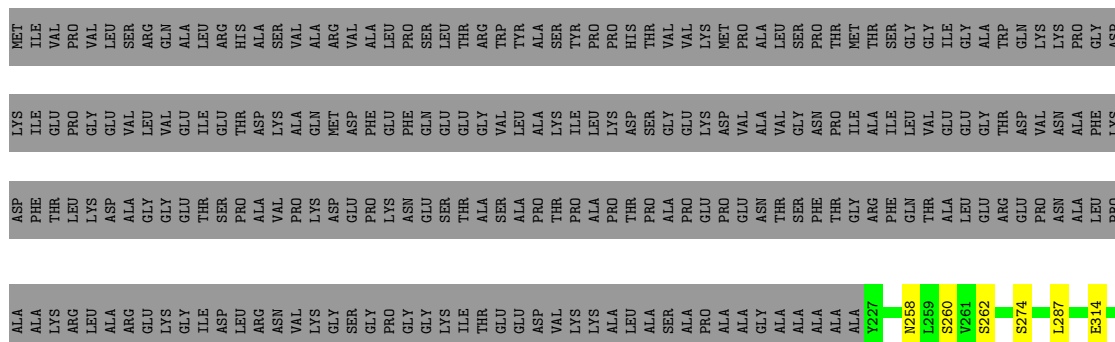
Response	Percentage
Doing a good job	49%
Not doing a good job	1%
Don't know	49%

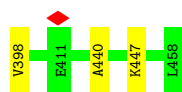


- Chain IB:  47% . 49%



- Chain JB:  48% 0 49%





- 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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/1779	0.33	0/2413
1	AA	0.24	0/1779	0.34	0/2413
1	AB	0.24	0/1779	0.34	0/2413
1	B	0.24	0/1779	0.33	0/2413
1	BA	0.24	0/1779	0.33	0/2413
1	C	0.24	0/1779	0.34	0/2413
1	CA	0.24	0/1779	0.34	0/2413
1	CB	0.24	0/1779	0.33	0/2413
1	D	0.24	0/1779	0.33	0/2413
1	DB	0.24	0/1779	0.33	0/2413
1	E	0.24	0/1779	0.34	0/2413
1	EA	0.24	0/1779	0.33	0/2413
1	EB	0.24	0/1779	0.34	0/2413
1	F	0.24	0/1779	0.33	0/2413
1	FA	0.24	0/1779	0.33	0/2413
1	FB	0.24	0/1779	0.33	0/2413
1	G	0.24	0/1779	0.33	0/2413
1	GA	0.24	0/1779	0.34	0/2413
1	GB	0.24	0/1779	0.35	0/2413
1	H	0.24	0/1779	0.34	0/2413
1	HA	0.24	0/1779	0.33	0/2413
1	I	0.24	0/1779	0.33	0/2413
1	IA	0.24	0/1779	0.35	0/2413
1	IB	0.24	0/1779	0.33	0/2413
1	J	0.24	0/1779	0.35	0/2413
1	JB	0.24	0/1779	0.33	0/2413
1	KA	0.24	0/1779	0.33	0/2413
1	KB	0.24	0/1779	0.34	0/2413
1	L	0.24	0/1779	0.33	0/2413
1	LA	0.24	0/1779	0.33	0/2413
1	LB	0.24	0/1779	0.33	0/2413
1	M	0.24	0/1779	0.33	0/2413
1	MA	0.24	0/1779	0.34	0/2413
1	MB	0.24	0/1779	0.34	0/2413

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	N	0.24	0/1779	0.34	0/2413
1	NA	0.24	0/1779	0.33	0/2413
1	O	0.24	0/1779	0.33	0/2413
1	OA	0.24	0/1779	0.34	0/2413
1	OB	0.24	0/1779	0.33	0/2413
1	P	0.24	0/1779	0.34	0/2413
1	PB	0.24	0/1779	0.33	0/2413
1	QA	0.24	0/1779	0.33	0/2413
1	QB	0.24	0/1779	0.34	0/2413
1	R	0.24	0/1779	0.33	0/2413
1	RA	0.24	0/1779	0.33	0/2413
1	RB	0.24	0/1779	0.33	0/2413
1	S	0.24	0/1779	0.33	0/2413
1	SA	0.24	0/1779	0.34	0/2413
1	SB	0.24	0/1779	0.34	0/2413
1	T	0.24	0/1779	0.34	0/2413
1	TA	0.24	0/1779	0.33	0/2413
1	UA	0.24	0/1779	0.34	0/2413
1	V	0.24	0/1779	0.33	0/2413
1	W	0.24	0/1779	0.34	0/2413
1	WA	0.24	0/1779	0.33	0/2413
1	XA	0.24	0/1779	0.33	0/2413
1	Y	0.24	0/1779	0.33	0/2413
1	YA	0.24	0/1779	0.34	0/2413
1	Z	0.24	0/1779	0.33	0/2413
1	ZA	0.24	0/1779	0.33	0/2413
All	All	0.24	0/106740	0.33	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

