



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 01:21 AM UTC

PDB ID : 9CCA / pdb_00009cca
EMDB ID : EMD-45440
Title : Cryo-EM structure of a designed pyridoxal phosphate (PLP) synthase fused to a designed circumsporozoite protein antigen from Plasmodium falciparum (CSP-P1-CSP and CSP-P2-CSP)
Authors : Shi, D.; Ma, R.; Tang, W.K.; Tolia, N.H.
Deposited on : 2024-06-21
Resolution : 2.95 Å (reported)
Based on initial models : 4ADT, 2ABW

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

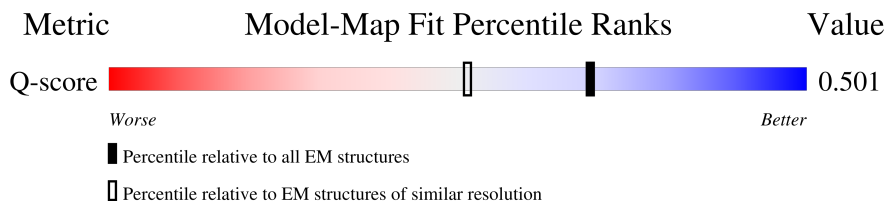
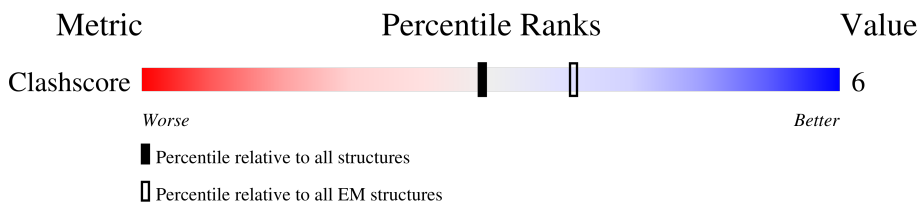
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.95 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.
















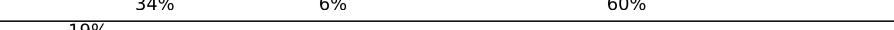




Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	13114 (2.45 - 3.45)

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	537	 41% 7% 52%
1	B	537	 42% 6% 52%
1	C	537	 42% 6% 52%
1	D	537	 42% 6% 52%
1	E	537	 42% 6% 52%
1	F	537	 41% 7% 52%

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Mol	Chain	Length	Quality of chain
1	M	537	
1	N	537	
1	O	537	
1	P	537	
1	Q	537	
1	R	537	
2	G	454	
2	H	454	
2	I	454	
2	J	454	
2	K	454	
2	L	454	
2	S	454	
2	T	454	
2	U	454	
2	V	454	
2	W	454	
2	X	454	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 82341 atoms, of which 41664 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 Circumsporozoite protein,Pyridoxal 5'-phosphate synthase subunit Pdx1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	257	Total	C	H	N	O	S	0	0
			3962	1231	2015	335	362	19		
1	B	258	Total	C	H	N	O	S	0	0
			3969	1233	2018	336	363	19		
1	C	258	Total	C	H	N	O	S	0	0
			3969	1233	2018	336	363	19		
1	D	258	Total	C	H	N	O	S	0	0
			3969	1233	2018	336	363	19		
1	E	258	Total	C	H	N	O	S	0	0
			3969	1233	2018	336	363	19		
1	F	258	Total	C	H	N	O	S	0	0
			3969	1233	2018	336	363	19		
1	M	258	Total	C	H	N	O	S	0	0
			3969	1233	2018	336	363	19		
1	N	258	Total	C	H	N	O	S	0	0
			3969	1233	2018	336	363	19		
1	O	258	Total	C	H	N	O	S	0	0
			3969	1233	2018	336	363	19		
1	P	258	Total	C	H	N	O	S	0	0
			3969	1233	2018	336	363	19		
1	Q	258	Total	C	H	N	O	S	0	0
			3969	1233	2018	336	363	19		
1	R	258	Total	C	H	N	O	S	0	0
			3969	1233	2018	336	363	19		

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q7K740
A	2	THR	-	cloning artifact	UNP Q7K740
A	3	GLY	-	cloning artifact	UNP Q7K740
A	112	GLY	-	linker	UNP Q7K740
A	113	GLY	-	linker	UNP Q7K740

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Chain	Residue	Modelled	Actual	Comment	Reference
A	114	SER	-	linker	UNP Q7K740
A	115	GLY	-	cloning artifact	UNP Q7K740
A	116	THR	-	cloning artifact	UNP Q7K740
A	198	ARG	LYS	engineered mutation	UNP C6KT50
A	289	CYS	LYS	engineered mutation	UNP C6KT50
A	293	CYS	SER	engineered mutation	UNP C6KT50
A	417	THR	-	cloning artifact	UNP C6KT50
A	418	GLY	-	cloning artifact	UNP C6KT50
A	527	GLY	-	linker	UNP Q7K740
A	528	GLY	-	linker	UNP Q7K740
A	529	SER	-	linker	UNP Q7K740
A	530	LEU	-	cloning artifact	UNP Q7K740
A	531	GLU	-	cloning artifact	UNP Q7K740
A	532	HIS	-	expression tag	UNP Q7K740
A	533	HIS	-	expression tag	UNP Q7K740
A	534	HIS	-	expression tag	UNP Q7K740
A	535	HIS	-	expression tag	UNP Q7K740
A	536	HIS	-	expression tag	UNP Q7K740
A	537	HIS	-	expression tag	UNP Q7K740
B	1	MET	-	initiating methionine	UNP Q7K740
B	2	THR	-	cloning artifact	UNP Q7K740
B	3	GLY	-	cloning artifact	UNP Q7K740
B	112	GLY	-	linker	UNP Q7K740
B	113	GLY	-	linker	UNP Q7K740
B	114	SER	-	linker	UNP Q7K740
B	115	GLY	-	cloning artifact	UNP Q7K740
B	116	THR	-	cloning artifact	UNP Q7K740
B	198	ARG	LYS	engineered mutation	UNP C6KT50
B	289	CYS	LYS	engineered mutation	UNP C6KT50
B	293	CYS	SER	engineered mutation	UNP C6KT50
B	417	THR	-	cloning artifact	UNP C6KT50
B	418	GLY	-	cloning artifact	UNP C6KT50
B	527	GLY	-	linker	UNP Q7K740
B	528	GLY	-	linker	UNP Q7K740
B	529	SER	-	linker	UNP Q7K740
B	530	LEU	-	cloning artifact	UNP Q7K740
B	531	GLU	-	cloning artifact	UNP Q7K740
B	532	HIS	-	expression tag	UNP Q7K740
B	533	HIS	-	expression tag	UNP Q7K740
B	534	HIS	-	expression tag	UNP Q7K740
B	535	HIS	-	expression tag	UNP Q7K740
B	536	HIS	-	expression tag	UNP Q7K740

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Chain	Residue	Modelled	Actual	Comment	Reference
B	537	HIS	-	expression tag	UNP Q7K740
C	1	MET	-	initiating methionine	UNP Q7K740
C	2	THR	-	cloning artifact	UNP Q7K740
C	3	GLY	-	cloning artifact	UNP Q7K740
C	112	GLY	-	linker	UNP Q7K740
C	113	GLY	-	linker	UNP Q7K740
C	114	SER	-	linker	UNP Q7K740
C	115	GLY	-	cloning artifact	UNP Q7K740
C	116	THR	-	cloning artifact	UNP Q7K740
C	198	ARG	LYS	engineered mutation	UNP C6KT50
C	289	CYS	LYS	engineered mutation	UNP C6KT50
C	293	CYS	SER	engineered mutation	UNP C6KT50
C	417	THR	-	cloning artifact	UNP C6KT50
C	418	GLY	-	cloning artifact	UNP C6KT50
C	527	GLY	-	linker	UNP Q7K740
C	528	GLY	-	linker	UNP Q7K740
C	529	SER	-	linker	UNP Q7K740
C	530	LEU	-	cloning artifact	UNP Q7K740
C	531	GLU	-	cloning artifact	UNP Q7K740
C	532	HIS	-	expression tag	UNP Q7K740
C	533	HIS	-	expression tag	UNP Q7K740
C	534	HIS	-	expression tag	UNP Q7K740
C	535	HIS	-	expression tag	UNP Q7K740
C	536	HIS	-	expression tag	UNP Q7K740
C	537	HIS	-	expression tag	UNP Q7K740
D	1	MET	-	initiating methionine	UNP Q7K740
D	2	THR	-	cloning artifact	UNP Q7K740
D	3	GLY	-	cloning artifact	UNP Q7K740
D	112	GLY	-	linker	UNP Q7K740
D	113	GLY	-	linker	UNP Q7K740
D	114	SER	-	linker	UNP Q7K740
D	115	GLY	-	cloning artifact	UNP Q7K740
D	116	THR	-	cloning artifact	UNP Q7K740
D	198	ARG	LYS	engineered mutation	UNP C6KT50
D	289	CYS	LYS	engineered mutation	UNP C6KT50
D	293	CYS	SER	engineered mutation	UNP C6KT50
D	417	THR	-	cloning artifact	UNP C6KT50
D	418	GLY	-	cloning artifact	UNP C6KT50
D	527	GLY	-	linker	UNP Q7K740
D	528	GLY	-	linker	UNP Q7K740
D	529	SER	-	linker	UNP Q7K740
D	530	LEU	-	cloning artifact	UNP Q7K740

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Chain	Residue	Modelled	Actual	Comment	Reference
D	531	GLU	-	cloning artifact	UNP Q7K740
D	532	HIS	-	expression tag	UNP Q7K740
D	533	HIS	-	expression tag	UNP Q7K740
D	534	HIS	-	expression tag	UNP Q7K740
D	535	HIS	-	expression tag	UNP Q7K740
D	536	HIS	-	expression tag	UNP Q7K740
D	537	HIS	-	expression tag	UNP Q7K740
E	1	MET	-	initiating methionine	UNP Q7K740
E	2	THR	-	cloning artifact	UNP Q7K740
E	3	GLY	-	cloning artifact	UNP Q7K740
E	112	GLY	-	linker	UNP Q7K740
E	113	GLY	-	linker	UNP Q7K740
E	114	SER	-	linker	UNP Q7K740
E	115	GLY	-	cloning artifact	UNP Q7K740
E	116	THR	-	cloning artifact	UNP Q7K740
E	198	ARG	LYS	engineered mutation	UNP C6KT50
E	289	CYS	LYS	engineered mutation	UNP C6KT50
E	293	CYS	SER	engineered mutation	UNP C6KT50
E	417	THR	-	cloning artifact	UNP C6KT50
E	418	GLY	-	cloning artifact	UNP C6KT50
E	527	GLY	-	linker	UNP Q7K740
E	528	GLY	-	linker	UNP Q7K740
E	529	SER	-	linker	UNP Q7K740
E	530	LEU	-	cloning artifact	UNP Q7K740
E	531	GLU	-	cloning artifact	UNP Q7K740
E	532	HIS	-	expression tag	UNP Q7K740
E	533	HIS	-	expression tag	UNP Q7K740
E	534	HIS	-	expression tag	UNP Q7K740
E	535	HIS	-	expression tag	UNP Q7K740
E	536	HIS	-	expression tag	UNP Q7K740
E	537	HIS	-	expression tag	UNP Q7K740
F	1	MET	-	initiating methionine	UNP Q7K740
F	2	THR	-	cloning artifact	UNP Q7K740
F	3	GLY	-	cloning artifact	UNP Q7K740
F	112	GLY	-	linker	UNP Q7K740
F	113	GLY	-	linker	UNP Q7K740
F	114	SER	-	linker	UNP Q7K740
F	115	GLY	-	cloning artifact	UNP Q7K740
F	116	THR	-	cloning artifact	UNP Q7K740
F	198	ARG	LYS	engineered mutation	UNP C6KT50
F	289	CYS	LYS	engineered mutation	UNP C6KT50
F	293	CYS	SER	engineered mutation	UNP C6KT50

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Chain	Residue	Modelled	Actual	Comment	Reference
F	417	THR	-	cloning artifact	UNP C6KT50
F	418	GLY	-	cloning artifact	UNP C6KT50
F	527	GLY	-	linker	UNP Q7K740
F	528	GLY	-	linker	UNP Q7K740
F	529	SER	-	linker	UNP Q7K740
F	530	LEU	-	cloning artifact	UNP Q7K740
F	531	GLU	-	cloning artifact	UNP Q7K740
F	532	HIS	-	expression tag	UNP Q7K740
F	533	HIS	-	expression tag	UNP Q7K740
F	534	HIS	-	expression tag	UNP Q7K740
F	535	HIS	-	expression tag	UNP Q7K740
F	536	HIS	-	expression tag	UNP Q7K740
F	537	HIS	-	expression tag	UNP Q7K740
M	1	MET	-	initiating methionine	UNP Q7K740
M	2	THR	-	cloning artifact	UNP Q7K740
M	3	GLY	-	cloning artifact	UNP Q7K740
M	112	GLY	-	linker	UNP Q7K740
M	113	GLY	-	linker	UNP Q7K740
M	114	SER	-	linker	UNP Q7K740
M	115	GLY	-	cloning artifact	UNP Q7K740
M	116	THR	-	cloning artifact	UNP Q7K740
M	198	ARG	LYS	engineered mutation	UNP C6KT50
M	289	CYS	LYS	engineered mutation	UNP C6KT50
M	293	CYS	SER	engineered mutation	UNP C6KT50
M	417	THR	-	cloning artifact	UNP C6KT50
M	418	GLY	-	cloning artifact	UNP C6KT50
M	527	GLY	-	linker	UNP Q7K740
M	528	GLY	-	linker	UNP Q7K740
M	529	SER	-	linker	UNP Q7K740
M	530	LEU	-	cloning artifact	UNP Q7K740
M	531	GLU	-	cloning artifact	UNP Q7K740
M	532	HIS	-	expression tag	UNP Q7K740
M	533	HIS	-	expression tag	UNP Q7K740
M	534	HIS	-	expression tag	UNP Q7K740
M	535	HIS	-	expression tag	UNP Q7K740
M	536	HIS	-	expression tag	UNP Q7K740
M	537	HIS	-	expression tag	UNP Q7K740
N	1	MET	-	initiating methionine	UNP Q7K740
N	2	THR	-	cloning artifact	UNP Q7K740
N	3	GLY	-	cloning artifact	UNP Q7K740
N	112	GLY	-	linker	UNP Q7K740
N	113	GLY	-	linker	UNP Q7K740

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Chain	Residue	Modelled	Actual	Comment	Reference
N	114	SER	-	linker	UNP Q7K740
N	115	GLY	-	cloning artifact	UNP Q7K740
N	116	THR	-	cloning artifact	UNP Q7K740
N	198	ARG	LYS	engineered mutation	UNP C6KT50
N	289	CYS	LYS	engineered mutation	UNP C6KT50
N	293	CYS	SER	engineered mutation	UNP C6KT50
N	417	THR	-	cloning artifact	UNP C6KT50
N	418	GLY	-	cloning artifact	UNP C6KT50
N	527	GLY	-	linker	UNP Q7K740
N	528	GLY	-	linker	UNP Q7K740
N	529	SER	-	linker	UNP Q7K740
N	530	LEU	-	cloning artifact	UNP Q7K740
N	531	GLU	-	cloning artifact	UNP Q7K740
N	532	HIS	-	expression tag	UNP Q7K740
N	533	HIS	-	expression tag	UNP Q7K740
N	534	HIS	-	expression tag	UNP Q7K740
N	535	HIS	-	expression tag	UNP Q7K740
N	536	HIS	-	expression tag	UNP Q7K740
N	537	HIS	-	expression tag	UNP Q7K740
O	1	MET	-	initiating methionine	UNP Q7K740
O	2	THR	-	cloning artifact	UNP Q7K740
O	3	GLY	-	cloning artifact	UNP Q7K740
O	112	GLY	-	linker	UNP Q7K740
O	113	GLY	-	linker	UNP Q7K740
O	114	SER	-	linker	UNP Q7K740
O	115	GLY	-	cloning artifact	UNP Q7K740
O	116	THR	-	cloning artifact	UNP Q7K740
O	198	ARG	LYS	engineered mutation	UNP C6KT50
O	289	CYS	LYS	engineered mutation	UNP C6KT50
O	293	CYS	SER	engineered mutation	UNP C6KT50
O	417	THR	-	cloning artifact	UNP C6KT50
O	418	GLY	-	cloning artifact	UNP C6KT50
O	527	GLY	-	linker	UNP Q7K740
O	528	GLY	-	linker	UNP Q7K740
O	529	SER	-	linker	UNP Q7K740
O	530	LEU	-	cloning artifact	UNP Q7K740
O	531	GLU	-	cloning artifact	UNP Q7K740
O	532	HIS	-	expression tag	UNP Q7K740
O	533	HIS	-	expression tag	UNP Q7K740
O	534	HIS	-	expression tag	UNP Q7K740
O	535	HIS	-	expression tag	UNP Q7K740
O	536	HIS	-	expression tag	UNP Q7K740

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Chain	Residue	Modelled	Actual	Comment	Reference
O	537	HIS	-	expression tag	UNP Q7K740
P	1	MET	-	initiating methionine	UNP Q7K740
P	2	THR	-	cloning artifact	UNP Q7K740
P	3	GLY	-	cloning artifact	UNP Q7K740
P	112	GLY	-	linker	UNP Q7K740
P	113	GLY	-	linker	UNP Q7K740
P	114	SER	-	linker	UNP Q7K740
P	115	GLY	-	cloning artifact	UNP Q7K740
P	116	THR	-	cloning artifact	UNP Q7K740
P	198	ARG	LYS	engineered mutation	UNP C6KT50
P	289	CYS	LYS	engineered mutation	UNP C6KT50
P	293	CYS	SER	engineered mutation	UNP C6KT50
P	417	THR	-	cloning artifact	UNP C6KT50
P	418	GLY	-	cloning artifact	UNP C6KT50
P	527	GLY	-	linker	UNP Q7K740
P	528	GLY	-	linker	UNP Q7K740
P	529	SER	-	linker	UNP Q7K740
P	530	LEU	-	cloning artifact	UNP Q7K740
P	531	GLU	-	cloning artifact	UNP Q7K740
P	532	HIS	-	expression tag	UNP Q7K740
P	533	HIS	-	expression tag	UNP Q7K740
P	534	HIS	-	expression tag	UNP Q7K740
P	535	HIS	-	expression tag	UNP Q7K740
P	536	HIS	-	expression tag	UNP Q7K740
P	537	HIS	-	expression tag	UNP Q7K740
Q	1	MET	-	initiating methionine	UNP Q7K740
Q	2	THR	-	cloning artifact	UNP Q7K740
Q	3	GLY	-	cloning artifact	UNP Q7K740
Q	112	GLY	-	linker	UNP Q7K740
Q	113	GLY	-	linker	UNP Q7K740
Q	114	SER	-	linker	UNP Q7K740
Q	115	GLY	-	cloning artifact	UNP Q7K740
Q	116	THR	-	cloning artifact	UNP Q7K740
Q	198	ARG	LYS	engineered mutation	UNP C6KT50
Q	289	CYS	LYS	engineered mutation	UNP C6KT50
Q	293	CYS	SER	engineered mutation	UNP C6KT50
Q	417	THR	-	cloning artifact	UNP C6KT50
Q	418	GLY	-	cloning artifact	UNP C6KT50
Q	527	GLY	-	linker	UNP Q7K740
Q	528	GLY	-	linker	UNP Q7K740
Q	529	SER	-	linker	UNP Q7K740
Q	530	LEU	-	cloning artifact	UNP Q7K740

