

Aug 30, 2023 – 01:38 am BST

PDB ID	:	8P2L
EMDB ID	:	EMD-17369
Title	:	A CHIMERA construct containing human SARM1 ARM and SAM domains
		and C. elegans TIR domain.
Authors	:	Isupov, M.N.; Opatowsky, Y.
Deposited on	:	2023-05-16
Resolution	:	2.68 Å(reported)
Based on initial model	:	

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 (i) 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	FAILED
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.68 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 40776 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues		At	oms			AltConf	Trace
1	А	496	Total	С	Ν	0	S	0	0
			3845	2412	703	713	17	Ŭ	
1	В	496	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
1	D	450	3845	2412	703	713	17	0	0
1	C	406	Total	\mathbf{C}	Ν	0	\mathbf{S}	0	0
1	U	490	3845	2412	703	713	17	0	0
1	D	406	Total	С	Ν	0	S	0	0
1	D	490	3845	2412	703	713	17	0	0
1	Б	406	Total	С	Ν	0	S	0	0
	Ľ	490	3845	2412	703	713	17	0	0
1	Б	406	Total	С	Ν	0	S	0	0
1	Г	490	3845	2412	703	713	17	0	0
1	C	400	Total	С	Ν	0	S	0	0
1	G	490	3845	2412	703	713	17		
1	тт	400	Total	С	Ν	0	S	0	0
	п	490	3845	2412	703	713	17	0	U
1	т	1 4 0	Total	С	Ν	0	S	0	0
1	J	148	1208	776	206	221	5	0	0
1	т	140	Total	С	Ν	0	S	0	0
1	1	148	1208	776	206	221	5	0	
1	V	140	Total	С	Ν	0	S	0	0
1	n	148	1208	776	206	221	5	0	0
1	т	140	Total	С	Ν	0	S	0	0
1	L	148	1208	776	206	221	5	0	0
1	м	140	Total	С	Ν	0	S	0	0
1	IVI	148	1208	776	206	221	5	0	0
1	N	140	Total	С	Ν	0	S	0	0
	1 IN	148	1208	776	206	221	5	0	0
1	0	140	Total	С	Ν	0	S	0	0
	U	140	1208	776	206	221	5	U	U
1	р	140	Total	С	Ν	0	S	0	0
	Г	148	1208	776	206	221	5	U	U

• Molecule 1 is a protein called NAD(+) hydrolase SARM1,NAD(+) hydrolase tir-1.

There are 432 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
А	-1	MET	-	initiating methionine	UNP Q6SZW1
А	0	SER	-	expression tag	UNP Q6SZW1
А	1	TYR	-	expression tag	UNP Q6SZW1
А	2	HIS	-	expression tag	UNP Q6SZW1
А	3	HIS	-	expression tag	UNP Q6SZW1
А	4	HIS	-	expression tag	UNP Q6SZW1
А	5	HIS	-	expression tag	UNP Q6SZW1
А	6	HIS	-	expression tag	UNP Q6SZW1
А	7	HIS	-	expression tag	UNP Q6SZW1
А	8	ASP	-	expression tag	UNP Q6SZW1
А	9	TYR	-	expression tag	UNP Q6SZW1
А	10	ASP	-	expression tag	UNP Q6SZW1
А	11	ILE	-	expression tag	UNP Q6SZW1
А	12	PRO	-	expression tag	UNP Q6SZW1
А	13	THR	-	expression tag	UNP Q6SZW1
A	14	THR	-	expression tag	UNP Q6SZW1
А	15	GLU	-	expression tag	UNP Q6SZW1
А	16	ASN	-	expression tag	UNP Q6SZW1
А	17	LEU	-	expression tag	UNP Q6SZW1
А	18	TYR	-	expression tag	UNP Q6SZW1
А	19	PHE	-	expression tag	UNP Q6SZW1
А	20	GLN	-	expression tag	UNP Q6SZW1
А	21	GLY	-	expression tag	UNP Q6SZW1
А	22	ALA	-	expression tag	UNP Q6SZW1
А	23	MET	-	expression tag	UNP Q6SZW1
А	24	GLY	-	expression tag	UNP Q6SZW1
А	25	SER	-	expression tag	UNP Q6SZW1
В	-1	MET	-	initiating methionine	UNP Q6SZW1
В	0	SER	-	expression tag	UNP Q6SZW1
В	1	TYR	-	expression tag	UNP Q6SZW1
В	2	HIS	-	expression tag	UNP Q6SZW1
B	3	HIS	-	expression tag	UNP Q6SZW1
В	4	HIS	-	expression tag	UNP Q6SZW1
B	5	HIS	-	expression tag	UNP Q6SZW1
В	6	HIS	-	expression tag	UNP Q6SZW1
B	7	HIS	-	expression tag	UNP Q6SZW1
B	8	ASP	-	expression tag	UNP Q6SZW1
B	9	TYR	-	expression tag	UNP Q6SZW1
B	10	ASP	-	expression tag	UNP Q6SZW1
B	11	ILE	-	expression tag	UNP Q6SZW1
B	12	PRO	_	expression tag	UNP Q6SZW1
B	13	THR	-	expression tag	UNP Q6SZW1
В	14	THR	_	expression tag	UNP Q6SZW1