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	7	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	8	0
1	C	1751	1804	1811	9	0
1	CA	1751	1804	1811	6	0
1	CB	1751	1804	1811	8	0
1	D	1751	1804	1811	9	0
1	DB	1751	1804	1811	11	0
1	E	1751	1804	1811	5	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	5	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	12	0
1	J	1751	1804	1811	5	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	11	0
1	LA	1751	1804	1811	11	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	8	0
1	N	1751	1804	1811	10	0
1	NA	1751	1804	1811	8	0
1	O	1751	1804	1811	7	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	6	0
1	RA	1751	1804	1811	10	0
1	RB	1751	1804	1811	14	0
1	S	1751	1804	1811	11	0
1	SA	1751	1804	1811	13	0
1	SB	1751	1804	1811	8	0
1	T	1751	1804	1811	14	0
1	TA	1751	1804	1811	15	0
1	UA	1751	1804	1811	12	0
1	V	1751	1804	1811	16	0
1	W	1751	1804	1811	7	0
1	WA	1751	1804	1811	8	0
1	XA	1751	1804	1811	9	0
1	Y	1751	1804	1811	9	0
1	YA	1751	1804	1811	9	0
1	Z	1751	1804	1811	8	0
1	ZA	1751	1804	1811	7	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	492	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 (492) 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:I:262:SER:OG	1:I:420:ASP:OD1	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IB:262:SER:OG	1:IB:420:ASP:OD1	2.21	0.55
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:V:262:SER:OG	1:V:420:ASP:OD1	2.23	0.54
1:ZA:262:SER:OG	1:ZA:420:ASP:OD1	2.23	0.53
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: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:G:274:SER:O	1:G:274:SER:OG	2.27	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:TA:274:SER:O	1:TA:274:SER:OG	2.28	0.52
1:H:251:PRO:HB3	1:RA:247:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:274:SER:O	1:B:274:SER:OG	2.27	0.51
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:L:257:THR:OG1	1:IB:380:ALA:O	2.27	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: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:M:274:SER:O	1:M:274:SER:OG	2.27	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:L:249:GLU:OE1	1:IB:244:LYS:NZ	2.41	0.49
1:V:378:ASN:ND2	1:RB:440:ALA:HB1	2.28	0.49
1:RB:274:SER:O	1:RB:274:SER:OG	2.28	0.48
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:TA:249:GLU:OE1	1:RB:244:LYS:NZ	2.46	0.47
1:V:274:SER:O	1:V:274:SER:OG	2.28	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:C:408:VAL:O	1:C:416:GLY:N	2.48	0.46
1:T:380:ALA:O	1:UA:257:THR:OG1	2.26	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:T:230:VAL:C	1:UA:309:VAL:HG23	2.40	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:ZA:274:SER:O	1:ZA:274:SER:OG	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:377:MET:SD	1:FB:377:MET:N	2.89	0.45
1:V:232:ILE:HD12	1:RB:308:GLY:HA2	1.99	0.45
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:LA:257:THR:OG1	1:MB:380:ALA:O	2.31	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: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: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: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: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
1:JB:377:MET:SD	1:JB:377:MET:N	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:JB:260:SER:OG	1:JB:420:ASP:OD2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:274:SER:O	1:D:274:SER:OG	2.28	0.42
1:E:258:ASN:O	1:E:447:LYS:NZ	2.51	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:PB:258:ASN:O	1:PB:447:LYS:NZ	2.52	0.42
1:LA:420:ASP:OD1	1:LA:421:GLU:N	2.52	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:FA:258:ASN:O	1:FA:447:LYS:NZ	2.52	0.42
1:FB:300:THR:O	1:FB:303:SER:OG	2.30	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
1:MA:258:ASN:OD1	1:MA:258:ASN:N	2.53	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	1:YA:258:ASN:N	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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 ⓘ

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	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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 (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	378	ASN
1	D	452	ASN
1	G	382	GLN
1	H	284	ASN
1	I	452	ASN
1	N	378	ASN
1	O	452	ASN
1	V	452	ASN
1	BA	452	ASN
1	HA	452	ASN
1	LA	378	ASN
1	MA	378	ASN
1	NA	452	ASN
1	TA	452	ASN
1	XA	378	ASN
1	ZA	452	ASN
1	DB	382	GLN
1	FB	452	ASN
1	JB	378	ASN

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Mol	Chain	Res	Type
1	KB	378	ASN
1	LB	452	ASN
1	PB	382	GLN
1	RB	452	ASN
1	SB	378	ASN

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.

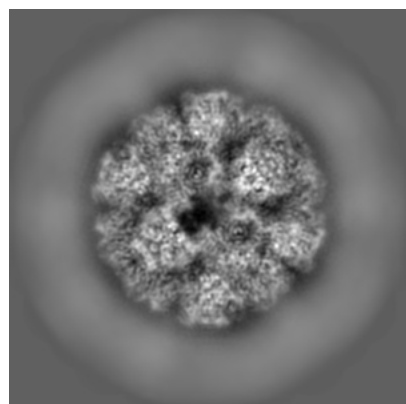
6 Map visualisation [i](#)

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

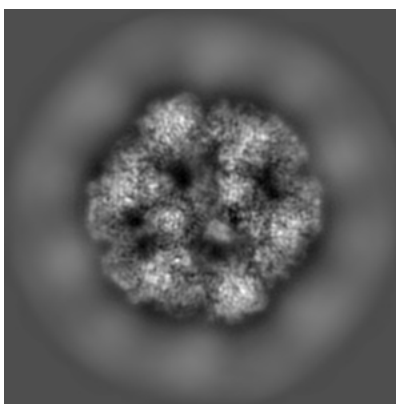
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

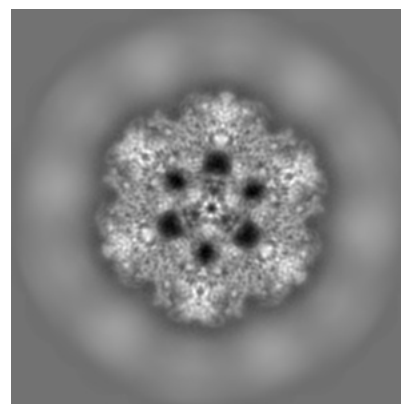
6.1.1 Primary map



X

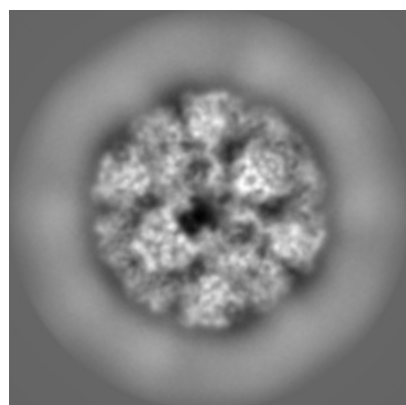


Y

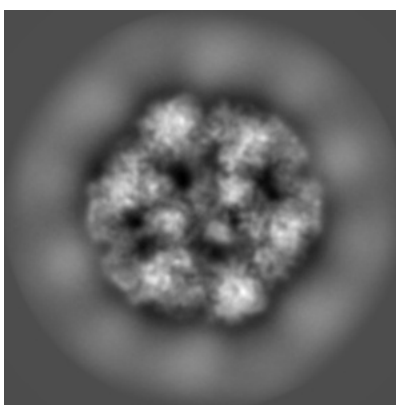


Z

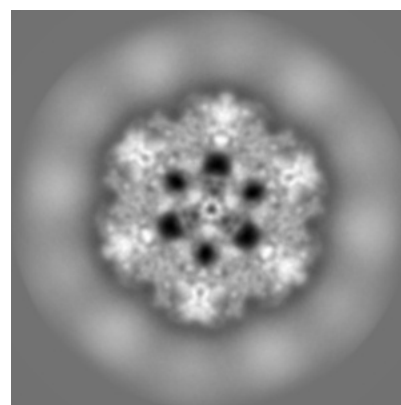
6.1.2 Raw map



X



Y

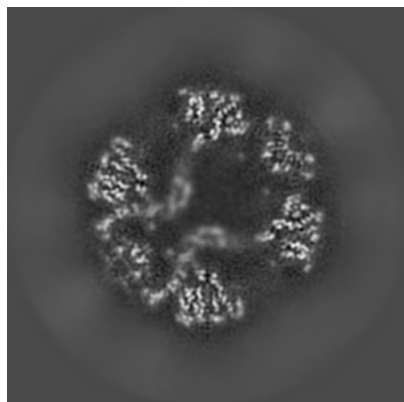


Z

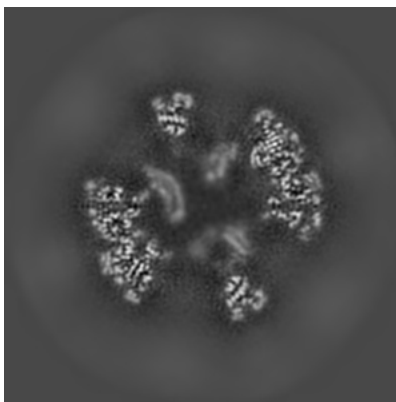
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