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	531	GLU	-	cloning artifact	UNP Q7K740
Q	532	HIS	-	expression tag	UNP Q7K740
Q	533	HIS	-	expression tag	UNP Q7K740
Q	534	HIS	-	expression tag	UNP Q7K740
Q	535	HIS	-	expression tag	UNP Q7K740
Q	536	HIS	-	expression tag	UNP Q7K740
Q	537	HIS	-	expression tag	UNP Q7K740
R	1	MET	-	initiating methionine	UNP Q7K740
R	2	THR	-	cloning artifact	UNP Q7K740
R	3	GLY	-	cloning artifact	UNP Q7K740
R	112	GLY	-	linker	UNP Q7K740
R	113	GLY	-	linker	UNP Q7K740
R	114	SER	-	linker	UNP Q7K740
R	115	GLY	-	cloning artifact	UNP Q7K740
R	116	THR	-	cloning artifact	UNP Q7K740
R	198	ARG	LYS	engineered mutation	UNP C6KT50
R	289	CYS	LYS	engineered mutation	UNP C6KT50
R	293	CYS	SER	engineered mutation	UNP C6KT50
R	417	THR	-	cloning artifact	UNP C6KT50
R	418	GLY	-	cloning artifact	UNP C6KT50
R	527	GLY	-	linker	UNP Q7K740
R	528	GLY	-	linker	UNP Q7K740
R	529	SER	-	linker	UNP Q7K740
R	530	LEU	-	cloning artifact	UNP Q7K740
R	531	GLU	-	cloning artifact	UNP Q7K740
R	532	HIS	-	expression tag	UNP Q7K740
R	533	HIS	-	expression tag	UNP Q7K740
R	534	HIS	-	expression tag	UNP Q7K740
R	535	HIS	-	expression tag	UNP Q7K740
R	536	HIS	-	expression tag	UNP Q7K740
R	537	HIS	-	expression tag	UNP Q7K740

- Molecule 2 is a protein called Circumsporozoite protein,Pyridoxal 5'-phosphate synthase subunit PDX2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	G	183	Total	C	H	N	O	S	0	0
			2900	934	1458	244	255	9		
2	H	182	Total	C	H	N	O	S	0	0
			2879	928	1446	242	254	9		
2	I	182	Total	C	H	N	O	S	0	0
			2879	928	1446	242	254	9		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	J	182	Total	C	H	N	O	S	0	0
			2879	928	1446	242	254	9		
2	K	182	Total	C	H	N	O	S	0	0
			2882	928	1448	243	254	9		
2	L	183	Total	C	H	N	O	S	0	0
			2901	934	1459	244	255	9		
2	S	183	Total	C	H	N	O	S	0	0
			2900	934	1458	244	255	9		
2	T	183	Total	C	H	N	O	S	0	0
			2900	934	1458	244	255	9		
2	U	183	Total	C	H	N	O	S	0	0
			2900	934	1458	244	255	9		
2	V	183	Total	C	H	N	O	S	0	0
			2900	934	1458	244	255	9		
2	W	183	Total	C	H	N	O	S	0	0
			2900	934	1458	244	255	9		
2	X	183	Total	C	H	N	O	S	0	0
			2900	934	1458	244	255	9		

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	initiating methionine	UNP Q7K740
G	2	THR	-	cloning artifact	UNP Q7K740
G	3	GLY	-	cloning artifact	UNP Q7K740
G	112	GLY	-	linker	UNP Q7K740
G	113	GLY	-	linker	UNP Q7K740
G	114	SER	-	linker	UNP Q7K740
G	115	GLY	-	cloning artifact	UNP Q7K740
G	116	THR	-	cloning artifact	UNP Q7K740
G	179	GLN	ASN	engineered mutation	UNP Q8IHK4
G	242	GLN	ASN	engineered mutation	UNP Q8IHK4
G	310	ASN	HIS	engineered mutation	UNP Q8IHK4
G	334	THR	-	cloning artifact	UNP Q8IHK4
G	335	GLY	-	cloning artifact	UNP Q8IHK4
G	444	GLY	-	linker	UNP Q7K740
G	445	GLY	-	linker	UNP Q7K740
G	446	SER	-	linker	UNP Q7K740
G	447	LEU	-	cloning artifact	UNP Q7K740
G	448	GLU	-	cloning artifact	UNP Q7K740
G	449	HIS	-	expression tag	UNP Q7K740
G	450	HIS	-	expression tag	UNP Q7K740
G	451	HIS	-	expression tag	UNP Q7K740

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Chain	Residue	Modelled	Actual	Comment	Reference
G	452	HIS	-	expression tag	UNP Q7K740
G	453	HIS	-	expression tag	UNP Q7K740
G	454	HIS	-	expression tag	UNP Q7K740
H	1	MET	-	initiating methionine	UNP Q7K740
H	2	THR	-	cloning artifact	UNP Q7K740
H	3	GLY	-	cloning artifact	UNP Q7K740
H	112	GLY	-	linker	UNP Q7K740
H	113	GLY	-	linker	UNP Q7K740
H	114	SER	-	linker	UNP Q7K740
H	115	GLY	-	cloning artifact	UNP Q7K740
H	116	THR	-	cloning artifact	UNP Q7K740
H	179	GLN	ASN	engineered mutation	UNP Q8IHK4
H	242	GLN	ASN	engineered mutation	UNP Q8IHK4
H	310	ASN	HIS	engineered mutation	UNP Q8IHK4
H	334	THR	-	cloning artifact	UNP Q8IHK4
H	335	GLY	-	cloning artifact	UNP Q8IHK4
H	444	GLY	-	linker	UNP Q7K740
H	445	GLY	-	linker	UNP Q7K740
H	446	SER	-	linker	UNP Q7K740
H	447	LEU	-	cloning artifact	UNP Q7K740
H	448	GLU	-	cloning artifact	UNP Q7K740
H	449	HIS	-	expression tag	UNP Q7K740
H	450	HIS	-	expression tag	UNP Q7K740
H	451	HIS	-	expression tag	UNP Q7K740
H	452	HIS	-	expression tag	UNP Q7K740
H	453	HIS	-	expression tag	UNP Q7K740
H	454	HIS	-	expression tag	UNP Q7K740
I	1	MET	-	initiating methionine	UNP Q7K740
I	2	THR	-	cloning artifact	UNP Q7K740
I	3	GLY	-	cloning artifact	UNP Q7K740
I	112	GLY	-	linker	UNP Q7K740
I	113	GLY	-	linker	UNP Q7K740
I	114	SER	-	linker	UNP Q7K740
I	115	GLY	-	cloning artifact	UNP Q7K740
I	116	THR	-	cloning artifact	UNP Q7K740
I	179	GLN	ASN	engineered mutation	UNP Q8IHK4
I	242	GLN	ASN	engineered mutation	UNP Q8IHK4
I	310	ASN	HIS	engineered mutation	UNP Q8IHK4
I	334	THR	-	cloning artifact	UNP Q8IHK4
I	335	GLY	-	cloning artifact	UNP Q8IHK4
I	444	GLY	-	linker	UNP Q7K740
I	445	GLY	-	linker	UNP Q7K740

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Chain	Residue	Modelled	Actual	Comment	Reference
I	446	SER	-	linker	UNP Q7K740
I	447	LEU	-	cloning artifact	UNP Q7K740
I	448	GLU	-	cloning artifact	UNP Q7K740
I	449	HIS	-	expression tag	UNP Q7K740
I	450	HIS	-	expression tag	UNP Q7K740
I	451	HIS	-	expression tag	UNP Q7K740
I	452	HIS	-	expression tag	UNP Q7K740
I	453	HIS	-	expression tag	UNP Q7K740
I	454	HIS	-	expression tag	UNP Q7K740
J	1	MET	-	initiating methionine	UNP Q7K740
J	2	THR	-	cloning artifact	UNP Q7K740
J	3	GLY	-	cloning artifact	UNP Q7K740
J	112	GLY	-	linker	UNP Q7K740
J	113	GLY	-	linker	UNP Q7K740
J	114	SER	-	linker	UNP Q7K740
J	115	GLY	-	cloning artifact	UNP Q7K740
J	116	THR	-	cloning artifact	UNP Q7K740
J	179	GLN	ASN	engineered mutation	UNP Q8IHK4
J	242	GLN	ASN	engineered mutation	UNP Q8IHK4
J	310	ASN	HIS	engineered mutation	UNP Q8IHK4
J	334	THR	-	cloning artifact	UNP Q8IHK4
J	335	GLY	-	cloning artifact	UNP Q8IHK4
J	444	GLY	-	linker	UNP Q7K740
J	445	GLY	-	linker	UNP Q7K740
J	446	SER	-	linker	UNP Q7K740
J	447	LEU	-	cloning artifact	UNP Q7K740
J	448	GLU	-	cloning artifact	UNP Q7K740
J	449	HIS	-	expression tag	UNP Q7K740
J	450	HIS	-	expression tag	UNP Q7K740
J	451	HIS	-	expression tag	UNP Q7K740
J	452	HIS	-	expression tag	UNP Q7K740
J	453	HIS	-	expression tag	UNP Q7K740
J	454	HIS	-	expression tag	UNP Q7K740
K	1	MET	-	initiating methionine	UNP Q7K740
K	2	THR	-	cloning artifact	UNP Q7K740
K	3	GLY	-	cloning artifact	UNP Q7K740
K	112	GLY	-	linker	UNP Q7K740
K	113	GLY	-	linker	UNP Q7K740
K	114	SER	-	linker	UNP Q7K740
K	115	GLY	-	cloning artifact	UNP Q7K740
K	116	THR	-	cloning artifact	UNP Q7K740
K	179	GLN	ASN	engineered mutation	UNP Q8IHK4

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Chain	Residue	Modelled	Actual	Comment	Reference
K	242	GLN	ASN	engineered mutation	UNP Q8IIK4
K	310	ASN	HIS	engineered mutation	UNP Q8IIK4
K	334	THR	-	cloning artifact	UNP Q8IIK4
K	335	GLY	-	cloning artifact	UNP Q8IIK4
K	444	GLY	-	linker	UNP Q7K740
K	445	GLY	-	linker	UNP Q7K740
K	446	SER	-	linker	UNP Q7K740
K	447	LEU	-	cloning artifact	UNP Q7K740
K	448	GLU	-	cloning artifact	UNP Q7K740
K	449	HIS	-	expression tag	UNP Q7K740
K	450	HIS	-	expression tag	UNP Q7K740
K	451	HIS	-	expression tag	UNP Q7K740
K	452	HIS	-	expression tag	UNP Q7K740
K	453	HIS	-	expression tag	UNP Q7K740
K	454	HIS	-	expression tag	UNP Q7K740
L	1	MET	-	initiating methionine	UNP Q7K740
L	2	THR	-	cloning artifact	UNP Q7K740
L	3	GLY	-	cloning artifact	UNP Q7K740
L	112	GLY	-	linker	UNP Q7K740
L	113	GLY	-	linker	UNP Q7K740
L	114	SER	-	linker	UNP Q7K740
L	115	GLY	-	cloning artifact	UNP Q7K740
L	116	THR	-	cloning artifact	UNP Q7K740
L	179	GLN	ASN	engineered mutation	UNP Q8IIK4
L	242	GLN	ASN	engineered mutation	UNP Q8IIK4
L	310	ASN	HIS	engineered mutation	UNP Q8IIK4
L	334	THR	-	cloning artifact	UNP Q8IIK4
L	335	GLY	-	cloning artifact	UNP Q8IIK4
L	444	GLY	-	linker	UNP Q7K740
L	445	GLY	-	linker	UNP Q7K740
L	446	SER	-	linker	UNP Q7K740
L	447	LEU	-	cloning artifact	UNP Q7K740
L	448	GLU	-	cloning artifact	UNP Q7K740
L	449	HIS	-	expression tag	UNP Q7K740
L	450	HIS	-	expression tag	UNP Q7K740
L	451	HIS	-	expression tag	UNP Q7K740
L	452	HIS	-	expression tag	UNP Q7K740
L	453	HIS	-	expression tag	UNP Q7K740
L	454	HIS	-	expression tag	UNP Q7K740
S	1	MET	-	initiating methionine	UNP Q7K740
S	2	THR	-	cloning artifact	UNP Q7K740
S	3	GLY	-	cloning artifact	UNP Q7K740

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Chain	Residue	Modelled	Actual	Comment	Reference
S	112	GLY	-	linker	UNP Q7K740
S	113	GLY	-	linker	UNP Q7K740
S	114	SER	-	linker	UNP Q7K740
S	115	GLY	-	cloning artifact	UNP Q7K740
S	116	THR	-	cloning artifact	UNP Q7K740
S	179	GLN	ASN	engineered mutation	UNP Q8IHK4
S	242	GLN	ASN	engineered mutation	UNP Q8IHK4
S	310	ASN	HIS	engineered mutation	UNP Q8IHK4
S	334	THR	-	cloning artifact	UNP Q8IHK4
S	335	GLY	-	cloning artifact	UNP Q8IHK4
S	444	GLY	-	linker	UNP Q7K740
S	445	GLY	-	linker	UNP Q7K740
S	446	SER	-	linker	UNP Q7K740
S	447	LEU	-	cloning artifact	UNP Q7K740
S	448	GLU	-	cloning artifact	UNP Q7K740
S	449	HIS	-	expression tag	UNP Q7K740
S	450	HIS	-	expression tag	UNP Q7K740
S	451	HIS	-	expression tag	UNP Q7K740
S	452	HIS	-	expression tag	UNP Q7K740
S	453	HIS	-	expression tag	UNP Q7K740
S	454	HIS	-	expression tag	UNP Q7K740
T	1	MET	-	initiating methionine	UNP Q7K740
T	2	THR	-	cloning artifact	UNP Q7K740
T	3	GLY	-	cloning artifact	UNP Q7K740
T	112	GLY	-	linker	UNP Q7K740
T	113	GLY	-	linker	UNP Q7K740
T	114	SER	-	linker	UNP Q7K740
T	115	GLY	-	cloning artifact	UNP Q7K740
T	116	THR	-	cloning artifact	UNP Q7K740
T	179	GLN	ASN	engineered mutation	UNP Q8IHK4
T	242	GLN	ASN	engineered mutation	UNP Q8IHK4
T	310	ASN	HIS	engineered mutation	UNP Q8IHK4
T	334	THR	-	cloning artifact	UNP Q8IHK4
T	335	GLY	-	cloning artifact	UNP Q8IHK4
T	444	GLY	-	linker	UNP Q7K740
T	445	GLY	-	linker	UNP Q7K740
T	446	SER	-	linker	UNP Q7K740
T	447	LEU	-	cloning artifact	UNP Q7K740
T	448	GLU	-	cloning artifact	UNP Q7K740
T	449	HIS	-	expression tag	UNP Q7K740
T	450	HIS	-	expression tag	UNP Q7K740
T	451	HIS	-	expression tag	UNP Q7K740

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Chain	Residue	Modelled	Actual	Comment	Reference
T	452	HIS	-	expression tag	UNP Q7K740
T	453	HIS	-	expression tag	UNP Q7K740
T	454	HIS	-	expression tag	UNP Q7K740
U	1	MET	-	initiating methionine	UNP Q7K740
U	2	THR	-	cloning artifact	UNP Q7K740
U	3	GLY	-	cloning artifact	UNP Q7K740
U	112	GLY	-	linker	UNP Q7K740
U	113	GLY	-	linker	UNP Q7K740
U	114	SER	-	linker	UNP Q7K740
U	115	GLY	-	cloning artifact	UNP Q7K740
U	116	THR	-	cloning artifact	UNP Q7K740
U	179	GLN	ASN	engineered mutation	UNP Q8IHK4
U	242	GLN	ASN	engineered mutation	UNP Q8IHK4
U	310	ASN	HIS	engineered mutation	UNP Q8IHK4
U	334	THR	-	cloning artifact	UNP Q8IHK4
U	335	GLY	-	cloning artifact	UNP Q8IHK4
U	444	GLY	-	linker	UNP Q7K740
U	445	GLY	-	linker	UNP Q7K740
U	446	SER	-	linker	UNP Q7K740
U	447	LEU	-	cloning artifact	UNP Q7K740
U	448	GLU	-	cloning artifact	UNP Q7K740
U	449	HIS	-	expression tag	UNP Q7K740
U	450	HIS	-	expression tag	UNP Q7K740
U	451	HIS	-	expression tag	UNP Q7K740
U	452	HIS	-	expression tag	UNP Q7K740
U	453	HIS	-	expression tag	UNP Q7K740
U	454	HIS	-	expression tag	UNP Q7K740
V	1	MET	-	initiating methionine	UNP Q7K740
V	2	THR	-	cloning artifact	UNP Q7K740
V	3	GLY	-	cloning artifact	UNP Q7K740
V	112	GLY	-	linker	UNP Q7K740
V	113	GLY	-	linker	UNP Q7K740
V	114	SER	-	linker	UNP Q7K740
V	115	GLY	-	cloning artifact	UNP Q7K740
V	116	THR	-	cloning artifact	UNP Q7K740
V	179	GLN	ASN	engineered mutation	UNP Q8IHK4
V	242	GLN	ASN	engineered mutation	UNP Q8IHK4
V	310	ASN	HIS	engineered mutation	UNP Q8IHK4
V	334	THR	-	cloning artifact	UNP Q8IHK4
V	335	GLY	-	cloning artifact	UNP Q8IHK4
V	444	GLY	-	linker	UNP Q7K740
V	445	GLY	-	linker	UNP Q7K740

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Chain	Residue	Modelled	Actual	Comment	Reference
V	446	SER	-	linker	UNP Q7K740
V	447	LEU	-	cloning artifact	UNP Q7K740
V	448	GLU	-	cloning artifact	UNP Q7K740
V	449	HIS	-	expression tag	UNP Q7K740
V	450	HIS	-	expression tag	UNP Q7K740
V	451	HIS	-	expression tag	UNP Q7K740
V	452	HIS	-	expression tag	UNP Q7K740
V	453	HIS	-	expression tag	UNP Q7K740
V	454	HIS	-	expression tag	UNP Q7K740
W	1	MET	-	initiating methionine	UNP Q7K740
W	2	THR	-	cloning artifact	UNP Q7K740
W	3	GLY	-	cloning artifact	UNP Q7K740
W	112	GLY	-	linker	UNP Q7K740
W	113	GLY	-	linker	UNP Q7K740
W	114	SER	-	linker	UNP Q7K740
W	115	GLY	-	cloning artifact	UNP Q7K740
W	116	THR	-	cloning artifact	UNP Q7K740
W	179	GLN	ASN	engineered mutation	UNP Q8IIK4
W	242	GLN	ASN	engineered mutation	UNP Q8IIK4
W	310	ASN	HIS	engineered mutation	UNP Q8IIK4
W	334	THR	-	cloning artifact	UNP Q8IIK4
W	335	GLY	-	cloning artifact	UNP Q8IIK4
W	444	GLY	-	linker	UNP Q7K740
W	445	GLY	-	linker	UNP Q7K740
W	446	SER	-	linker	UNP Q7K740
W	447	LEU	-	cloning artifact	UNP Q7K740
W	448	GLU	-	cloning artifact	UNP Q7K740
W	449	HIS	-	expression tag	UNP Q7K740
W	450	HIS	-	expression tag	UNP Q7K740
W	451	HIS	-	expression tag	UNP Q7K740
W	452	HIS	-	expression tag	UNP Q7K740
W	453	HIS	-	expression tag	UNP Q7K740
W	454	HIS	-	expression tag	UNP Q7K740
X	1	MET	-	initiating methionine	UNP Q7K740
X	2	THR	-	cloning artifact	UNP Q7K740
X	3	GLY	-	cloning artifact	UNP Q7K740
X	112	GLY	-	linker	UNP Q7K740
X	113	GLY	-	linker	UNP Q7K740
X	114	SER	-	linker	UNP Q7K740
X	115	GLY	-	cloning artifact	UNP Q7K740
X	116	THR	-	cloning artifact	UNP Q7K740
X	179	GLN	ASN	engineered mutation	UNP Q8IIK4