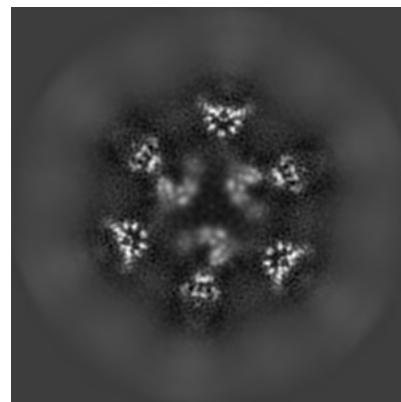
6.2.1 Primary map



X Index: 160

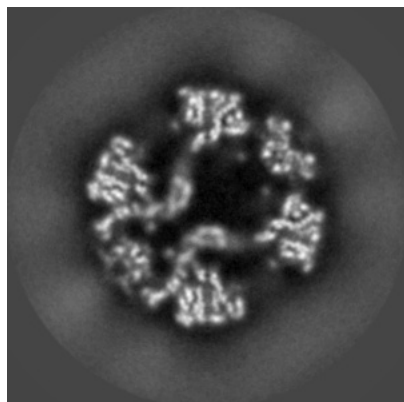


Y Index: 160

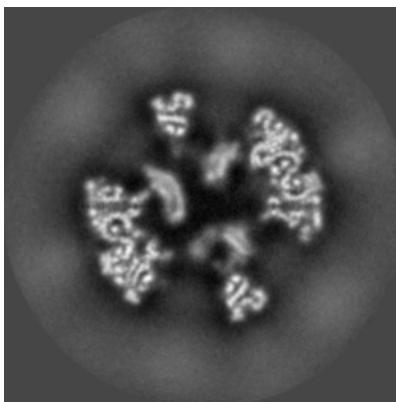


Z Index: 160

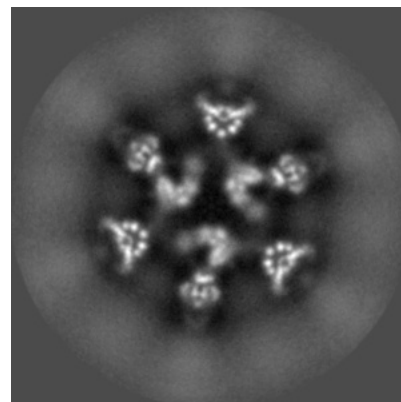
6.2.2 Raw map



X Index: 160



Y Index: 160

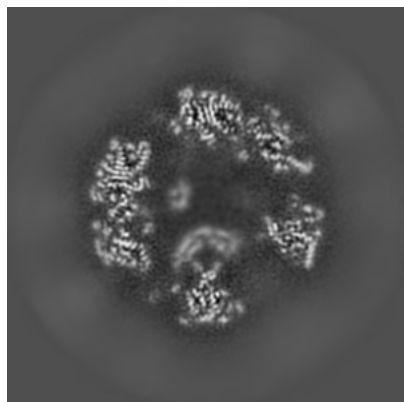


Z Index: 160

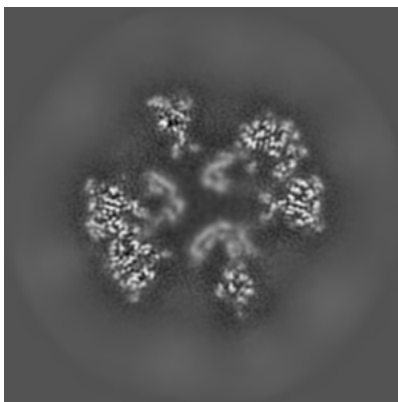
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

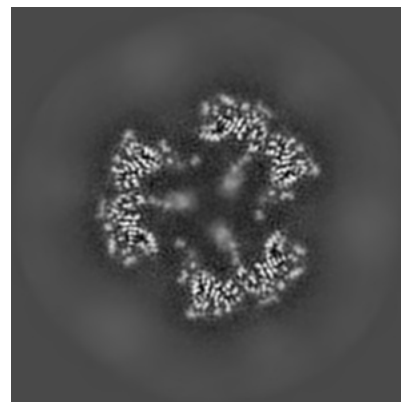
6.3.1 Primary map



X Index: 155

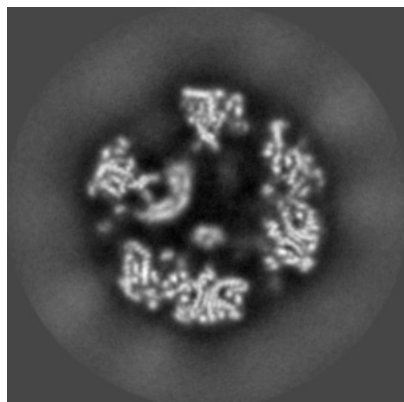


Y Index: 166

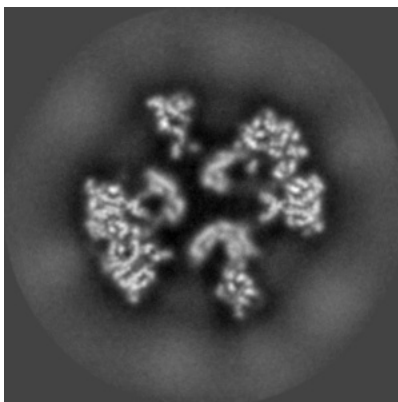


Z Index: 190

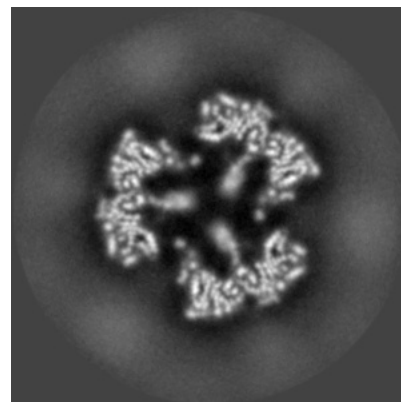
6.3.2 Raw map



X Index: 165



Y Index: 165

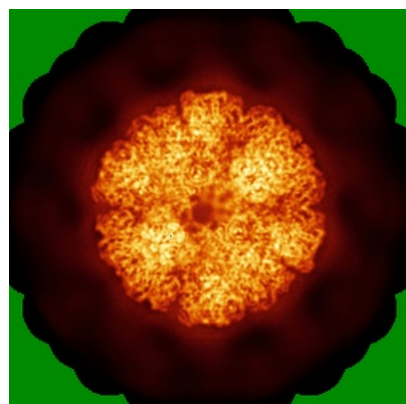


Z Index: 190

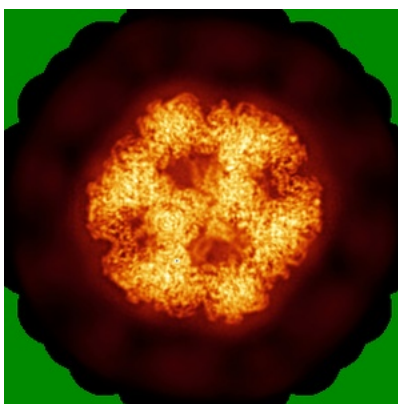
The images above show the largest variance slices of the map in three orthogonal directions.

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

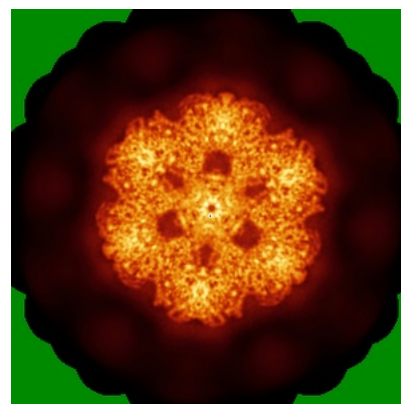
6.4.1 Primary map



X

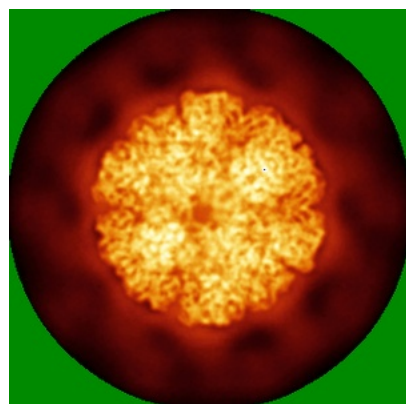


Y

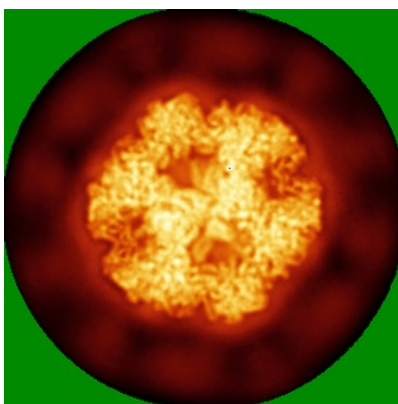


Z

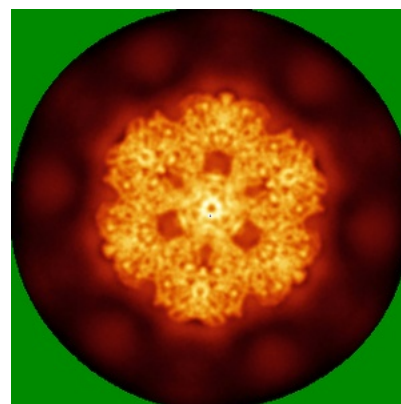
6.4.2 Raw map



X



Y

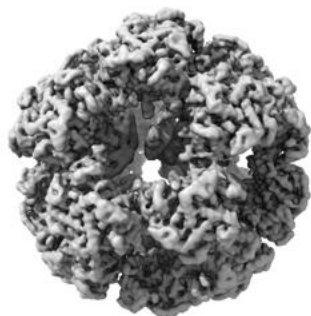


Z

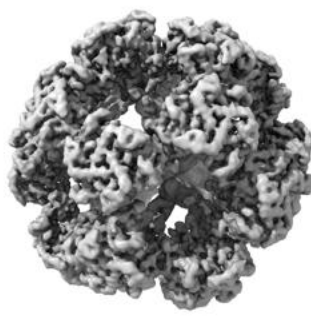
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