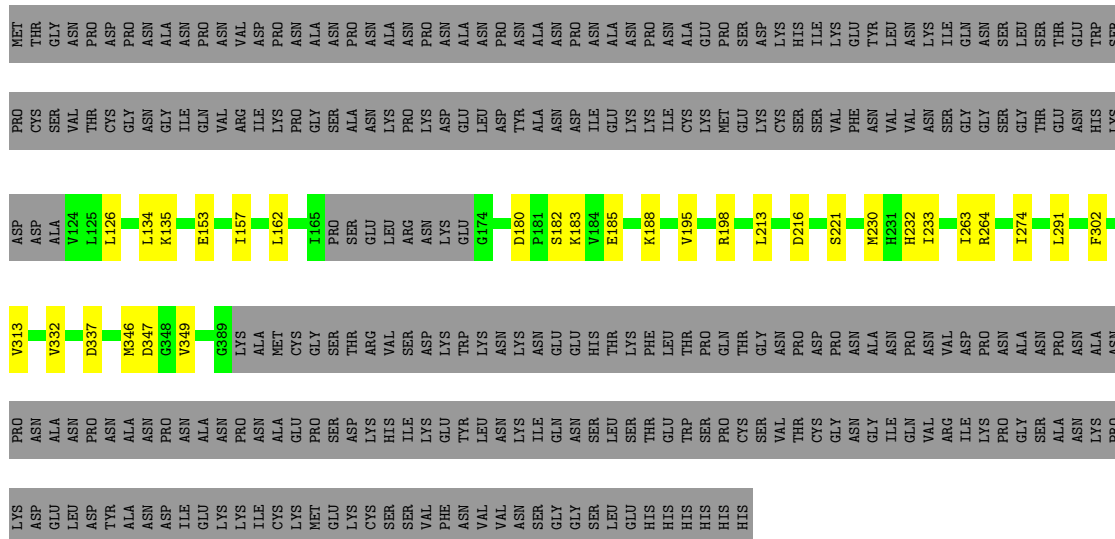
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Chain	Residue	Modelled	Actual	Comment	Reference
X	242	GLN	ASN	engineered mutation	UNP Q8IIK4
X	310	ASN	HIS	engineered mutation	UNP Q8IIK4
X	334	THR	-	cloning artifact	UNP Q8IIK4
X	335	GLY	-	cloning artifact	UNP Q8IIK4
X	444	GLY	-	linker	UNP Q7K740
X	445	GLY	-	linker	UNP Q7K740
X	446	SER	-	linker	UNP Q7K740
X	447	LEU	-	cloning artifact	UNP Q7K740
X	448	GLU	-	cloning artifact	UNP Q7K740
X	449	HIS	-	expression tag	UNP Q7K740
X	450	HIS	-	expression tag	UNP Q7K740
X	451	HIS	-	expression tag	UNP Q7K740
X	452	HIS	-	expression tag	UNP Q7K740
X	453	HIS	-	expression tag	UNP Q7K740
X	454	HIS	-	expression tag	UNP Q7K740

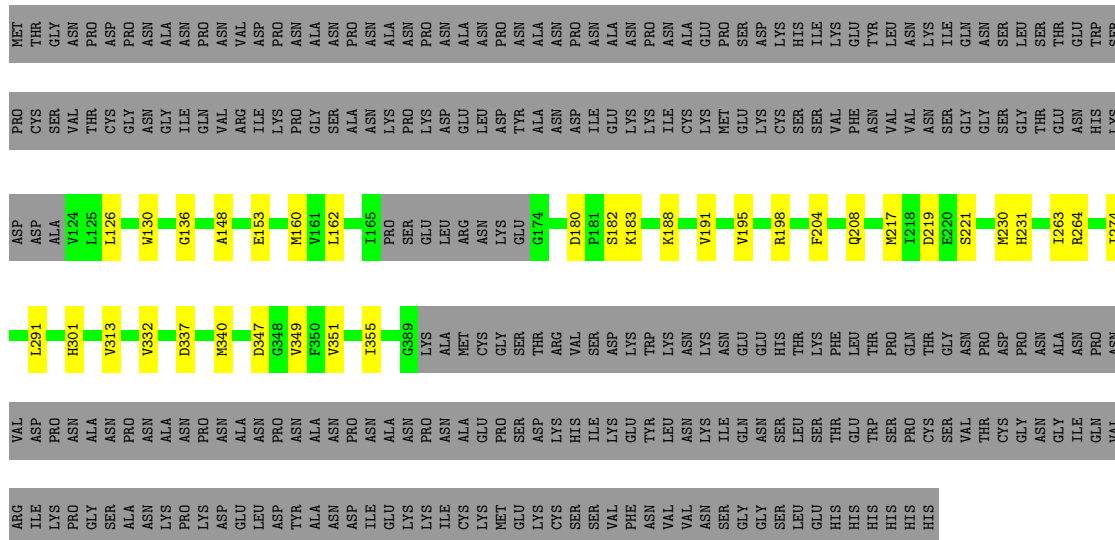
- Molecule 1: Circumsporozoite protein,Pyridoxal 5'-phosphate synthase subunit Pdx1

Chain C: 42% 6% 52%



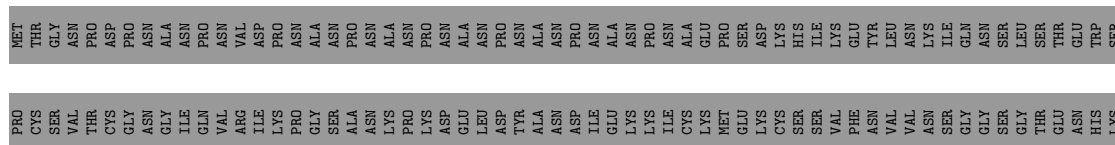
- Molecule 1: Circumsporozoite protein,Pyridoxal 5'-phosphate synthase subunit Pdx1

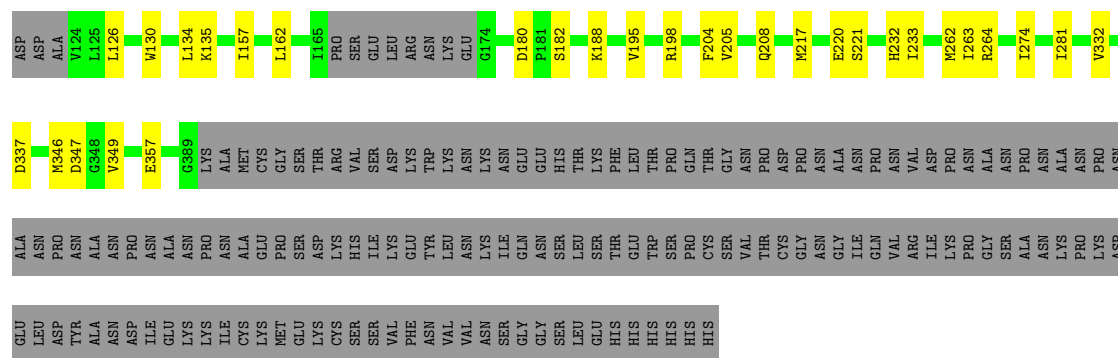
Chain D:  42% 6% 52%



- Molecule 1: Circumsporozoite protein,Pyridoxal 5'-phosphate synthase subunit Pdx1

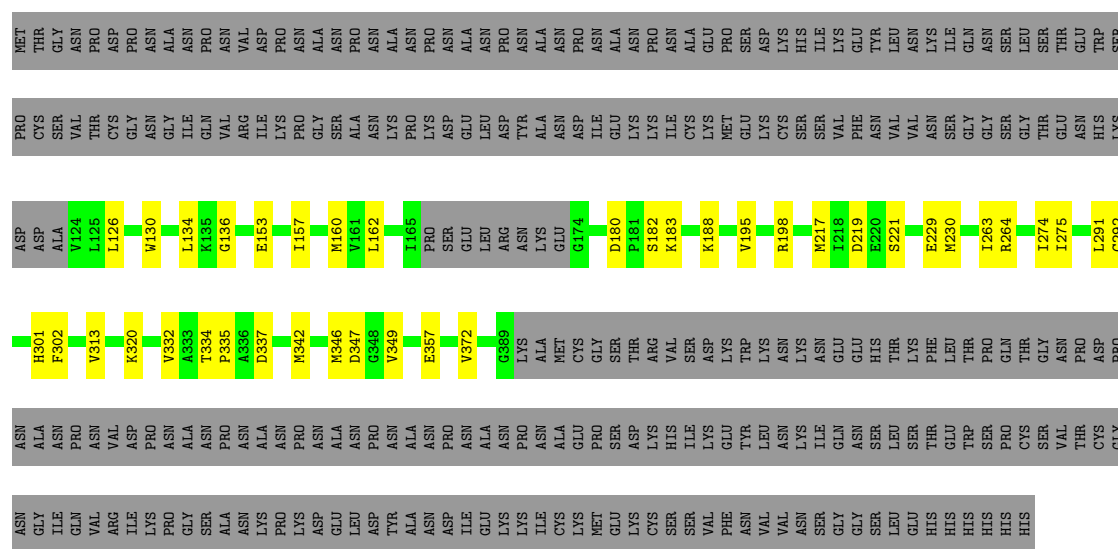
Chain E: 42% 6% 52%





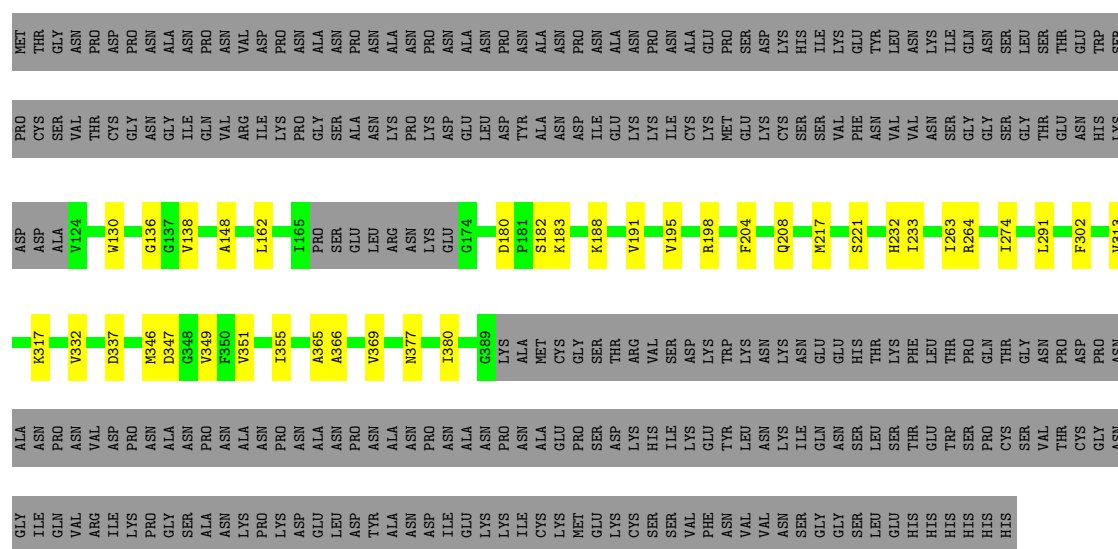
● Molecule 1: Circumsporozoite protein,Pyridoxal 5'-phosphate synthase subunit Pdx1

Chain F: 41% 7% 52%



● Molecule 1: Circumsporozoite protein,Pyridoxal 5'-phosphate synthase subunit Pdx1

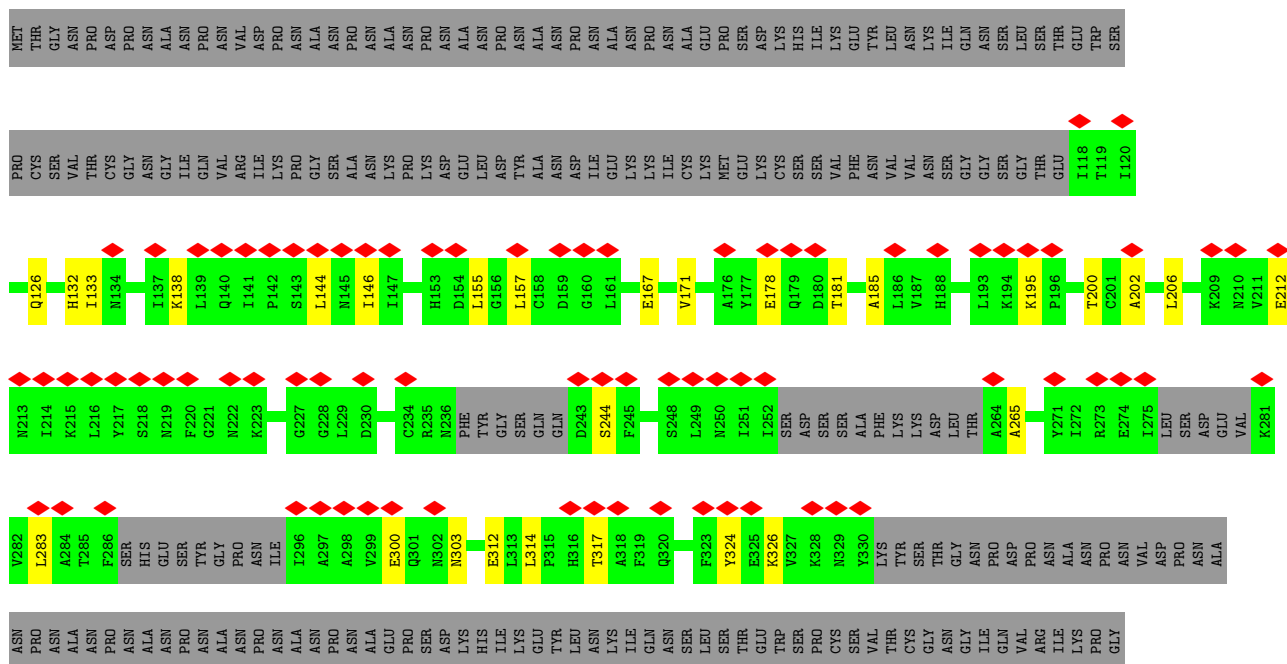
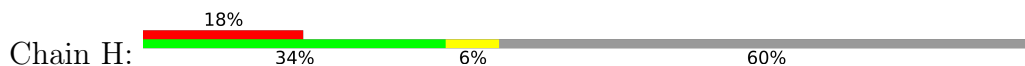
Chain M: 41% 7% 52%



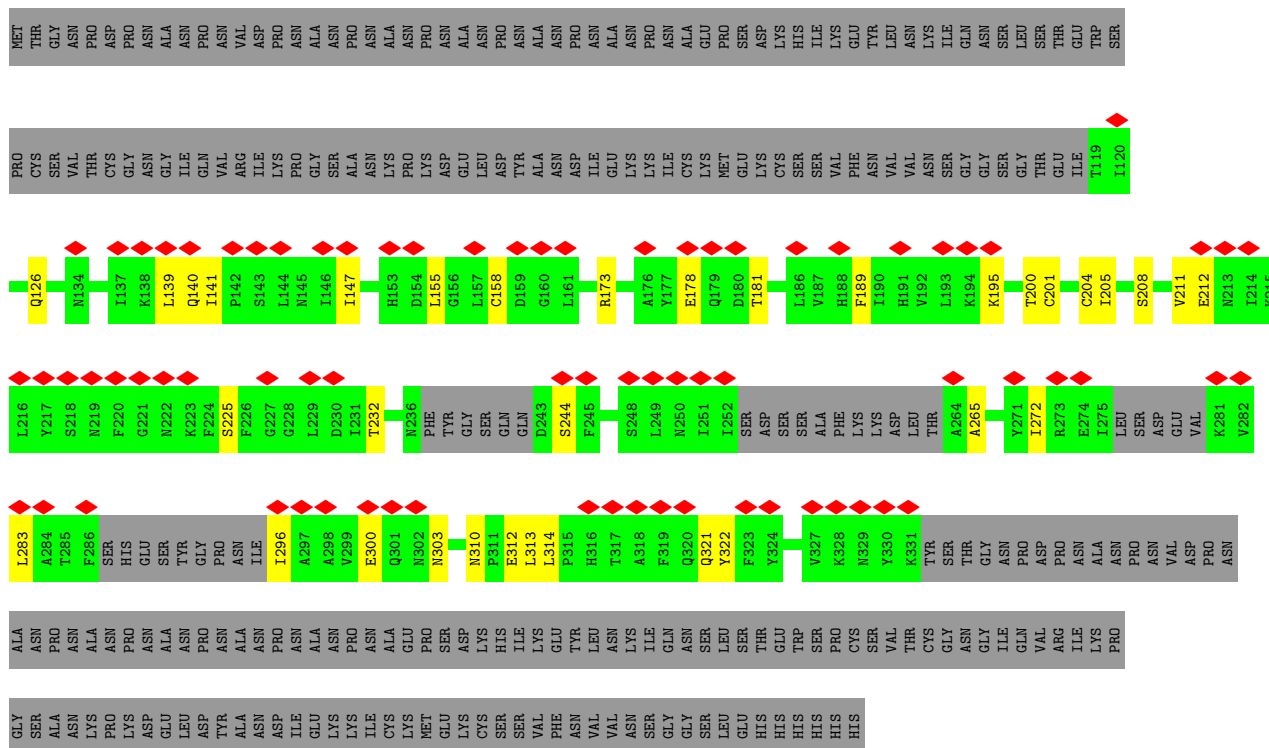
- Chain P: 41% 7% 52%

Category	Percentage
Green	41%
Yellow	7%
Grey	52%

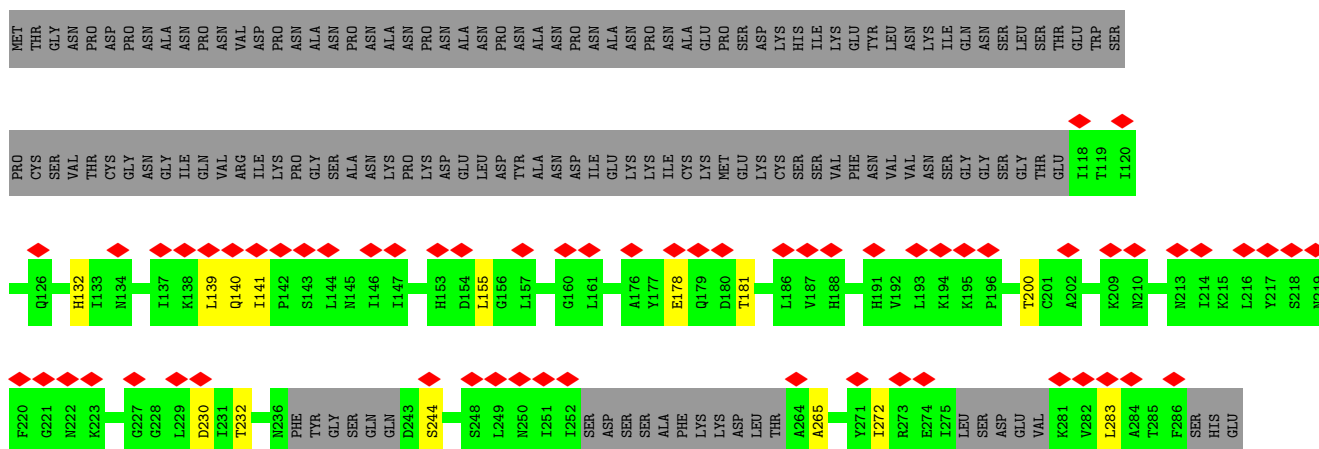
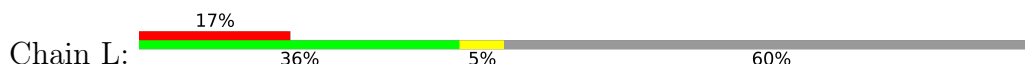
- Chain G: 