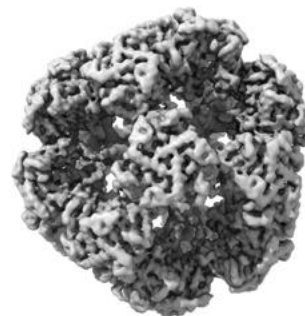
6.5.1 Primary map



X



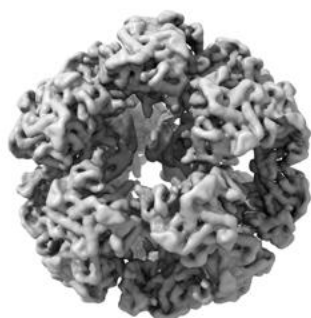
Y



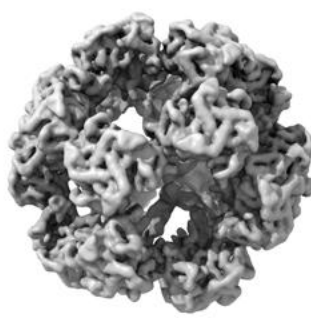
Z

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

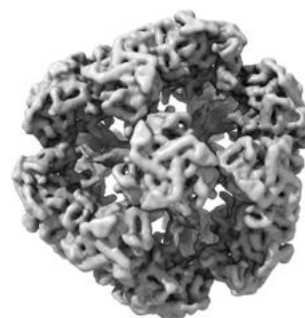
6.5.2 Raw map



X



Y



Z

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

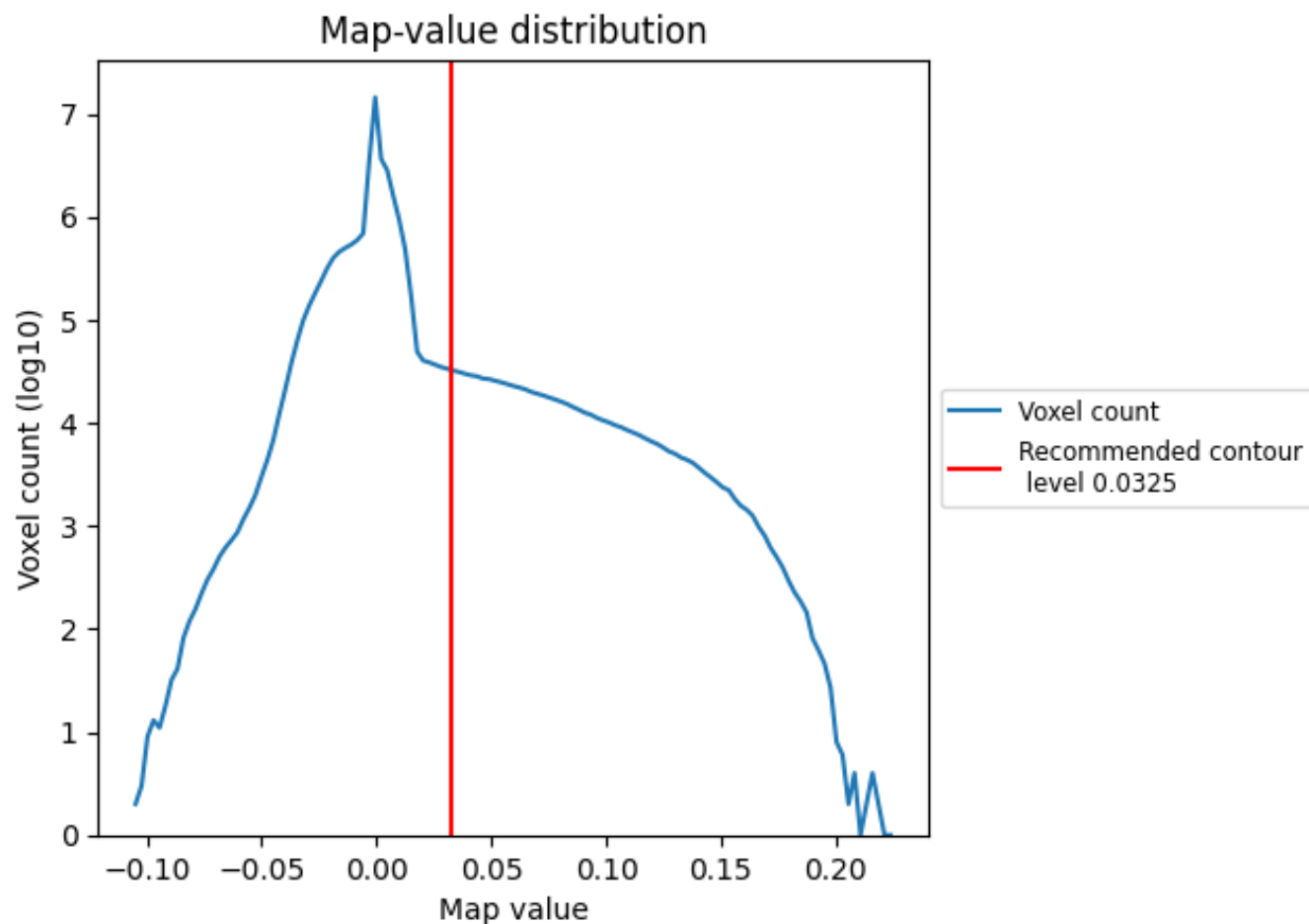
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

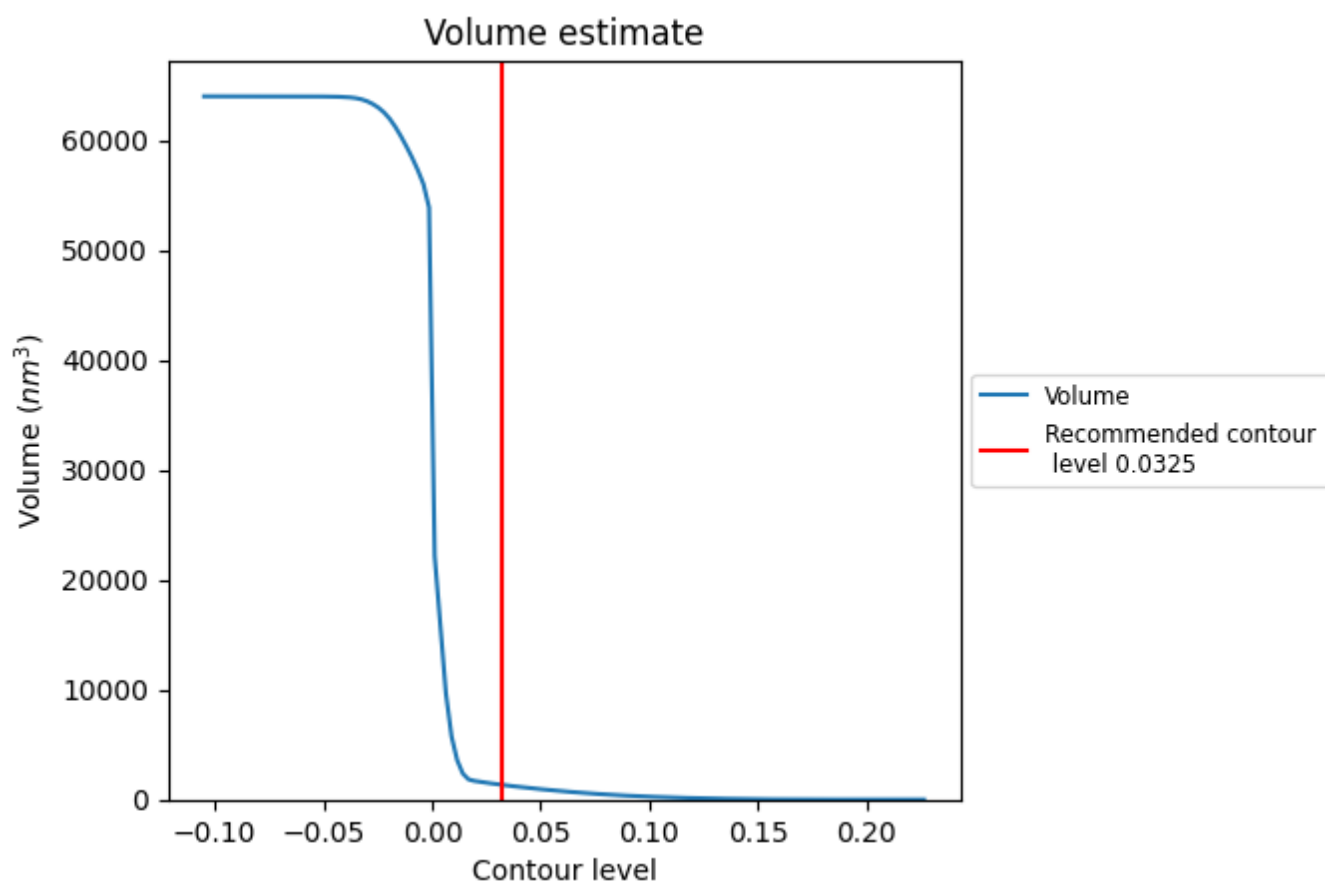
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

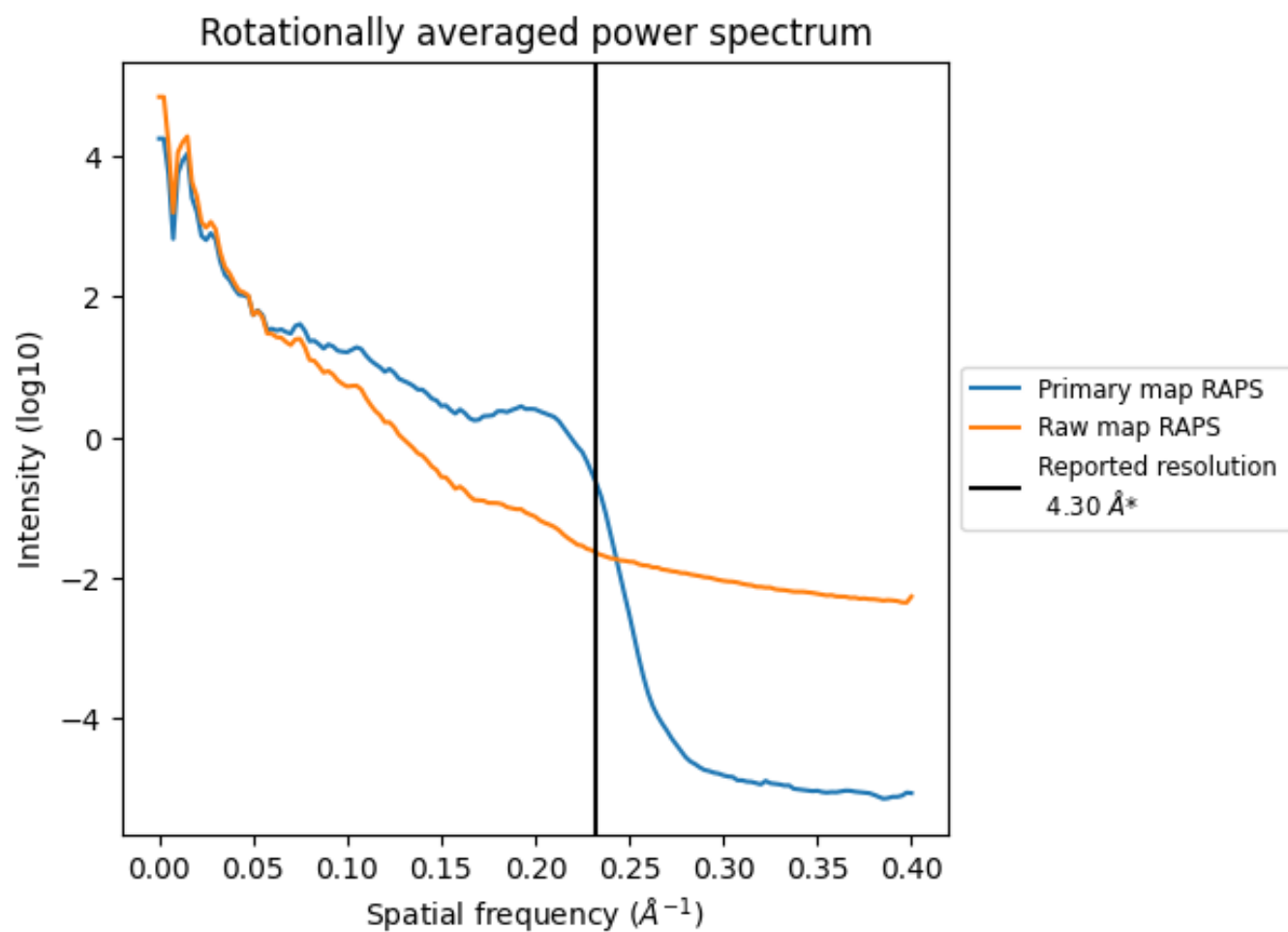
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1333 nm^3 ; 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 ⓘ