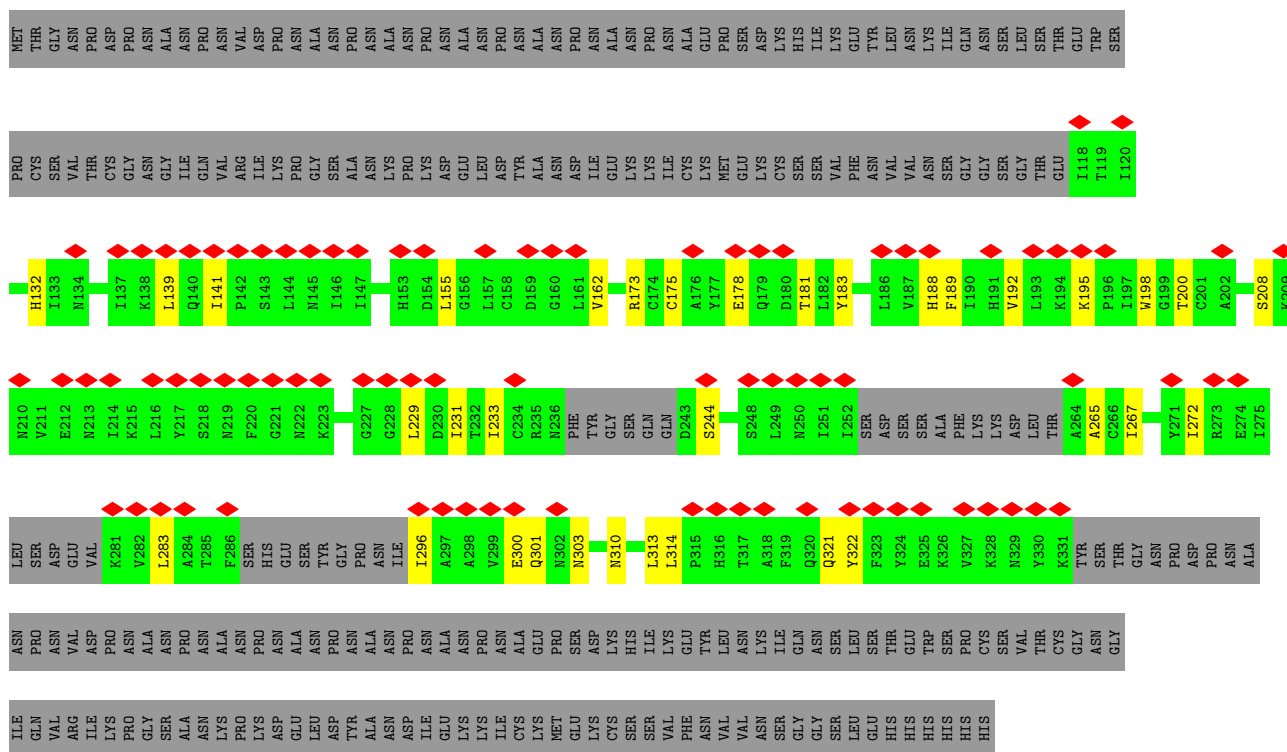
- Molecule 2: Circumsporozoite protein,Pyridoxal 5'-phosphate synthase subunit PDX2



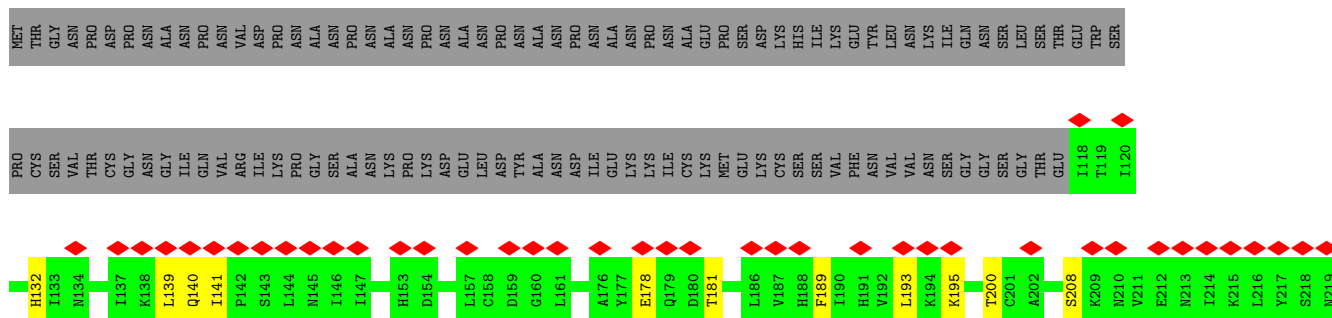
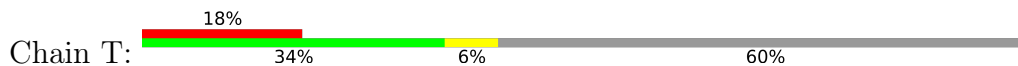
- Molecule 2: Circumsporozoite protein,Pyridoxal 5'-phosphate synthase subunit PDX2

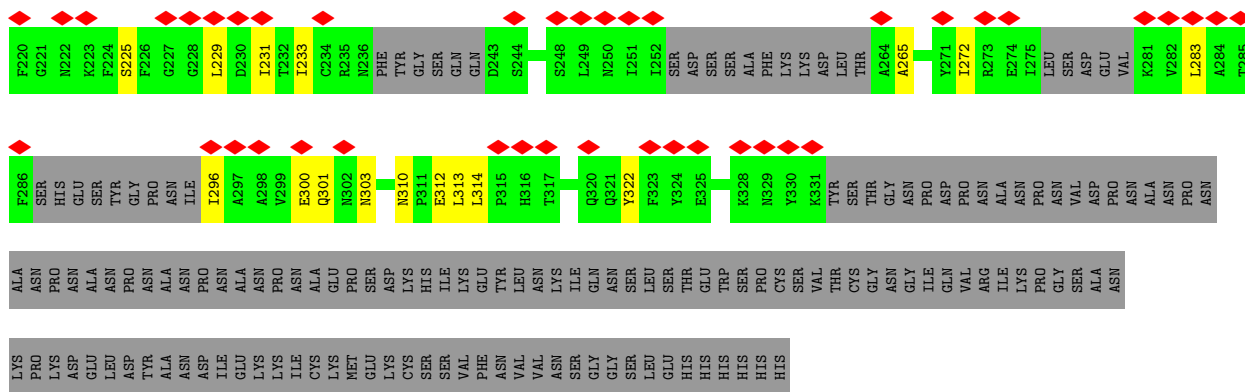


- Molecule 2: Circumsporozoite protein,Pyridoxal 5'-phosphate synthase subunit PDX2

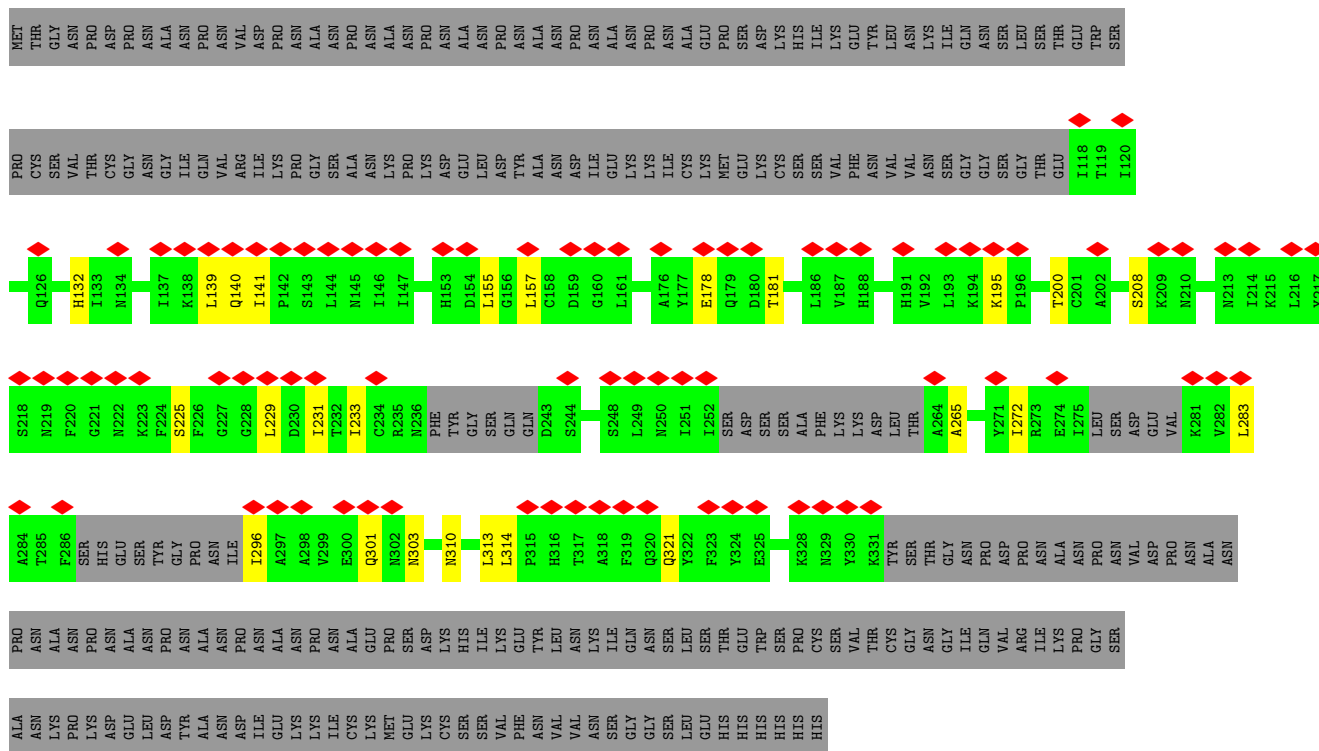
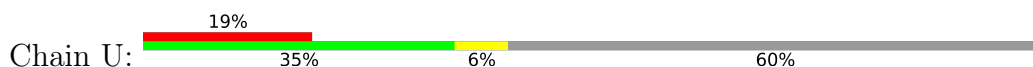


- Molecule 2: Circumsporozoite protein,Pyridoxal 5'-phosphate synthase subunit PDX2

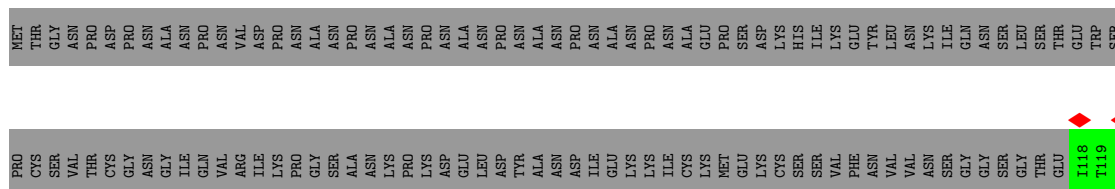
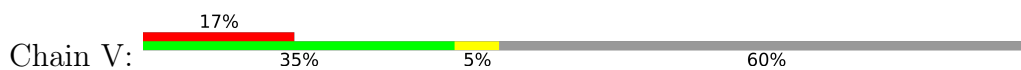


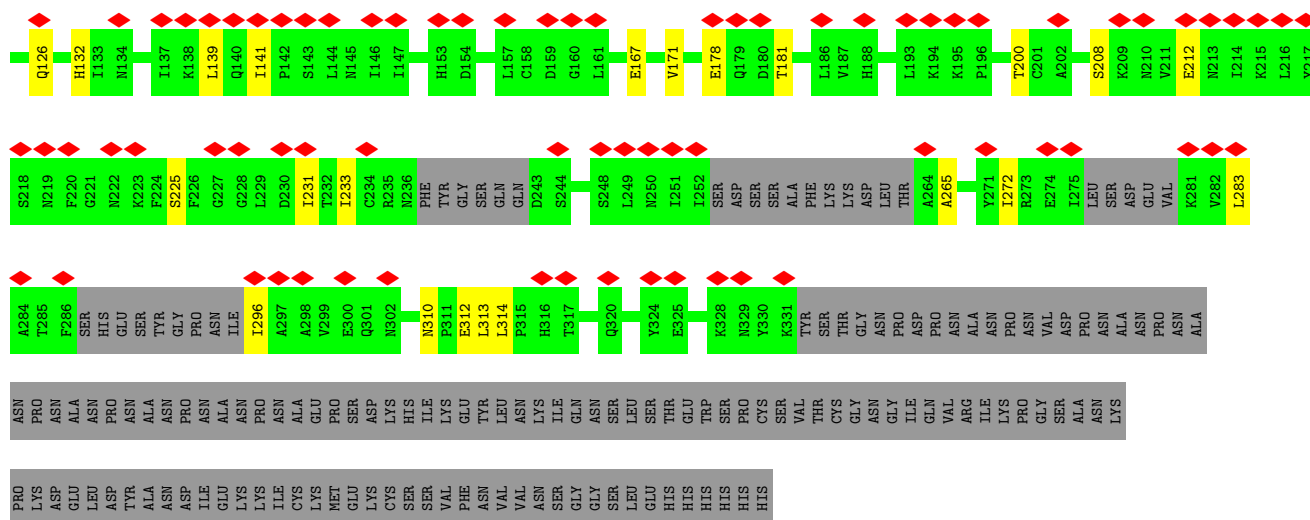


• Molecule 2: Circumsporozoite protein,Pyridoxal 5'-phosphate synthase subunit PDX2

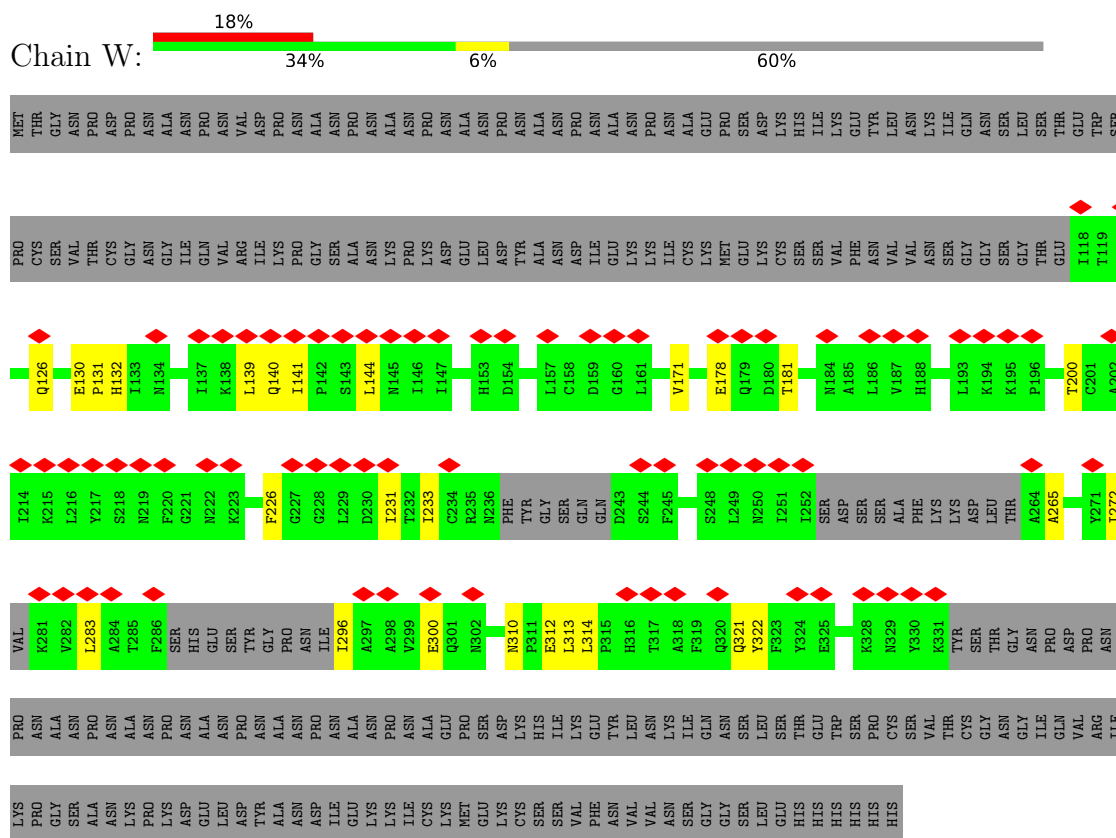


• Molecule 2: Circumsporozoite protein,Pyridoxal 5'-phosphate synthase subunit PDX2

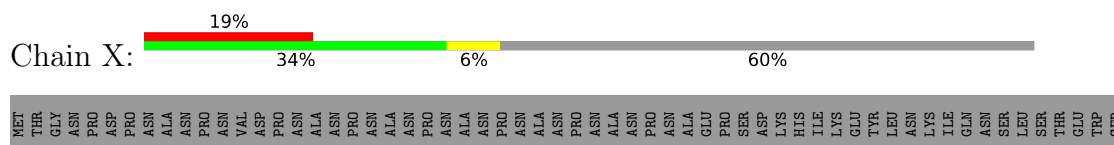


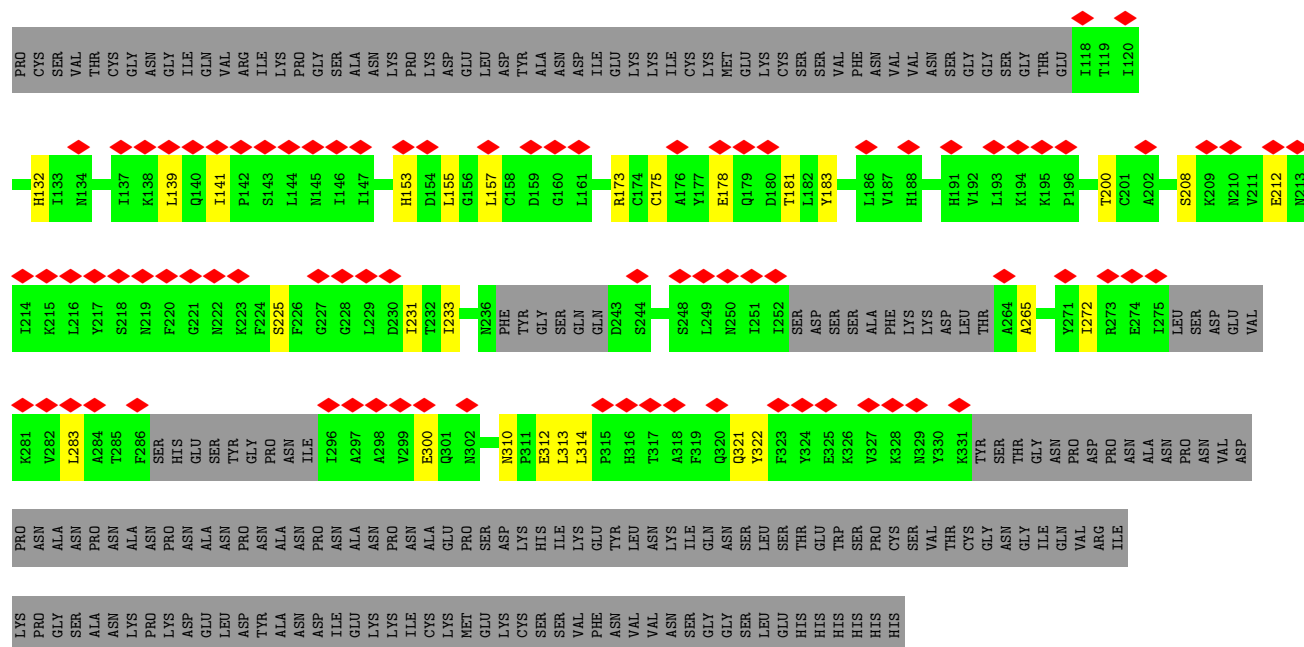


• Molecule 2: Circumsporozoite protein,Pyridoxal 5'-phosphate synthase subunit PDX2



• Molecule 2: Circumsporozoite protein,Pyridoxal 5'-phosphate synthase subunit PDX2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	251050	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.8	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	29.141	Depositor
Minimum map value	-18.289	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.76	Depositor
Map size (\AA)	270.336, 270.336, 270.336	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.056, 1.056, 1.056	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	0.23	0/1971	0.28	0/2653
1	B	0.22	0/1975	0.27	0/2658
1	C	0.22	0/1975	0.27	0/2658
1	D	0.22	0/1975	0.28	0/2658
1	E	0.22	0/1975	0.28	0/2658
1	F	0.22	0/1975	0.28	0/2658
1	M	0.22	0/1975	0.29	0/2658
1	N	0.22	0/1975	0.28	0/2658
1	O	0.22	0/1975	0.28	0/2658
1	P	0.22	0/1975	0.28	0/2658
1	Q	0.22	0/1975	0.28	0/2658
1	R	0.22	0/1975	0.28	0/2658
2	G	0.08	0/1470	0.23	0/1988
2	H	0.08	0/1461	0.23	0/1977
2	I	0.08	0/1461	0.24	0/1977
2	J	0.09	0/1461	0.24	0/1977
2	K	0.10	0/1462	0.25	0/1977
2	L	0.09	0/1470	0.23	0/1988
2	S	0.10	0/1470	0.26	0/1988
2	T	0.09	0/1470	0.23	0/1988
2	U	0.09	0/1470	0.23	0/1988
2	V	0.08	0/1470	0.22	0/1988
2	W	0.09	0/1470	0.25	0/1988
2	X	0.09	0/1470	0.24	0/1988
All	All	0.18	0/41301	0.26	0/55703

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	1947	2015	2015	24	0
1	B	1951	2018	2018	22	0
1	C	1951	2018	2018	21	0
1	D	1951	2018	2018	23	0
1	E	1951	2018	2018	22	0
1	F	1951	2018	2018	27	0
1	M	1951	2018	2018	27	0
1	N	1951	2018	2018	23	0
1	O	1951	2018	2018	16	0
1	P	1951	2018	2018	32	0
1	Q	1951	2018	2018	26	0
1	R	1951	2018	2018	16	0
2	G	1442	1458	1455	14	0
2	H	1433	1446	1442	18	0
2	I	1433	1446	1442	22	0
2	J	1433	1446	1440	20	0
2	K	1434	1448	1444	27	0
2	L	1442	1459	1455	15	0
2	S	1442	1458	1455	26	0
2	T	1442	1458	1455	16	0
2	U	1442	1458	1455	19	0
2	V	1442	1458	1455	15	0
2	W	1442	1458	1455	18	0
2	X	1442	1458	1455	21	0
All	All	40677	41664	41621	476	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 6.

All (476) 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:O:180:ASP:OD2	1:O:182:SER:OG	1.83	0.96
1:B:180:ASP:OD2	1:B:182:SER:OG	1.85	0.93
1:P:134:LEU:HD23	1:P:262:MET:HE1	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:LEU:HD23	1:E:262:MET:HE1	1.60	0.84
1:N:180:ASP:OD1	1:N:182:SER:OG	1.96	0.83
1:C:180:ASP:OD1	1:C:182:SER:OG	1.96	0.83
1:Q:180:ASP:OD1	1:Q:182:SER:OG	1.97	0.81
1:B:357:GLU:N	1:B:357:GLU:OE2	2.13	0.81
1:A:180:ASP:OD1	1:A:182:SER:OG	1.97	0.80
1:R:180:ASP:OD1	1:R:182:SER:OG	2.03	0.77
1:E:357:GLU:OE2	1:E:357:GLU:N	2.18	0.76
1:M:332:VAL:HG11	1:M:349:VAL:HG11	1.66	0.76
1:A:332:VAL:HG11	1:A:349:VAL:HG11	1.68	0.76
1:D:332:VAL:HG11	1:D:349:VAL:HG11	1.68	0.74
1:M:180:ASP:OD1	1:M:182:SER:OG	2.05	0.74
1:F:357:GLU:OE2	1:F:357:GLU:N	2.21	0.74
2:J:296:ILE:HD12	2:J:296:ILE:O	1.87	0.73
2:L:300:GLU:OE1	2:L:322:TYR:OH	2.05	0.73
1:B:126:LEU:HD21	2:I:244:SER:HB2	1.70	0.72
2:J:212:GLU:N	2:J:212:GLU:OE1	2.23	0.71
1:D:230:MET:HE1	1:Q:301:HIS:NE2	2.06	0.71
2:L:272:ILE:HD12	2:L:296:ILE:HD13	1.72	0.71
1:F:180:ASP:OD1	1:F:182:SER:OG	2.07	0.70
1:P:332:VAL:HG11	1:P:349:VAL:HG11	1.72	0.70
2:H:195:LYS:O	2:H:303:ASN:ND2	2.25	0.70
1:P:162:LEU:O	1:P:183:LYS:NZ	2.25	0.70
1:E:180:ASP:OD1	1:E:182:SER:OG	2.07	0.70
1:F:332:VAL:HG11	1:F:349:VAL:HG11	1.73	0.69
2:K:300:GLU:OE1	2:K:322:TYR:OH	2.10	0.69
1:E:332:VAL:HG11	1:E:349:VAL:HG11	1.75	0.69
1:C:162:LEU:O	1:C:183:LYS:NZ	2.26	0.68
2:U:296:ILE:HD12	2:U:296:ILE:O	1.93	0.68
2:H:212:GLU:N	2:H:212:GLU:OE1	2.28	0.67
2:H:178:GLU:O	2:H:181:THR:OG1	2.11	0.67
2:S:178:GLU:O	2:S:181:THR:OG1	2.12	0.67
2:G:300:GLU:OE1	2:G:322:TYR:OH	2.11	0.67
1:N:332:VAL:HG11	1:N:349:VAL:HG11	1.76	0.66
2:J:272:ILE:HD12	2:J:296:ILE:HD13	1.76	0.66
2:S:296:ILE:HD12	2:S:296:ILE:O	1.94	0.66
1:F:229:GLU:OE2	1:F:229:GLU:N	2.28	0.66
1:A:126:LEU:HD21	2:L:244:SER:HB2	1.77	0.66
2:I:178:GLU:O	2:I:181:THR:OG1	2.13	0.65
1:Q:332:VAL:HG11	1:Q:349:VAL:HG11	1.76	0.65
1:F:130:TRP:HZ3	1:F:217:MET:HE3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:300:GLU:OE1	2:S:322:TYR:OH	2.15	0.65
2:T:300:GLU:OE1	2:T:322:TYR:OH	2.14	0.65
2:X:178:GLU:O	2:X:181:THR:OG1	2.14	0.65
2:K:178:GLU:O	2:K:181:THR:OG1	2.15	0.64
2:V:296:ILE:HD12	2:V:296:ILE:O	1.98	0.64
1:C:126:LEU:HD21	2:J:244:SER:HB2	1.78	0.64
2:U:178:GLU:O	2:U:181:THR:OG1	2.15	0.63
2:I:139:LEU:HG	2:I:141:ILE:HD13	1.81	0.63
2:W:300:GLU:OE1	2:W:322:TYR:OH	2.17	0.63
2:K:195:LYS:O	2:K:303:ASN:ND2	2.31	0.62
2:W:178:GLU:O	2:W:181:THR:OG1	2.16	0.62
1:B:162:LEU:O	1:B:183:LYS:NZ	2.32	0.62
1:O:134:LEU:HG	1:O:157:ILE:HD12	1.80	0.62
1:Q:291:LEU:HD11	1:Q:313:VAL:HG13	1.81	0.62
2:X:139:LEU:HD21	2:X:141:ILE:HD12	1.80	0.61
2:V:178:GLU:O	2:V:181:THR:OG1	2.17	0.61
2:K:212:GLU:N	2:K:212:GLU:OE1	2.33	0.61
2:T:178:GLU:O	2:T:181:THR:OG1	2.19	0.61
1:Q:134:LEU:HG	1:Q:157:ILE:HD12	1.83	0.60
1:R:136:GLY:N	1:R:347:ASP:O	2.31	0.60
2:L:310:ASN:HB3	2:L:313:LEU:HD13	1.83	0.60
1:F:162:LEU:O	1:F:183:LYS:NZ	2.34	0.60
2:S:310:ASN:HB3	2:S:313:LEU:HD13	1.83	0.60
1:D:351:VAL:HG11	1:D:355:ILE:HD11	1.83	0.60
1:B:134:LEU:HG	1:B:157:ILE:HD12	1.83	0.60
2:T:310:ASN:HB3	2:T:313:LEU:HD13	1.84	0.60
2:W:296:ILE:HD12	2:W:296:ILE:O	2.02	0.59
1:C:291:LEU:HD11	1:C:313:VAL:HG13	1.84	0.59
1:M:180:ASP:OD1	1:M:182:SER:N	2.33	0.59
2:K:296:ILE:HD12	2:K:296:ILE:O	2.02	0.59
2:J:132:HIS:CE1	2:J:200:THR:HG21	2.38	0.59
1:B:153:GLU:OE2	1:B:362:ARG:NH2	2.34	0.59
1:Q:162:LEU:O	1:Q:183:LYS:NZ	2.32	0.58
1:A:134:LEU:HG	1:A:157:ILE:HD12	1.84	0.58
1:D:301:HIS:NE2	1:Q:230:MET:HE1	2.18	0.58
1:F:134:LEU:HG	1:F:157:ILE:HD12	1.85	0.58
1:Q:135:LYS:NZ	1:Q:347:ASP:OD2	2.36	0.58
1:B:291:LEU:HD11	1:B:313:VAL:HG13	1.85	0.57
2:H:132:HIS:NE2	2:H:200:THR:HG21	2.19	0.57
1:M:366:ALA:HB1	2:X:173:ARG:HH21	1.68	0.57
2:J:195:LYS:O	2:J:303:ASN:ND2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:140:GLN:O	2:I:141:ILE:HD12	2.05	0.57
1:Q:188:LYS:HA	1:Q:195:VAL:HG21	1.87	0.57
1:B:136:GLY:N	1:B:347:ASP:O	2.32	0.57
1:P:369:VAL:HG12	2:S:173:ARG:NH1	2.20	0.57
1:F:180:ASP:OD1	1:F:182:SER:N	2.38	0.56
1:E:134:LEU:HG	1:E:157:ILE:HD12	1.87	0.56
2:T:195:LYS:O	2:T:303:ASN:ND2	2.37	0.56
2:V:139:LEU:HD21	2:V:141:ILE:HD12	1.87	0.56
1:C:185:GLU:HG2	1:C:213:LEU:HD11	1.86	0.56
2:L:265:ALA:H	2:L:314:LEU:HD21	1.70	0.56
1:O:136:GLY:N	1:O:347:ASP:O	2.30	0.56
2:I:310:ASN:HB3	2:I:313:LEU:HD13	1.88	0.56
1:A:180:ASP:OD1	1:A:182:SER:N	2.38	0.56
1:M:291:LEU:HD11	1:M:313:VAL:HG13	1.86	0.56
1:R:332:VAL:HG21	1:R:349:VAL:CG2	2.36	0.56
1:E:134:LEU:CD2	1:E:262:MET:HE1	2.34	0.56
1:F:346:MET:HE2	1:F:346:MET:HA	1.88	0.56
1:N:160:MET:HE1	1:N:219:ASP:OD2	2.04	0.56
1:N:180:ASP:OD1	1:N:182:SER:N	2.38	0.56
1:P:134:LEU:HG	1:P:157:ILE:HD12	1.88	0.55
2:I:132:HIS:NE2	2:I:200:THR:HG21	2.21	0.55
1:B:162:LEU:HD21	1:B:198:ARG:HH12	1.70	0.55
1:E:162:LEU:HD21	1:E:198:ARG:NH1	2.21	0.55
2:J:178:GLU:O	2:J:181:THR:OG1	2.24	0.55
1:Q:180:ASP:OD1	1:Q:182:SER:N	2.39	0.55
1:M:162:LEU:O	1:M:183:LYS:NZ	2.36	0.55
1:O:291:LEU:HD11	1:O:313:VAL:HG13	1.88	0.55
1:D:126:LEU:HD21	2:G:244:SER:HB2	1.88	0.55
2:X:212:GLU:OE1	2:X:212:GLU:N	2.38	0.55
2:X:310:ASN:HB3	2:X:313:LEU:HD13	1.88	0.55
2:I:135:HIS:NE2	2:I:312:GLU:O	2.40	0.55
1:P:134:LEU:HD11	1:P:194:ASN:ND2	2.22	0.55
2:T:139:LEU:HD21	2:T:141:ILE:HD12	1.88	0.55
1:M:366:ALA:HB1	2:X:173:ARG:NH2	2.22	0.55
1:C:153:GLU:O	2:J:173:ARG:NE	2.39	0.54
1:D:162:LEU:O	1:D:183:LYS:NZ	2.40	0.54
1:P:291:LEU:HD11	1:P:313:VAL:HG13	1.90	0.54
1:C:134:LEU:HG	1:C:157:ILE:HD12	1.90	0.54
1:C:180:ASP:OD1	1:C:182:SER:N	2.40	0.54
2:K:140:GLN:O	2:K:141:ILE:HD12	2.07	0.54
2:S:272:ILE:HD12	2:S:296:ILE:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:132:HIS:NE2	2:X:200:THR:HG21	2.22	0.54
2:S:175:CYS:O	2:S:183:TYR:N	2.41	0.54
2:X:153:HIS:ND1	2:X:153:HIS:C	2.66	0.54
1:B:162:LEU:HD21	1:B:198:ARG:NH1	2.23	0.54
2:K:139:LEU:HG	2:K:141:ILE:HD13	1.89	0.54
1:P:180:ASP:OD1	1:P:182:SER:N	2.34	0.54
2:J:188:HIS:O	2:J:188:HIS:ND1	2.41	0.54
1:F:292:CYS:SG	1:F:320:LYS:NZ	2.80	0.53
1:N:134:LEU:HG	1:N:157:ILE:HD12	1.90	0.53
1:R:188:LYS:HA	1:R:195:VAL:HG21	1.90	0.53
1:E:281:ILE:HG23	1:E:346:MET:HE3	1.91	0.53
1:F:291:LEU:HD11	1:F:313:VAL:HG13	1.90	0.53
1:P:130:TRP:HZ3	1:P:217:MET:HE3	1.73	0.53
2:U:139:LEU:HD21	2:U:141:ILE:HD12	1.89	0.53
2:L:139:LEU:HD21	2:L:141:ILE:HD12	1.90	0.53
2:G:310:ASN:HB3	2:G:313:LEU:HD13	1.90	0.53
1:N:162:LEU:O	1:N:183:LYS:NZ	2.33	0.53
1:P:180:ASP:OD1	1:P:182:SER:OG	2.23	0.53
2:T:231:ILE:HD12	2:T:233:ILE:HD11	1.90	0.53
2:U:195:LYS:O	2:U:303:ASN:ND2	2.41	0.53
1:E:126:LEU:HD21	2:H:244:SER:HB2	1.90	0.53
2:L:178:GLU:O	2:L:181:THR:OG1	2.26	0.53
2:G:132:HIS:NE2	2:G:200:THR:HG21	2.24	0.53
2:S:195:LYS:O	2:S:303:ASN:ND2	2.37	0.53
1:C:188:LYS:HA	1:C:195:VAL:HG21	1.91	0.52
2:K:310:ASN:HB3	2:K:313:LEU:HD13	1.91	0.52
2:G:195:LYS:O	2:G:303:ASN:ND2	2.38	0.52
2:J:206:LEU:O	2:J:226:PHE:N	2.42	0.52
2:K:321:GLN:C	2:K:321:GLN:OE1	2.53	0.52
1:D:162:LEU:HD11	1:D:198:ARG:NH1	2.24	0.52
2:G:312:GLU:OE1	2:G:312:GLU:N	2.38	0.52
1:N:130:TRP:HZ3	1:N:217:MET:HE3	1.75	0.52
2:U:233:ILE:HD12	2:U:272:ILE:HG12	1.92	0.52
1:P:188:LYS:HA	1:P:195:VAL:HG21	1.92	0.52
1:M:274:ILE:HD12	1:M:337:ASP:HB3	1.91	0.52
1:P:366:ALA:HB1	2:S:173:ARG:HH21	1.75	0.52
2:V:132:HIS:NE2	2:V:200:THR:HG21	2.25	0.52
2:V:231:ILE:HD12	2:V:233:ILE:HD11	1.90	0.52
1:O:188:LYS:HA	1:O:195:VAL:HG21	1.92	0.52
1:M:346:MET:HA	1:M:346:MET:HE2	1.92	0.52
2:K:272:ILE:HD12	2:K:296:ILE:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:321:GLN:C	2:L:321:GLN:OE1	2.54	0.51
1:O:162:LEU:O	1:O:183:LYS:NZ	2.42	0.51
1:D:274:ILE:HD12	1:D:337:ASP:HB3	1.93	0.51
1:E:220:GLU:OE1	1:E:232:HIS:ND1	2.40	0.51
1:F:301:HIS:CE1	1:O:230:MET:HE3	2.46	0.51
2:H:265:ALA:H	2:H:314:LEU:HD21	1.75	0.51
1:O:275:ILE:HD11	1:P:229:GLU:HB3	1.93	0.51
2:U:310:ASN:HB3	2:U:313:LEU:HD13	1.92	0.51
1:B:153:GLU:O	2:I:173:ARG:NE	2.41	0.51
1:F:153:GLU:O	2:K:173:ARG:NE	2.44	0.51
2:J:155:LEU:HD23	2:J:185:ALA:HB1	1.91	0.51
2:S:321:GLN:OE1	2:S:321:GLN:C	2.54	0.51
2:W:139:LEU:HD21	2:W:141:ILE:HD12	1.92	0.51
2:S:231:ILE:HD12	2:S:233:ILE:HD11	1.91	0.51
2:G:140:GLN:O	2:G:140:GLN:HG2	2.10	0.51
1:Q:136:GLY:N	1:Q:347:ASP:O	2.34	0.51
1:A:162:LEU:O	1:A:183:LYS:NZ	2.39	0.51
1:D:180:ASP:OD1	1:D:182:SER:N	2.40	0.51
2:K:155:LEU:C	2:K:155:LEU:HD23	2.36	0.51
1:P:366:ALA:O	2:S:173:ARG:NH2	2.37	0.51
1:Q:160:MET:HE1	1:Q:219:ASP:OD2	2.11	0.51
2:J:300:GLU:OE2	2:J:326:LYS:NZ	2.35	0.50
1:A:188:LYS:HA	1:A:195:VAL:HG21	1.93	0.50
1:F:274:ILE:HD12	1:F:337:ASP:HB3	1.92	0.50
1:Q:198:ARG:HD2	1:Q:221:SER:CB	2.41	0.50
2:W:321:GLN:C	2:W:321:GLN:OE1	2.54	0.50
2:X:300:GLU:OE1	2:X:322:TYR:OH	2.28	0.50
2:I:195:LYS:O	2:I:303:ASN:ND2	2.42	0.50
1:N:198:ARG:HD2	1:N:221:SER:CB	2.41	0.50
1:N:220:GLU:OE1	1:N:232:HIS:ND1	2.44	0.50
2:T:132:HIS:NE2	2:T:200:THR:HG21	2.26	0.50
1:A:160:MET:HE1	1:A:219:ASP:OD1	2.12	0.50
1:B:188:LYS:HA	1:B:195:VAL:HG21	1.93	0.50
1:C:135:LYS:NZ	1:C:347:ASP:OD2	2.43	0.50
1:E:188:LYS:HA	1:E:195:VAL:HG21	1.94	0.50
1:F:188:LYS:HA	1:F:195:VAL:HG21	1.94	0.50
2:U:321:GLN:OE1	2:U:321:GLN:C	2.54	0.50
1:E:180:ASP:OD1	1:E:182:SER:N	2.42	0.49
2:K:147:ILE:HD11	2:K:158:CYS:SG	2.51	0.49
1:M:291:LEU:HD12	1:M:302:PHE:CD2	2.47	0.49
2:U:155:LEU:C	2:U:155:LEU:HD23	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:162:LEU:O	1:R:183:LYS:NZ	2.42	0.49
2:U:272:ILE:HD12	2:U:296:ILE:HD13	1.94	0.49
2:K:205:ILE:HG23	2:K:211:VAL:HG11	1.94	0.49
1:M:188:LYS:HA	1:M:195:VAL:HG21	1.94	0.49
2:S:155:LEU:C	2:S:155:LEU:HD23	2.37	0.49
2:T:140:GLN:HG2	2:T:140:GLN:O	2.12	0.49
2:T:296:ILE:O	2:T:296:ILE:HD12	2.11	0.49
2:V:310:ASN:HB3	2:V:313:LEU:HD13	1.94	0.49
2:X:321:GLN:OE1	2:X:321:GLN:C	2.55	0.49
1:C:274:ILE:HD12	1:C:337:ASP:HB3	1.94	0.49
1:A:220:GLU:OE1	1:A:232:HIS:ND1	2.41	0.49
2:W:208:SER:OG	2:W:231:ILE:O	2.28	0.49
2:X:155:LEU:C	2:X:155:LEU:HD23	2.37	0.49
1:B:274:ILE:HD12	1:B:337:ASP:HB3	1.93	0.49
2:J:321:GLN:C	2:J:321:GLN:OE1	2.56	0.49
1:C:346:MET:HA	1:C:346:MET:HE2	1.95	0.49
2:V:212:GLU:OE1	2:V:212:GLU:N	2.44	0.48
1:O:135:LYS:NZ	1:O:347:ASP:OD2	2.45	0.48
1:P:134:LEU:HD23	1:P:262:MET:CE	2.38	0.48
2:W:231:ILE:HD12	2:W:233:ILE:HD11	1.94	0.48
1:D:188:LYS:HA	1:D:195:VAL:HG21	1.95	0.48
1:N:188:LYS:HA	1:N:195:VAL:HG21	1.95	0.48
2:I:157:LEU:HD23	2:I:157:LEU:O	2.14	0.48
1:R:274:ILE:HD12	1:R:337:ASP:HB3	1.95	0.48
2:S:162:VAL:HG12	2:S:198:TRP:HB3	1.94	0.48
2:K:200:THR:O	2:K:204:CYS:N	2.36	0.48
2:S:132:HIS:NE2	2:S:200:THR:HG21	2.29	0.48
1:F:230:MET:HA	1:F:230:MET:HE2	1.96	0.48
2:G:231:ILE:HD12	2:G:233:ILE:HD11	1.95	0.48
1:R:135:LYS:NZ	1:R:347:ASP:OD2	2.47	0.48