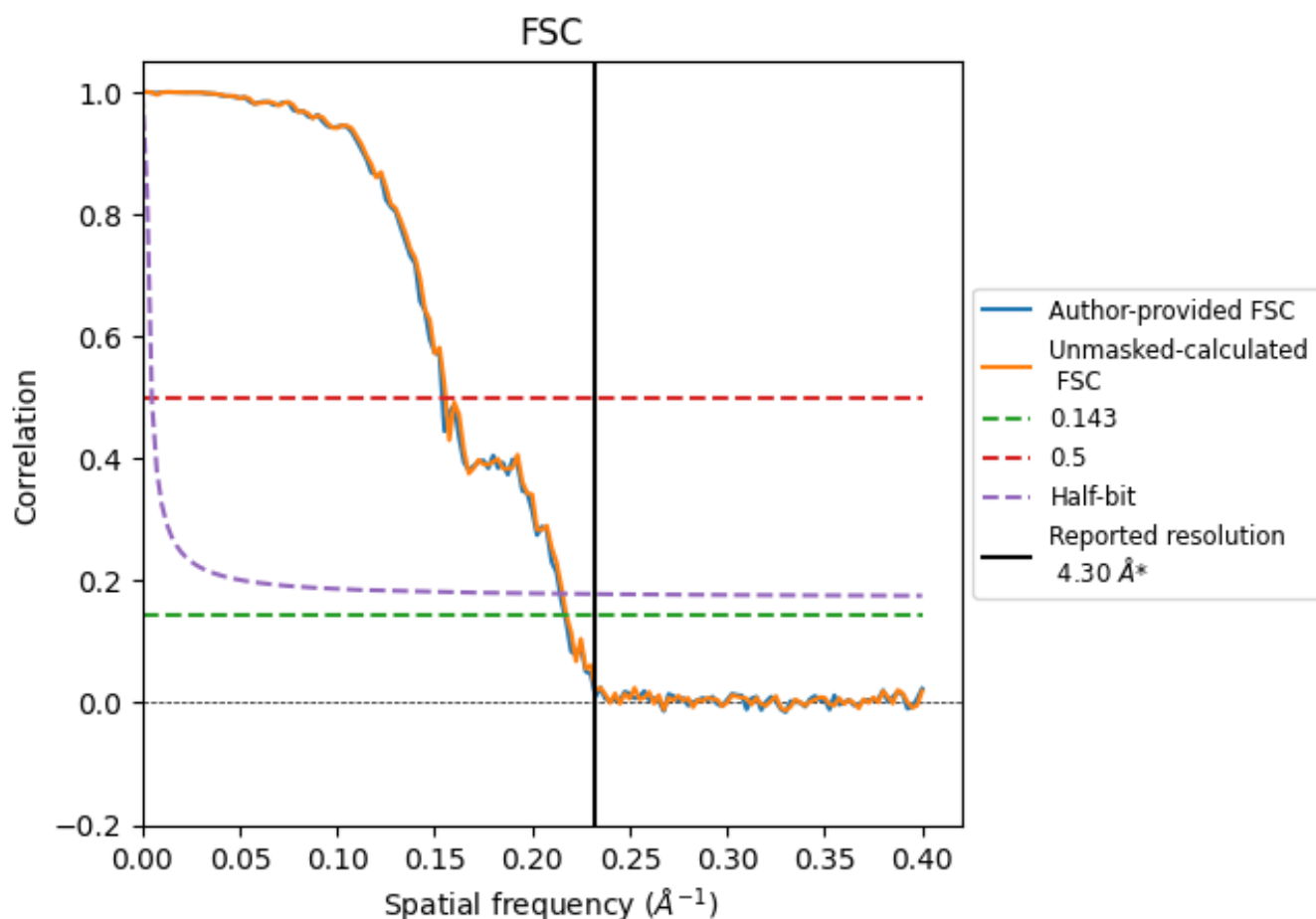


*Reported resolution corresponds to spatial frequency of 0.233 $\text{\AA}^{-1}$

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

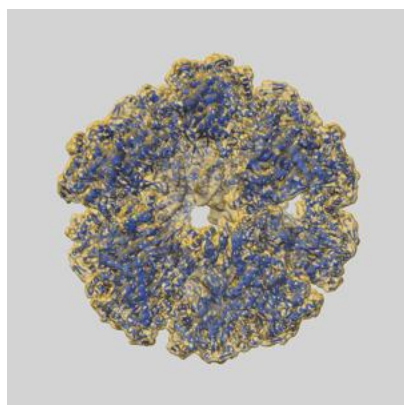
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.61	6.50	4.66
Unmasked-calculated*	4.60	6.43	4.64

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

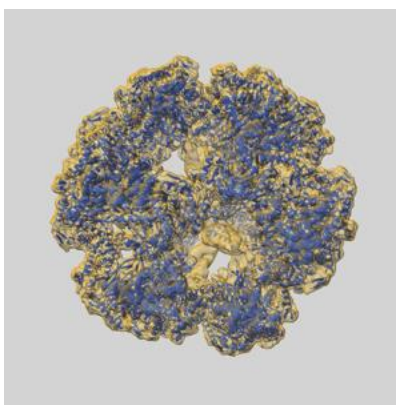
9 Map-model fit [i](#)

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.

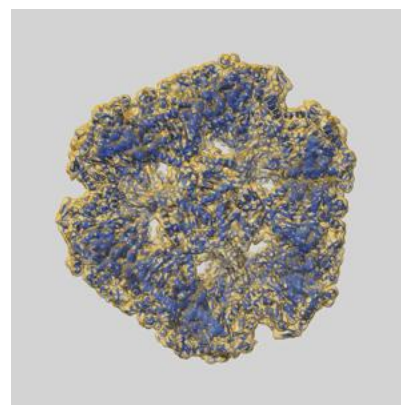
9.1 Map-model overlay [i](#)



X



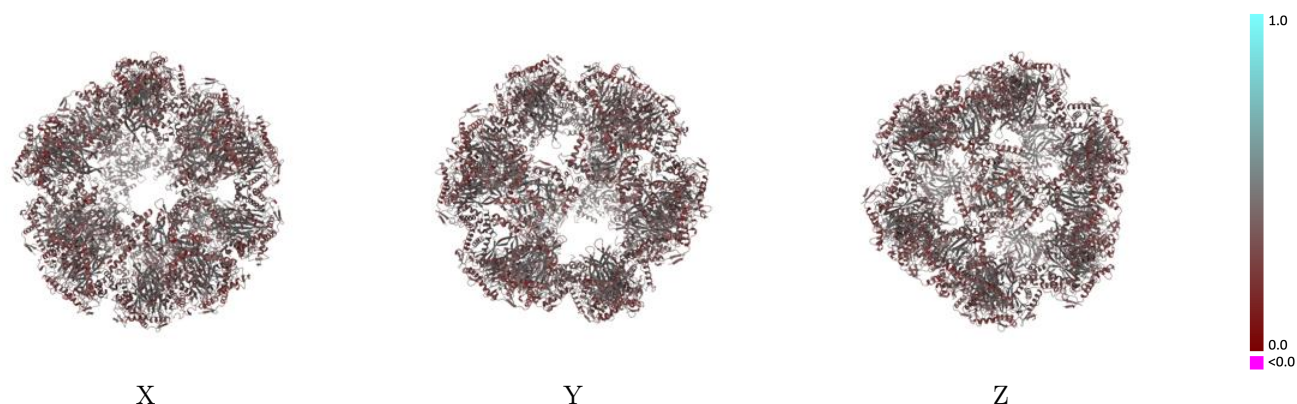
Y



Z

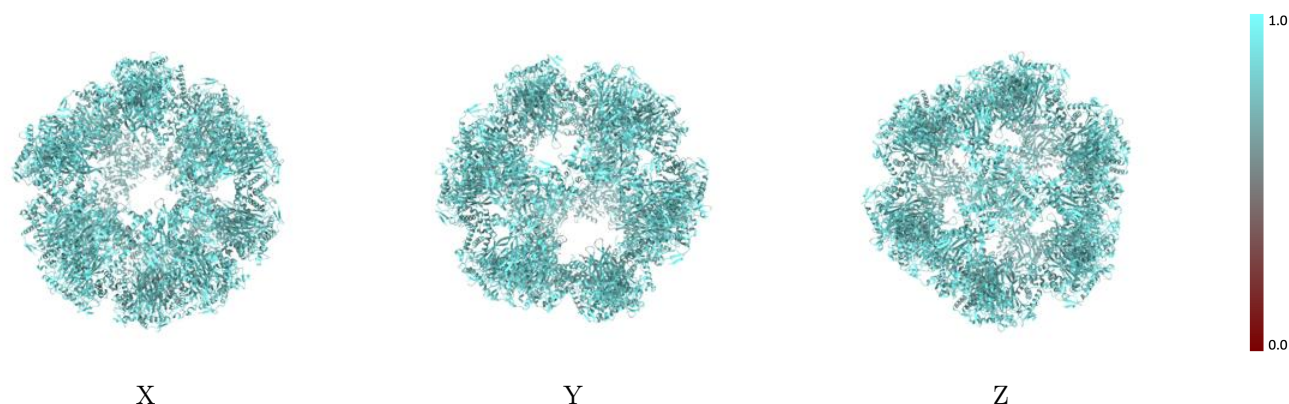
The images above show the 3D surface view of the map at the recommended contour level 0.0325 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