2:U:132:HIS:NE2	2:U:200:THR:HG21	2.29	0.48
1:P:369:VAL:HG12	2:S:173:ARG:HH12	1.78	0.47
1:Q:291:LEU:HD12	1:Q:302:PHE:CD2	2.49	0.47
2:W:132:HIS:NE2	2:W:200:THR:HG21	2.29	0.47
1:A:198:ARG:HD2	1:A:221:SER:CB	2.44	0.47
2:L:155:LEU:C	2:L:155:LEU:HD23	2.39	0.47
1:D:180:ASP:OD1	1:D:182:SER:OG	2.16	0.47
1:N:134:LEU:HD11	1:N:194:ASN:ND2	2.29	0.47
1:P:135:LYS:NZ	1:P:347:ASP:OD2	2.45	0.47
2:X:233:ILE:HD12	2:X:272:ILE:HG12	1.95	0.47
1:O:204:PHE:O	1:O:208:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:233:ILE:HD12	2:G:272:ILE:HG12	1.97	0.47
2:I:206:LEU:O	2:I:225:SER:OG	2.27	0.47
1:M:130:TRP:HZ3	1:M:217:MET:HE3	1.78	0.47
2:V:233:ILE:HD12	2:V:272:ILE:HG12	1.97	0.47
1:C:332:VAL:HG21	1:C:349:VAL:CG2	2.44	0.47
1:E:274:ILE:HD12	1:E:337:ASP:HB3	1.96	0.47
2:G:265:ALA:H	2:G:314:LEU:HD21	1.78	0.47
2:K:200:THR:OG1	2:K:201:CYS:N	2.42	0.47
1:P:274:ILE:HD12	1:P:337:ASP:HB3	1.95	0.47
1:A:274:ILE:HD12	1:A:337:ASP:HB3	1.96	0.47
1:D:130:TRP:HZ3	1:D:217:MET:HE3	1.79	0.47
2:K:283:LEU:HD13	2:K:283:LEU:C	2.40	0.47
2:X:157:LEU:HD23	2:X:157:LEU:O	2.15	0.47
1:E:162:LEU:HD21	1:E:198:ARG:HH12	1.80	0.47
2:H:133:ILE:HG23	2:H:146:ILE:HG21	1.95	0.47
1:N:136:GLY:N	1:N:347:ASP:O	2.35	0.47
1:C:291:LEU:HD12	1:C:302:PHE:CD2	2.51	0.47
2:I:140:GLN:C	2:I:141:ILE:HD12	2.40	0.47
1:C:198:ARG:HD2	1:C:221:SER:HB2	1.97	0.46
1:E:204:PHE:O	1:E:208:GLN:HG3	2.15	0.46
2:K:140:GLN:O	2:K:140:GLN:HG2	2.16	0.46
2:U:265:ALA:H	2:U:314:LEU:HD21	1.79	0.46
2:V:208:SER:OG	2:V:231:ILE:O	2.32	0.46
2:H:157:LEU:HD23	2:H:157:LEU:O	2.15	0.46
2:K:312:GLU:OE1	2:K:312:GLU:N	2.35	0.46
1:R:332:VAL:HG11	1:R:349:VAL:HG21	1.96	0.46
2:W:233:ILE:HD12	2:W:272:ILE:HG12	1.96	0.46
1:R:204:PHE:O	1:R:208:GLN:HG3	2.16	0.46
1:R:291:LEU:HD11	1:R:313:VAL:HG13	1.97	0.46
1:D:160:MET:HE1	1:D:219:ASP:OD2	2.15	0.46
2:I:283:LEU:HD13	2:I:283:LEU:C	2.41	0.46
1:M:198:ARG:HD2	1:M:221:SER:CB	2.46	0.46
1:Q:153:GLU:OE2	1:Q:362:ARG:NE	2.48	0.46
2:X:139:LEU:CD2	2:X:141:ILE:HD12	2.46	0.46
2:G:208:SER:O	2:G:225:SER:OG	2.24	0.46
2:L:283:LEU:C	2:L:283:LEU:HD13	2.41	0.46
2:S:283:LEU:HD13	2:S:283:LEU:C	2.41	0.46
1:D:136:GLY:N	1:D:347:ASP:O	2.34	0.45
1:F:291:LEU:HD12	1:F:302:PHE:CD2	2.51	0.45
1:D:291:LEU:HD11	1:D:313:VAL:HG13	1.97	0.45
2:U:231:ILE:HD12	2:U:233:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:283:LEU:C	2:V:283:LEU:HD13	2.41	0.45
2:W:265:ALA:H	2:W:314:LEU:HD21	1.80	0.45
1:B:160:MET:HE3	1:B:198:ARG:HD3	1.97	0.45
2:K:208:SER:O	2:K:225:SER:OG	2.33	0.45
2:U:283:LEU:HD13	2:U:283:LEU:C	2.41	0.45
2:W:283:LEU:HD13	2:W:283:LEU:C	2.41	0.45
2:X:231:ILE:HD12	2:X:233:ILE:HD11	1.98	0.45
2:T:283:LEU:C	2:T:283:LEU:HD13	2.42	0.45
2:X:208:SER:O	2:X:225:SER:OG	2.33	0.45
2:X:283:LEU:HD13	2:X:283:LEU:C	2.42	0.45
2:G:283:LEU:HD13	2:G:283:LEU:C	2.41	0.45
1:M:263:ILE:HG22	1:M:264:ARG:N	2.31	0.45
1:O:291:LEU:HD21	1:O:317:LYS:HB2	1.98	0.45
2:V:265:ALA:H	2:V:314:LEU:HD21	1.81	0.45
2:I:155:LEU:HD23	2:I:185:ALA:HB1	1.97	0.45
2:I:206:LEU:O	2:I:226:PHE:N	2.50	0.45
1:N:274:ILE:HD12	1:N:337:ASP:HB3	1.99	0.45
1:P:130:TRP:CZ3	1:P:217:MET:HE3	2.52	0.45
1:M:136:GLY:N	1:M:347:ASP:O	2.39	0.45
1:M:346:MET:HE2	1:M:346:MET:CA	2.47	0.45
1:M:377:ASN:OD1	1:M:380:ILE:HD12	2.17	0.45
2:T:208:SER:O	2:T:225:SER:OG	2.33	0.45
1:A:217:MET:HE1	1:A:243:VAL:HB	1.98	0.45
2:H:283:LEU:C	2:H:283:LEU:HD13	2.41	0.45
2:T:265:ALA:H	2:T:314:LEU:HD21	1.81	0.45
2:U:157:LEU:HD23	2:U:157:LEU:O	2.17	0.45
2:V:126:GLN:NE2	2:V:171:VAL:HG21	2.31	0.45
2:K:126:GLN:N	2:K:126:GLN:OE1	2.49	0.44
1:N:263:ILE:HG22	1:N:264:ARG:N	2.31	0.44
2:S:233:ILE:HD12	2:S:272:ILE:HG12	2.00	0.44
2:H:300:GLU:OE2	2:H:326:LYS:NZ	2.43	0.44
1:O:263:ILE:HG22	1:O:264:ARG:N	2.32	0.44
1:P:198:ARG:HD2	1:P:221:SER:HB2	1.99	0.44
2:X:175:CYS:O	2:X:183:TYR:N	2.51	0.44
2:L:132:HIS:NE2	2:L:200:THR:HG21	2.32	0.44
1:Q:220:GLU:OE1	1:Q:232:HIS:ND1	2.45	0.44
2:S:265:ALA:H	2:S:314:LEU:HD21	1.80	0.44
2:U:229:LEU:HD23	2:U:301:GLN:HB3	1.98	0.44
2:I:208:SER:O	2:I:225:SER:OG	2.35	0.44
2:J:310:ASN:HB3	2:J:313:LEU:HD13	2.00	0.44
1:R:263:ILE:HG22	1:R:264:ARG:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:312:GLU:OE1	2:T:312:GLU:N	2.40	0.44
1:P:204:PHE:O	1:P:208:GLN:HG3	2.18	0.44
2:S:229:LEU:HD23	2:S:301:GLN:HB3	1.98	0.44
1:C:263:ILE:HG22	1:C:264:ARG:N	2.33	0.44
2:H:126:GLN:NE2	2:H:171:VAL:HG21	2.33	0.44
2:K:155:LEU:HD21	2:K:189:PHE:CD2	2.53	0.44
2:T:229:LEU:HD23	2:T:301:GLN:HB3	1.99	0.44
1:D:162:LEU:HD11	1:D:198:ARG:HH12	1.81	0.44
1:D:198:ARG:HD3	1:D:221:SER:CB	2.48	0.44
2:H:138:LYS:HE2	2:H:317:THR:HG21	1.98	0.44
1:M:204:PHE:O	1:M:208:GLN:HG3	2.17	0.44
1:P:263:ILE:HG22	1:P:264:ARG:N	2.33	0.44
1:Q:217:MET:HE3	1:Q:243:VAL:HB	2.00	0.44
2:T:233:ILE:HD12	2:T:272:ILE:HG12	1.98	0.44
1:F:136:GLY:N	1:F:347:ASP:O	2.38	0.44
2:I:144:LEU:HD21	2:I:146:ILE:HD11	2.00	0.44
1:F:263:ILE:HG22	1:F:264:ARG:N	2.33	0.43
1:P:346:MET:HE2	1:P:346:MET:HA	2.00	0.43
2:X:265:ALA:H	2:X:314:LEU:HD21	1.82	0.43
2:H:202:ALA:O	2:H:206:LEU:HD22	2.18	0.43
2:K:265:ALA:H	2:K:314:LEU:HD21	1.82	0.43
1:N:291:LEU:HD11	1:N:313:VAL:HG13	2.00	0.43
2:W:140:GLN:O	2:W:140:GLN:HG2	2.17	0.43
1:D:263:ILE:HG22	1:D:264:ARG:N	2.33	0.43
1:M:347:ASP:OD1	1:M:347:ASP:N	2.51	0.43
1:N:291:LEU:HD21	1:N:317:LYS:HB2	2.01	0.43
2:W:310:ASN:HB3	2:W:313:LEU:HD13	2.01	0.43
2:J:206:LEU:O	2:J:225:SER:OG	2.36	0.43
2:L:140:GLN:O	2:L:140:GLN:HG2	2.18	0.43
1:M:198:ARG:HD2	1:M:221:SER:HB2	2.01	0.43
1:C:230:MET:HE3	1:R:301:HIS:CE1	2.54	0.43
2:H:312:GLU:OE1	2:H:312:GLU:N	2.41	0.43
1:P:126:LEU:HD11	2:S:244:SER:CB	2.49	0.43
2:U:139:LEU:CD2	2:U:141:ILE:HD12	2.49	0.43
1:B:134:LEU:HD23	1:B:262:MET:HE1	2.01	0.43
1:Q:128:HIS:NE2	1:Q:324:VAL:HG12	2.33	0.43
2:U:140:GLN:O	2:U:140:GLN:HG2	2.18	0.43
1:E:263:ILE:HG22	1:E:264:ARG:N	2.33	0.43
2:I:229:LEU:HD23	2:I:301:GLN:HB3	2.00	0.43
2:K:232:THR:O	2:K:272:ILE:HG23	2.19	0.43
1:Q:347:ASP:OD1	1:Q:347:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:PHE:O	1:D:208:GLN:HG3	2.18	0.43
1:B:263:ILE:HG22	1:B:264:ARG:N	2.33	0.43
1:M:332:VAL:HG21	1:M:349:VAL:HG13	2.01	0.43
2:T:189:PHE:HA	2:T:193:LEU:HD23	2.01	0.43
1:F:160:MET:HE1	1:F:219:ASP:OD2	2.19	0.42
2:J:162:VAL:HG23	2:J:162:VAL:O	2.19	0.42
1:M:355:ILE:HG21	1:M:365:ALA:HB2	2.01	0.42
1:A:135:LYS:NZ	1:A:347:ASP:OD2	2.51	0.42
1:A:263:ILE:HG22	1:A:264:ARG:N	2.33	0.42
1:D:148:ALA:HB1	1:D:191:VAL:HG11	2.00	0.42
1:D:153:GLU:O	2:G:173:ARG:NE	2.52	0.42
1:P:291:LEU:HD12	1:P:302:PHE:CD2	2.54	0.42
2:W:126:GLN:NE2	2:W:171:VAL:HG21	2.34	0.42
1:M:232:HIS:O	1:M:233:ILE:C	2.62	0.42
1:N:347:ASP:OD1	1:N:347:ASP:N	2.51	0.42
2:X:208:SER:OG	2:X:231:ILE:O	2.33	0.42
1:A:229:GLU:HB3	1:F:275:ILE:HD11	2.01	0.42
1:B:126:LEU:HD21	2:I:244:SER:CB	2.46	0.42
1:B:291:LEU:HD12	1:B:302:PHE:CD2	2.54	0.42
1:E:130:TRP:HZ3	1:E:217:MET:HE3	1.84	0.42
1:F:347:ASP:N	1:F:347:ASP:OD1	2.51	0.42
2:J:188:HIS:HD1	2:J:188:HIS:C	2.28	0.42
2:X:312:GLU:OE1	2:X:312:GLU:N	2.40	0.42
1:D:340:MET:HA	1:E:205:VAL:HG21	2.01	0.42
1:F:126:LEU:HD21	2:K:244:SER:CB	2.49	0.42
2:L:232:THR:O	2:L:272:ILE:HG23	2.20	0.42
1:N:340:MET:HA	1:O:205:VAL:HG21	2.01	0.42
2:U:208:SER:O	2:U:225:SER:OG	2.26	0.42
1:N:309:PRO:O	1:N:313:VAL:HG23	2.19	0.42
2:U:208:SER:OG	2:U:231:ILE:O	2.35	0.42
1:C:232:HIS:O	1:C:233:ILE:C	2.63	0.42
1:F:342:MET:SD	1:F:372:VAL:HG13	2.60	0.42
1:P:136:GLY:N	1:P:347:ASP:O	2.37	0.42
2:S:188:HIS:CD2	2:S:192:VAL:HG21	2.55	0.42
1:B:198:ARG:HD2	1:B:221:SER:HB2	2.02	0.42
1:O:232:HIS:O	1:O:233:ILE:C	2.63	0.42
2:L:139:LEU:CD2	2:L:141:ILE:HD12	2.50	0.42
1:P:275:ILE:HD11	1:Q:229:GLU:HB3	2.01	0.42
1:P:357:GLU:OE2	1:P:357:GLU:CA	2.68	0.42
1:C:216:ASP:OD1	2:J:268:ARG:NH2	2.53	0.41
1:D:231:HIS:NE2	1:Q:298:GLU:OE1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:ARG:HD2	1:E:221:SER:HB2	2.02	0.41
1:F:198:ARG:HD2	1:F:221:SER:HB2	2.02	0.41
1:O:198:ARG:HD2	1:O:221:SER:HB2	2.01	0.41
1:C:185:GLU:CG	1:C:213:LEU:HD11	2.50	0.41
1:P:198:ARG:HD2	1:P:221:SER:CB	2.49	0.41
1:Q:263:ILE:HG22	1:Q:264:ARG:N	2.34	0.41
2:H:155:LEU:HD23	2:H:185:ALA:HB1	2.02	0.41
1:N:232:HIS:O	1:N:233:ILE:C	2.63	0.41
2:S:139:LEU:HG	2:S:141:ILE:HG13	2.01	0.41
2:S:155:LEU:HD21	2:S:189:PHE:CD2	2.55	0.41
2:W:312:GLU:OE1	2:W:312:GLU:N	2.42	0.41
2:H:167:GLU:O	2:H:171:VAL:HG23	2.20	0.41
2:J:300:GLU:OE1	2:J:322:TYR:OH	2.29	0.41
1:Q:362:ARG:NH1	1:Q:362:ARG:HB2	2.35	0.41
1:A:136:GLY:N	1:A:347:ASP:O	2.33	0.41
1:C:198:ARG:HD2	1:C:221:SER:CB	2.49	0.41
1:E:126:LEU:HD11	2:H:244:SER:HB3	2.02	0.41
1:M:291:LEU:HD21	1:M:317:LYS:HB2	2.02	0.41
2:V:167:GLU:O	2:V:171:VAL:HG23	2.21	0.41
1:B:130:TRP:HZ3	1:B:217:MET:CE	2.33	0.41
1:E:135:LYS:NZ	1:E:347:ASP:OD1	2.52	0.41
1:E:232:HIS:O	1:E:233:ILE:C	2.64	0.41
2:H:144:LEU:HD23	2:H:324:TYR:CD1	2.55	0.41
1:A:291:LEU:HD11	1:A:313:VAL:HG13	2.02	0.41
1:A:347:ASP:OD1	1:A:347:ASP:N	2.53	0.41
1:B:232:HIS:O	1:B:233:ILE:C	2.64	0.41
1:F:346:MET:HE2	1:F:346:MET:CA	2.49	0.41
2:I:212:GLU:OE1	2:I:212:GLU:N	2.53	0.41
1:M:351:VAL:HG12	1:M:355:ILE:HD13	2.03	0.41
2:V:208:SER:O	2:V:225:SER:OG	2.34	0.41
1:A:230:MET:HE1	1:N:301:HIS:CE1	2.56	0.41
2:G:208:SER:OG	2:G:231:ILE:O	2.37	0.41
2:J:211:VAL:HG12	2:J:233:ILE:HB	2.03	0.41
2:K:200:THR:O	2:K:201:CYS:C	2.64	0.41
2:W:144:LEU:C	2:W:144:LEU:HD13	2.46	0.41
1:A:355:ILE:HG13	1:A:364:MET:HG3	2.04	0.40
1:B:291:LEU:HD21	1:B:317:LYS:HB2	2.02	0.40
1:Q:357:GLU:OE2	1:Q:357:GLU:CA	2.69	0.40
1:R:275:ILE:HG23	1:R:276:GLU:N	2.36	0.40
2:S:208:SER:OG	2:S:231:ILE:O	2.36	0.40
1:A:162:LEU:HD21	1:A:198:ARG:NH1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:134:LEU:HD23	1:N:262:MET:CE	2.52	0.40
1:A:217:MET:CE	1:A:243:VAL:HB	2.52	0.40
1:A:334:THR:HG22	1:A:335:PRO:HD2	2.02	0.40
2:L:230:ASP:OD1	2:L:230:ASP:N	2.54	0.40
1:M:138:VAL:HG21	1:M:369:VAL:HA	2.03	0.40
1:P:232:HIS:O	1:P:233:ILE:C	2.63	0.40
1:Q:232:HIS:O	1:Q:233:ILE:C	2.64	0.40
1:R:232:HIS:O	1:R:233:ILE:C	2.63	0.40
2:W:130:GLU:HB3	2:W:131:PRO:HD3	2.03	0.40
1:A:144:SER:OG	1:A:146:GLU:OE1	2.38	0.40
2:I:147:ILE:HD11	2:I:158:CYS:SG	2.61	0.40
2:K:296:ILE:HD12	2:K:296:ILE:C	2.46	0.40
1:P:134:LEU:HD11	1:P:194:ASN:HD22	1.85	0.40
1:R:130:TRP:HZ3	1:R:217:MET:CE	2.34	0.40
2:V:312:GLU:OE1	2:V:312:GLU:N	2.41	0.40
1:F:334:THR:HG22	1:F:335:PRO:HD2	2.04	0.40
2:I:200:THR:O	2:I:201:CYS:C	2.63	0.40
1:M:148:ALA:HB1	1:M:191:VAL:HG11	2.03	0.40
1:N:275:ILE:HD11	1:O:229:GLU:HB3	2.03	0.40
1:P:126:LEU:HD12	2:S:267:ILE:HD12	2.04	0.40
1:Q:340:MET:HA	1:R:205:VAL:HG21	2.04	0.40
2:W:206:LEU:O	2:W:226:PHE:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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.

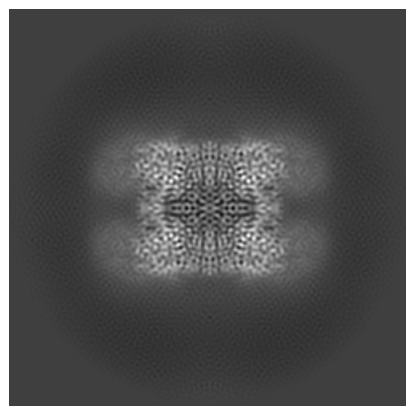
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45440. These allow visual inspection of the internal detail of the map and identification of artifacts.

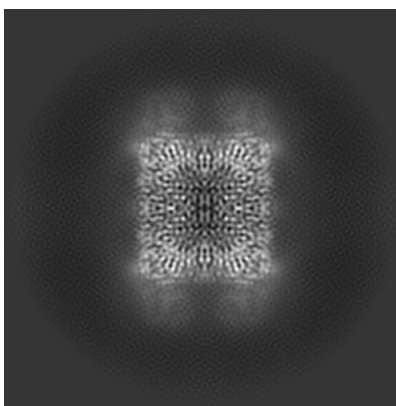
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

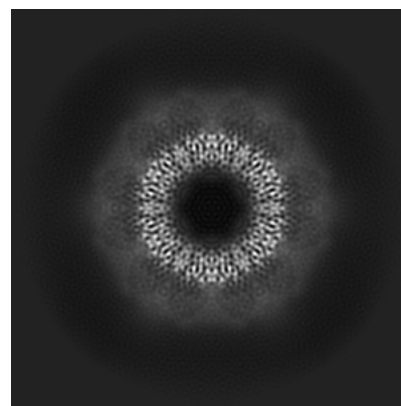
6.1.1 Primary map



X

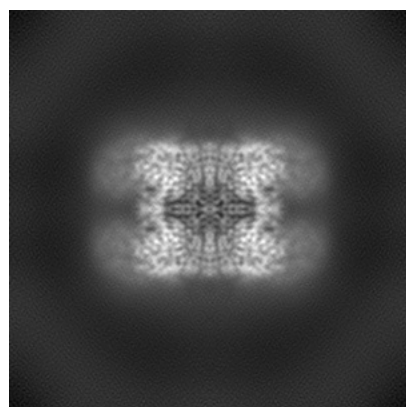


Y

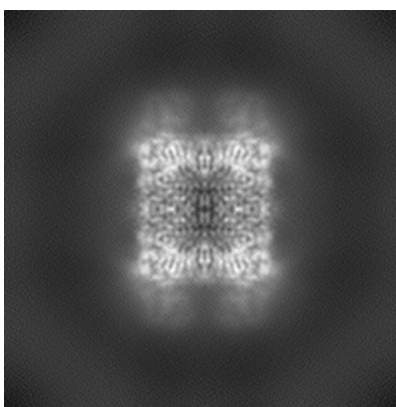


Z

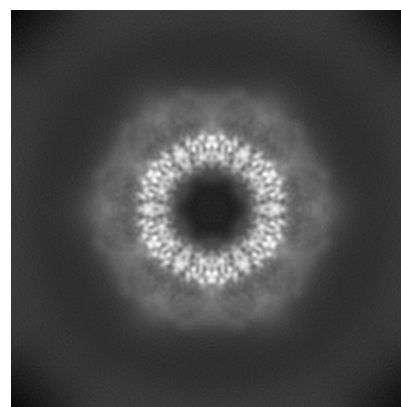
6.1.2 Raw map



X



Y

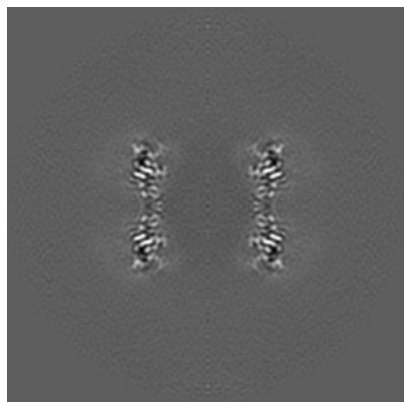


Z

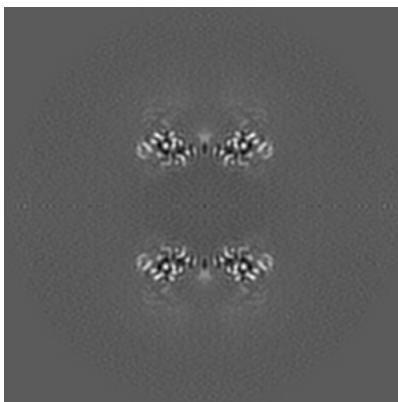
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

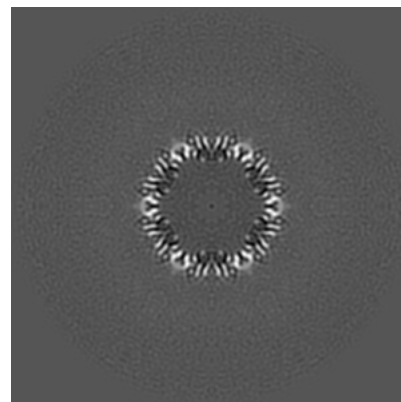
6.2.1 Primary map



X Index: 128

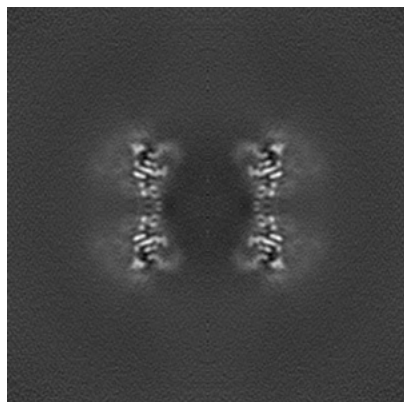


Y Index: 128

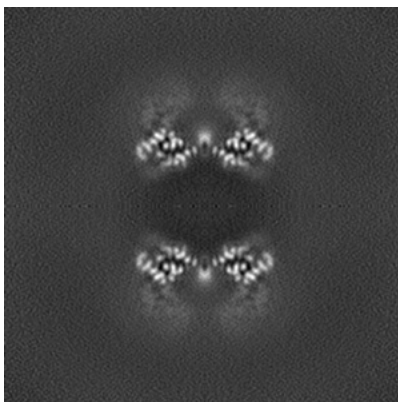


Z Index: 128

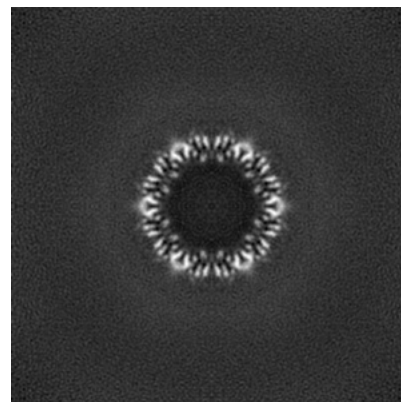
6.2.2 Raw map



X Index: 128



Y Index: 128

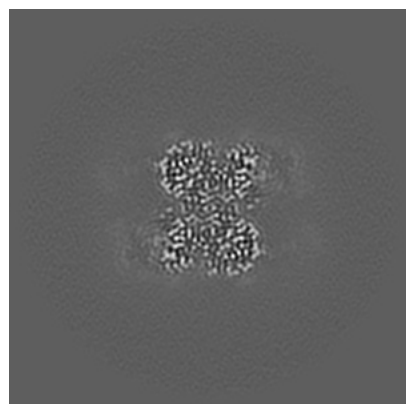


Z Index: 128

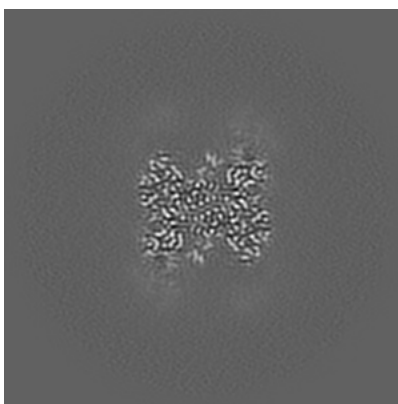
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

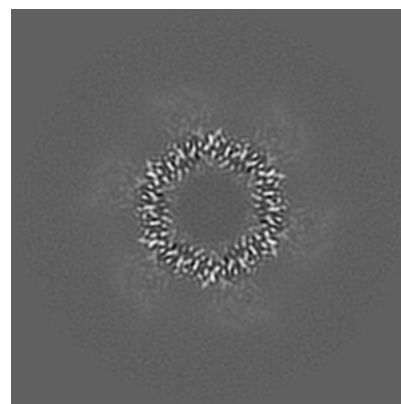
6.3.1 Primary map



X Index: 92

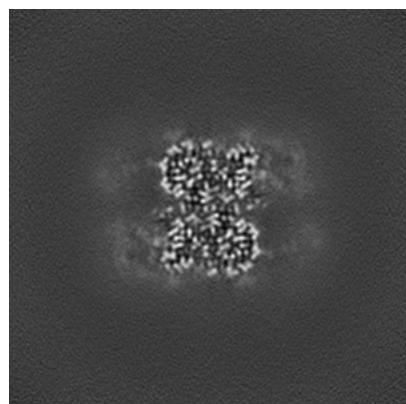


Y Index: 93

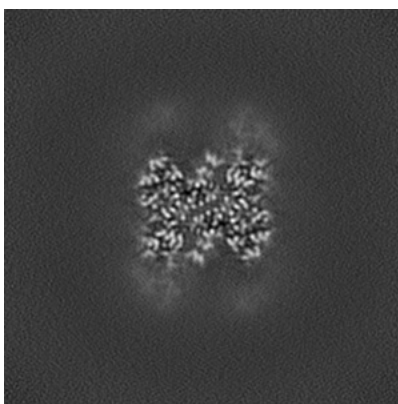


Z Index: 108

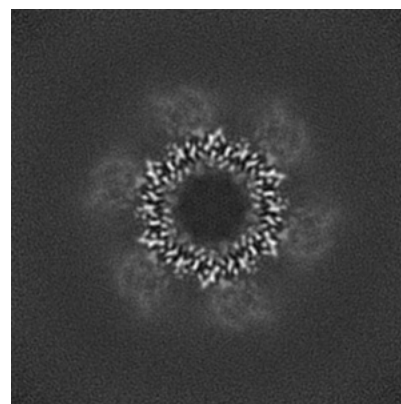
6.3.2 Raw map



X Index: 92



Y Index: 93

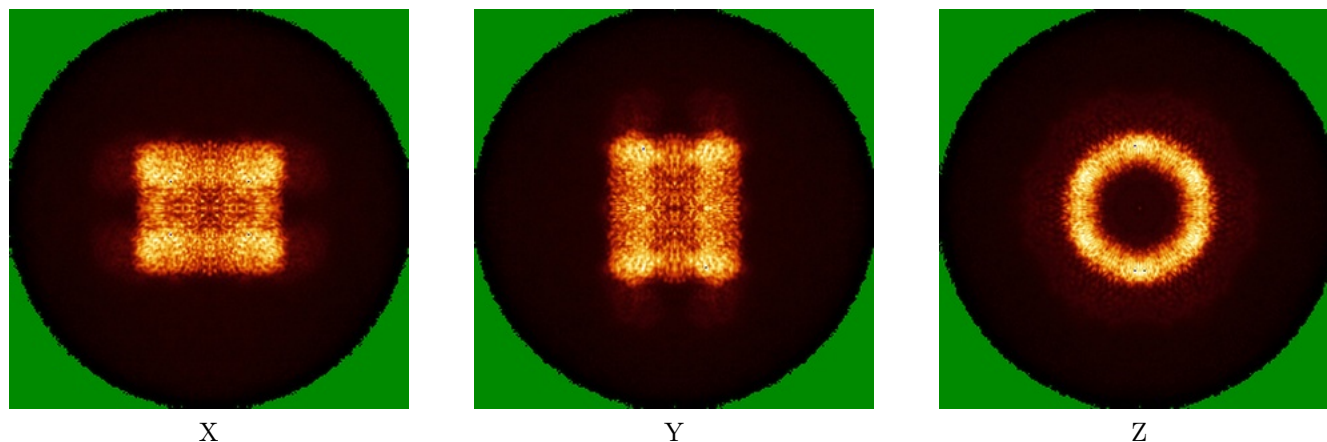


Z Index: 108

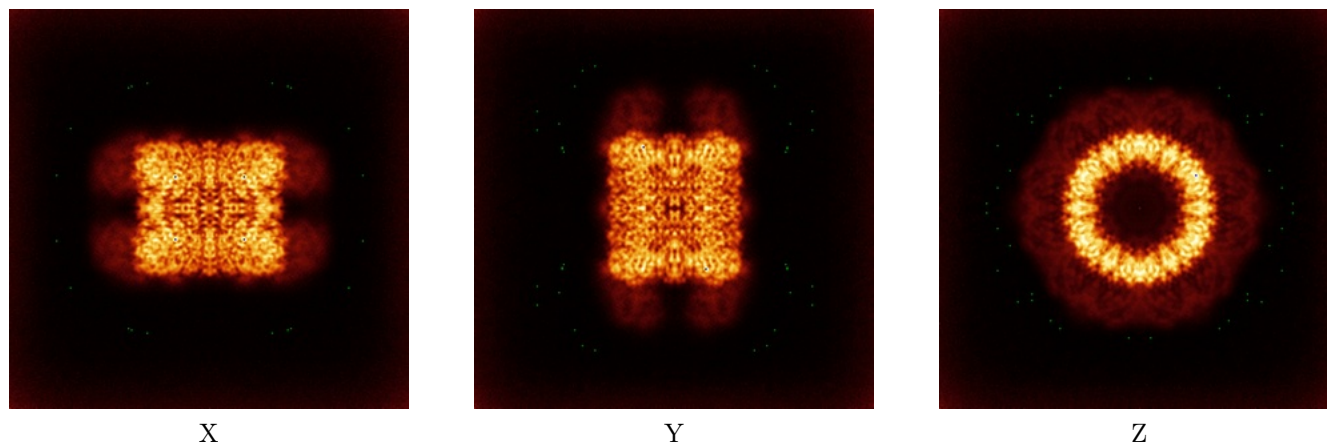
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



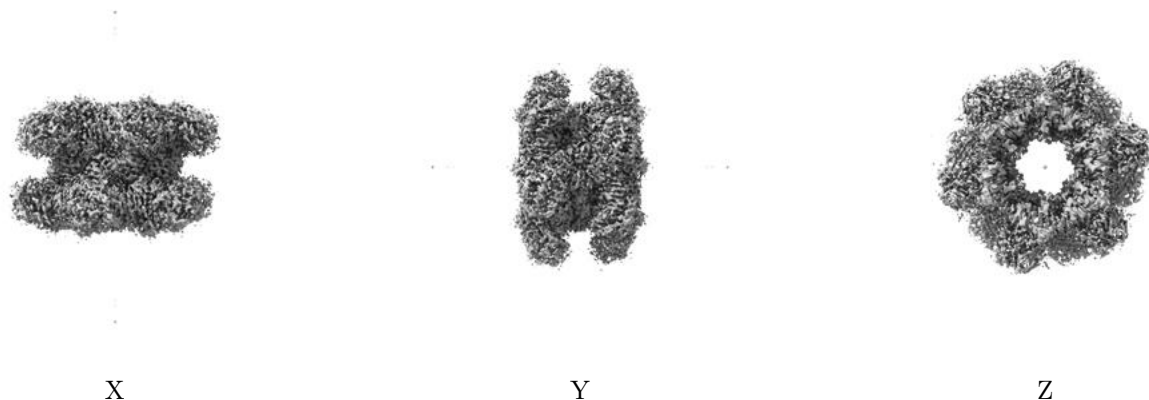
6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.76. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

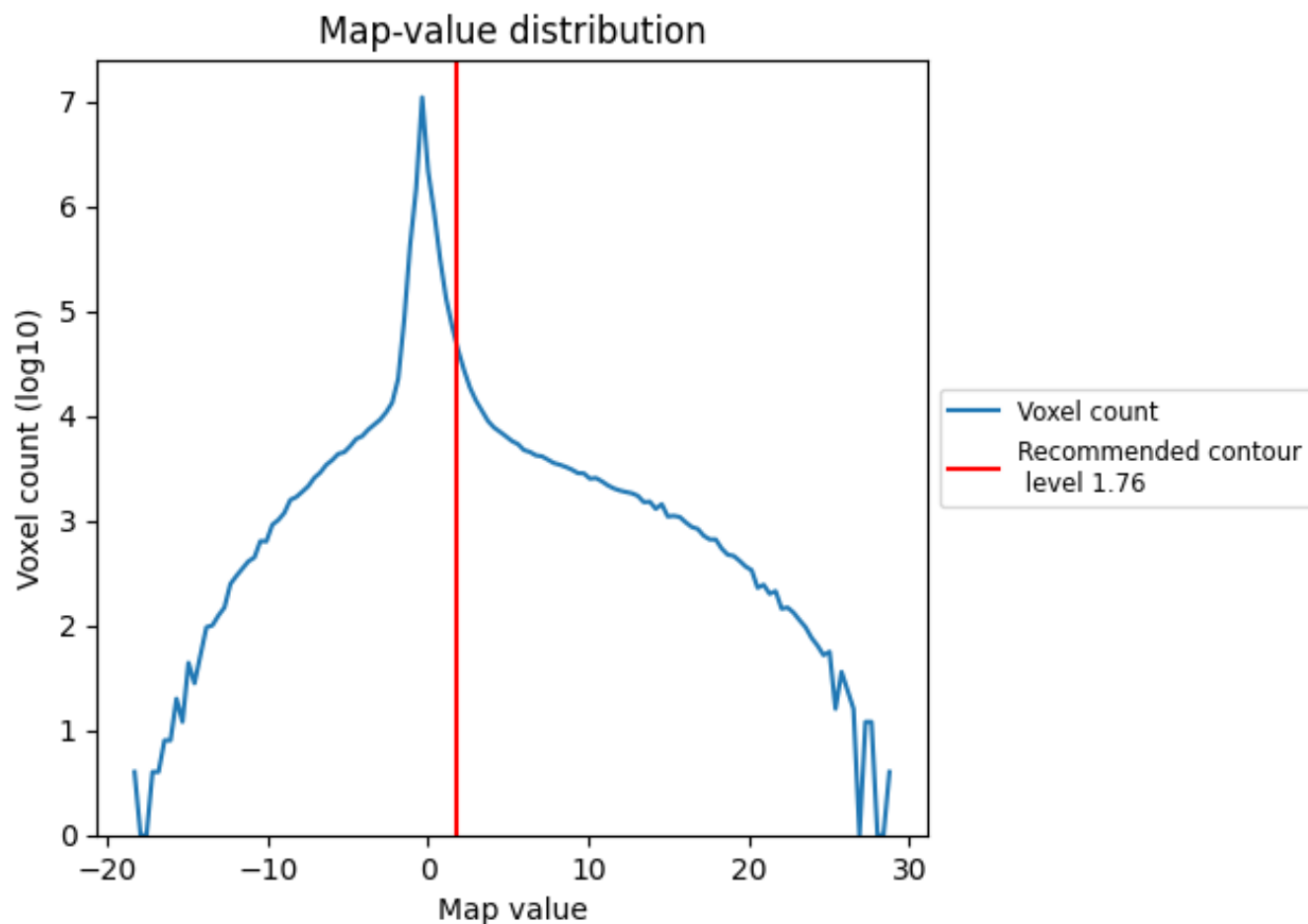
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