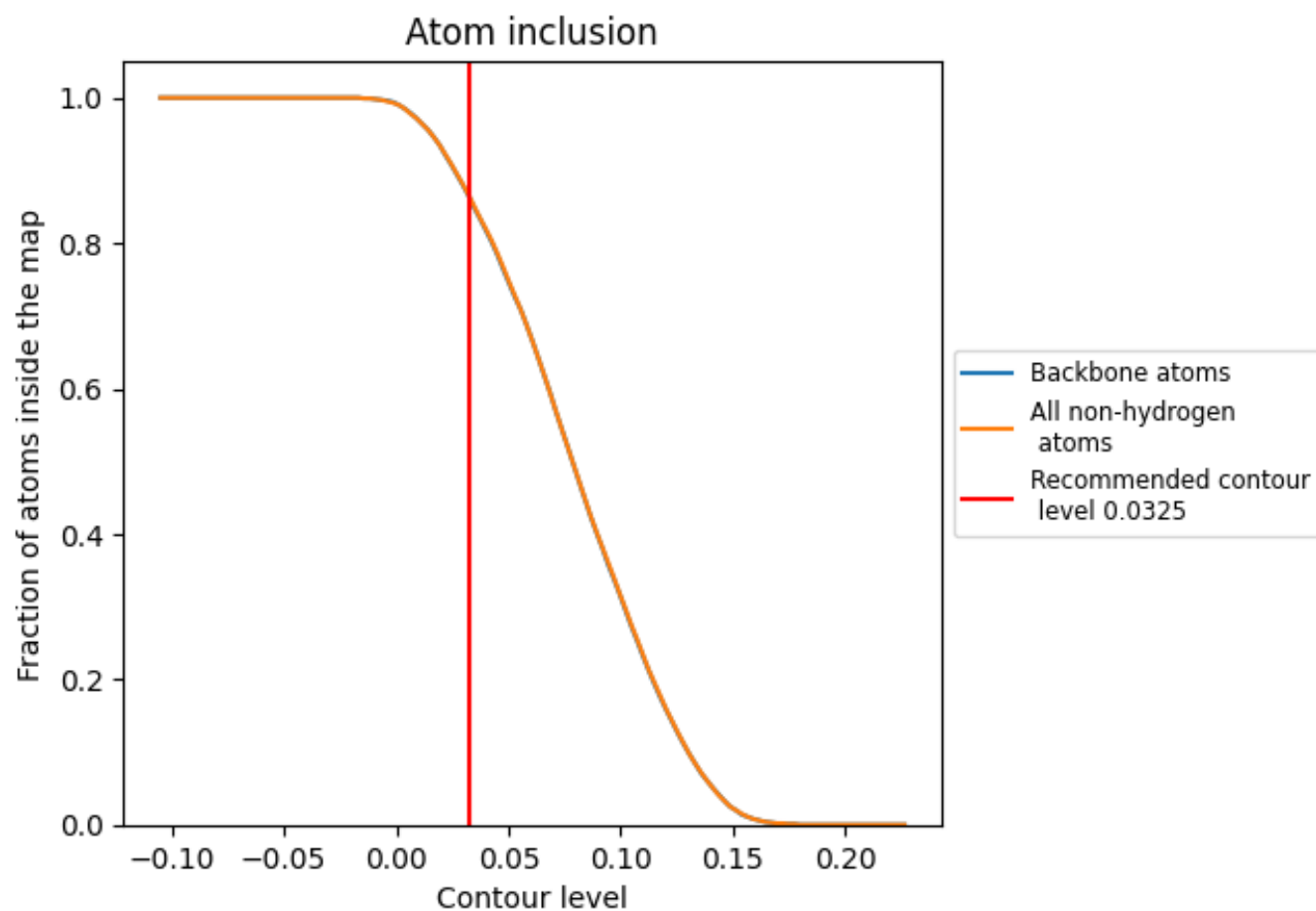
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.8650	 0.3730
A	 0.8720	 0.3790
AA	 0.8660	 0.3680
AB	 0.8710	 0.3740
B	 0.8670	 0.3740
BA	 0.8710	 0.3770
BB	 1.0000	 0.4400
C	 0.8670	 0.3720
CA	 0.8730	 0.3750
CB	 0.8650	 0.3740
D	 0.8690	 0.3760
DA	 1.0000	 0.4390
DB	 0.8720	 0.3730
E	 0.8740	 0.3750
EA	 0.8660	 0.3760
EB	 0.8710	 0.3720
F	 0.8690	 0.3780
FA	 0.8730	 0.3740
FB	 0.8700	 0.3760
G	 0.8700	 0.3730
GA	 0.8680	 0.3700
GB	 0.8690	 0.3740
H	 0.8670	 0.3720
HA	 0.8720	 0.3760
HB	 1.0000	 0.4410
I	 0.8720	 0.3770
IA	 0.8720	 0.3740
IB	 0.8710	 0.3740
J	 0.8740	 0.3730
JA	 1.0000	 0.4440
JB	 0.8760	 0.3760
K	 1.0000	 0.4480
KA	 0.8740	 0.3700
KB	 0.8670	 0.3720
L	 0.8720	 0.3700



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
LA	 0.8760	 0.3740
LB	 0.8670	 0.3750
M	 0.8770	 0.3770
MA	 0.8630	 0.3690
MB	 0.8670	 0.3710
N	 0.8610	 0.3710
NA	 0.8670	 0.3690
NB	 1.0000	 0.4300
O	 0.8660	 0.3710
OA	 0.8670	 0.3610
OB	 0.8640	 0.3750
P	 0.8690	 0.3650
PA	 1.0000	 0.4370
PB	 0.8690	 0.3720
Q	 1.0000	 0.4370
QA	 0.8620	 0.3710
QB	 0.8670	 0.3690
R	 0.8620	 0.3740
RA	 0.8660	 0.3680
RB	 0.8730	 0.3740
S	 0.8730	 0.3680
SA	 0.8730	 0.3660
SB	 0.8660	 0.3770
T	 0.8740	 0.3660
TA	 0.8670	 0.3680
TB	 1.0000	 0.4450
UA	 0.8670	 0.3730
V	 0.8720	 0.3690
VA	 0.9850	 0.4480
W	 0.8670	 0.3750
WA	 0.8710	 0.3740
X	 0.9850	 0.4430
XA	 0.8760	 0.3780
XC	 1.0000	 0.4470
Y	 0.8690	 0.3740
YA	 0.8670	 0.3730
Z	 0.8730	 0.3770
ZA	 0.8690	 0.3730