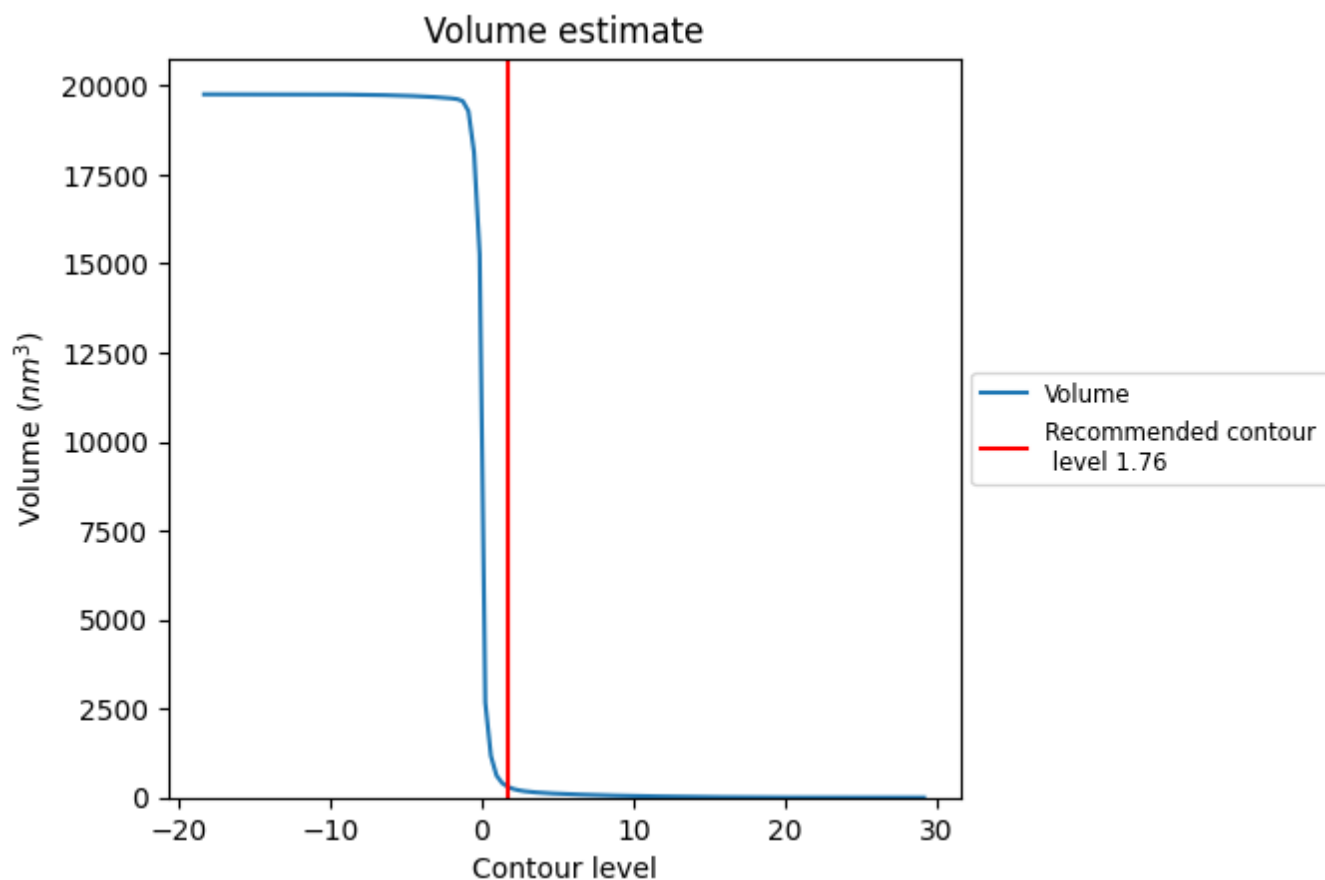
This section contains the results of statistical analysis of the map.

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.

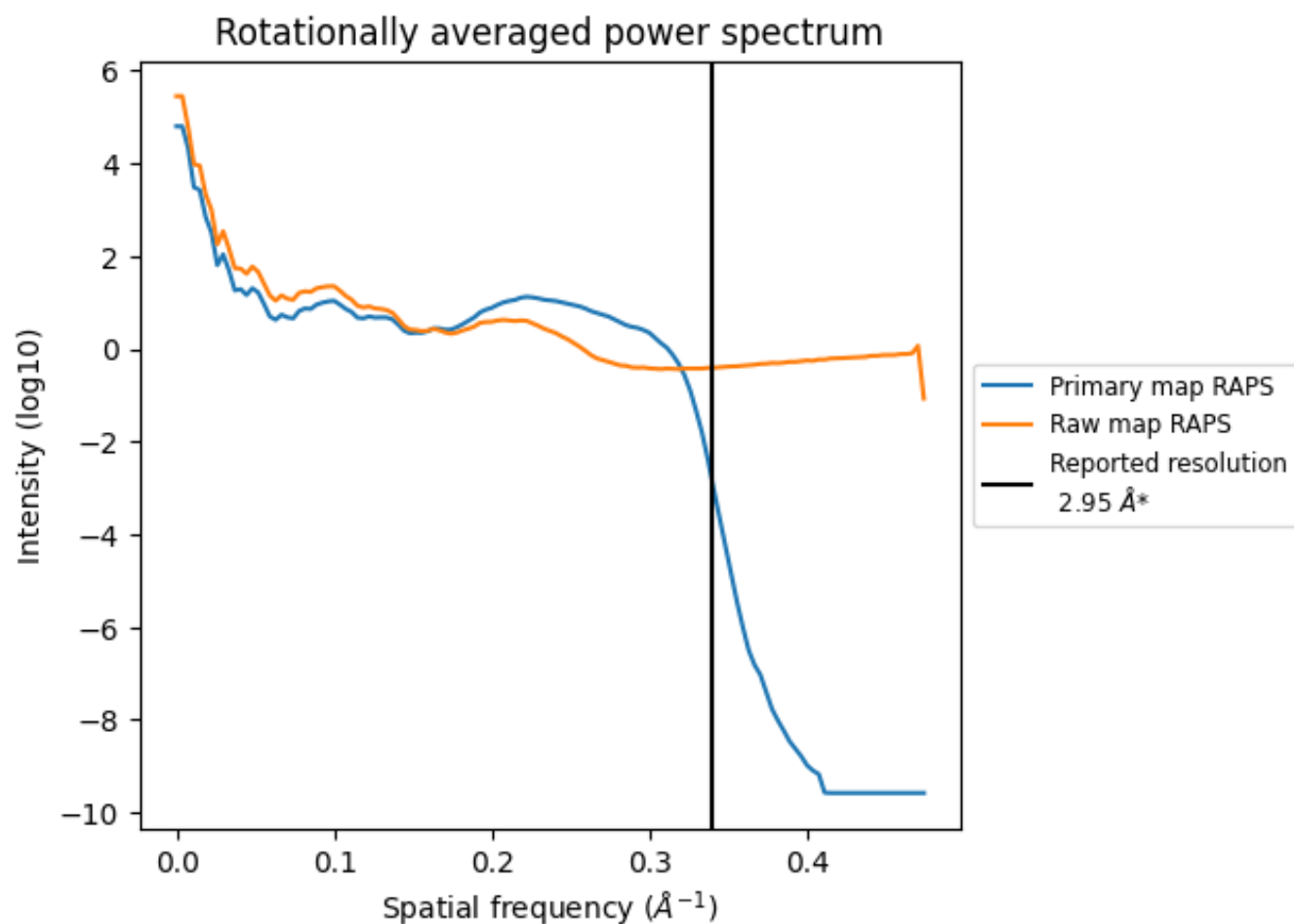
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 296 nm³; this corresponds to an approximate mass of 268 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 ⓘ

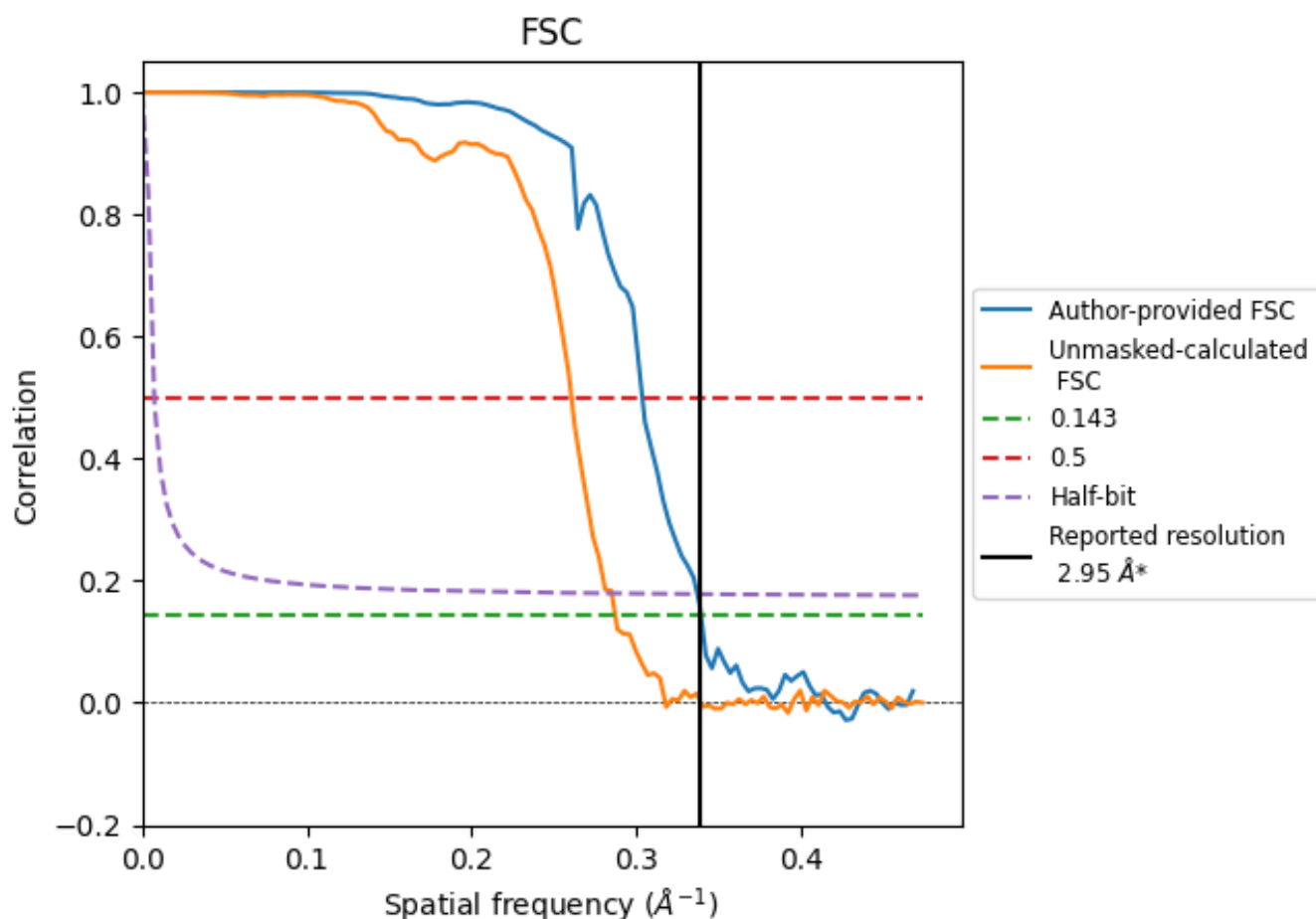


*Reported resolution corresponds to spatial frequency of 0.339 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.339 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	2.95	3.29	2.97
Unmasked-calculated*	3.48	3.84	3.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.48 differs from the reported value 2.95 by more than 10 %

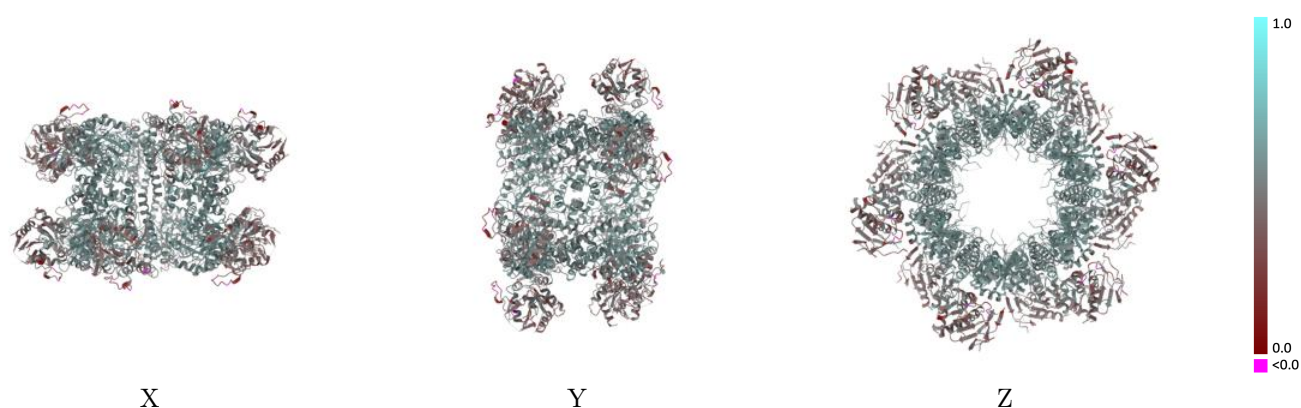
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-45440 and PDB model 9CCA. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)

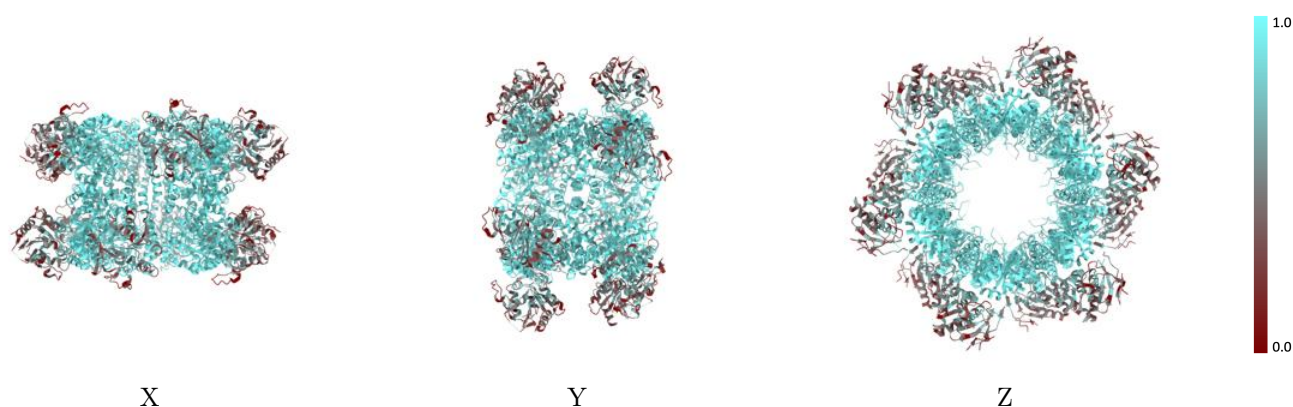
This section was not generated.

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



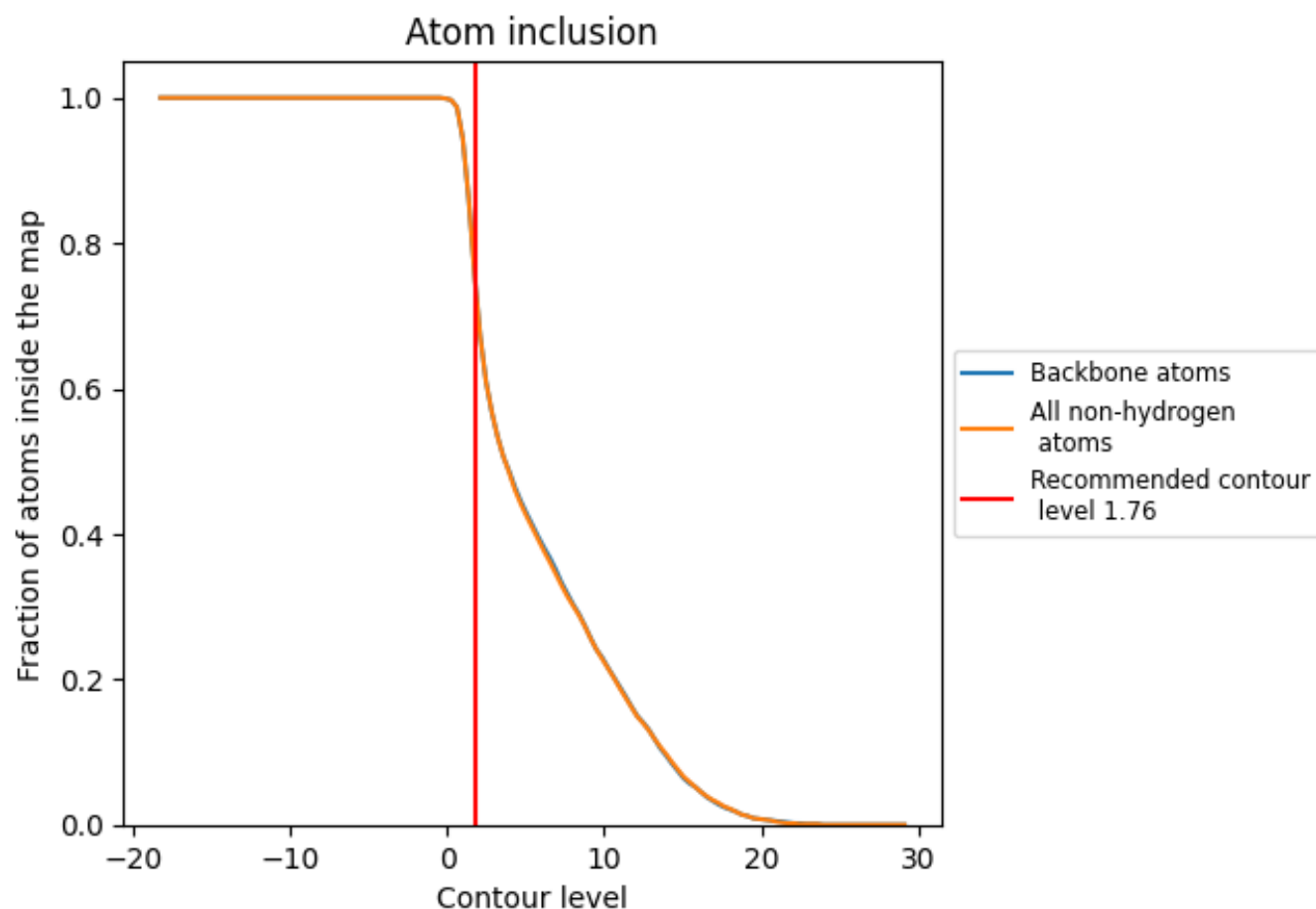
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.76).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 75% 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 (1.76) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7480	 0.5010
A	 0.9640	 0.5700
B	 0.9650	 0.5720
C	 0.9640	 0.5700
D	 0.9670	 0.5690
E	 0.9660	 0.5690
F	 0.9690	 0.5720
G	 0.4470	 0.4110
H	 0.4530	 0.4060
I	 0.4480	 0.4060
J	 0.4590	 0.4120
K	 0.4590	 0.4150
L	 0.4560	 0.4050
M	 0.9650	 0.5720
N	 0.9630	 0.5700
O	 0.9620	 0.5690
P	 0.9660	 0.5700
Q	 0.9650	 0.5710
R	 0.9640	 0.5720
S	 0.4420	 0.3990
T	 0.4470	 0.4080
U	 0.4460	 0.4050
V	 0.4460	 0.4040
W	 0.4470	 0.4010
X	 0.4420	 0.4010