Chain	Residue	Modelled	Actual	Comment	Reference
В	15	GLU	-	expression tag	UNP Q6SZW1
В	16	ASN	-	expression tag	UNP Q6SZW1
В	17	LEU	-	expression tag	UNP Q6SZW1
В	18	TYR	-	expression tag	UNP Q6SZW1
В	19	PHE	-	expression tag	UNP Q6SZW1
В	20	GLN	-	expression tag	UNP Q6SZW1
В	21	GLY	-	expression tag	UNP Q6SZW1
В	22	ALA	-	expression tag	UNP Q6SZW1
В	23	MET	-	expression tag	UNP Q6SZW1
В	24	GLY	-	expression tag	UNP Q6SZW1
В	25	SER	-	expression tag	UNP Q6SZW1
С	-1	MET	-	initiating methionine	UNP Q6SZW1
С	0	SER	-	expression tag	UNP Q6SZW1
С	1	TYR	-	expression tag	UNP Q6SZW1
С	2	HIS	-	expression tag	UNP Q6SZW1
С	3	HIS	-	expression tag	UNP Q6SZW1
С	4	HIS	-	expression tag	UNP Q6SZW1
С	5	HIS	-	expression tag	UNP Q6SZW1
С	6	HIS	-	expression tag	UNP Q6SZW1
С	7	HIS	-	expression tag	UNP Q6SZW1
С	8	ASP	-	expression tag	UNP Q6SZW1
С	9	TYR	-	expression tag	UNP Q6SZW1
С	10	ASP	-	expression tag	UNP Q6SZW1
С	11	ILE	-	expression tag	UNP Q6SZW1
С	12	PRO	-	expression tag	UNP Q6SZW1
С	13	THR	-	expression tag	UNP Q6SZW1
С	14	THR	-	expression tag	UNP Q6SZW1
С	15	GLU	-	expression tag	UNP Q6SZW1
С	16	ASN	-	expression tag	UNP Q6SZW1
С	17	LEU	-	expression tag	UNP Q6SZW1
С	18	TYR	-	expression tag	UNP Q6SZW1
С	19	PHE	-	expression tag	UNP Q6SZW1
С	20	GLN	-	expression tag	UNP Q6SZW1
С	21	GLY	-	expression tag	UNP Q6SZW1
С	22	ALA	-	expression tag	UNP Q6SZW1
С	23	MET	-	expression tag	UNP Q6SZW1
С	24	GLY	-	expression tag	UNP Q6SZW1
С	25	SER	-	expression tag	UNP Q6SZW1
D	-1	MET	-	initiating methionine	UNP Q6SZW1
D	0	SER	-	expression tag	UNP Q6SZW1
D	1	TYR	-	expression tag	UNP Q6SZW1
D	2	HIS	-	expression tag	UNP Q6SZW1



Chain	Residue	Modelled	Actual	Comment	Reference
D	3	HIS	_	expression tag	UNP Q6SZW1
D	4	HIS	-	expression tag	UNP Q6SZW1
D	5	HIS	-	expression tag	UNP Q6SZW1
D	6	HIS	-	expression tag	UNP Q6SZW1
D	7	HIS	-	expression tag	UNP Q6SZW1
D	8	ASP	-	expression tag	UNP Q6SZW1
D	9	TYR	-	expression tag	UNP Q6SZW1
D	10	ASP	-	expression tag	UNP Q6SZW1
D	11	ILE	-	expression tag	UNP Q6SZW1
D	12	PRO	-	expression tag	UNP Q6SZW1
D	13	THR	-	expression tag	UNP Q6SZW1
D	14	THR	-	expression tag	UNP Q6SZW1
D	15	GLU	-	expression tag	UNP Q6SZW1
D	16	ASN	-	expression tag	UNP Q6SZW1
D	17	LEU	-	expression tag	UNP Q6SZW1
D	18	TYR	_	expression tag	UNP Q6SZW1
D	19	PHE	-	expression tag	UNP Q6SZW1
D	20	GLN	_	expression tag	UNP Q6SZW1
D	21	GLY	_	expression tag	UNP Q6SZW1
D	22	ALA	_	expression tag	UNP Q6SZW1
D	23	MET	_	expression tag	UNP Q6SZW1
D	24	GLY	_	expression tag	UNP Q6SZW1
D	25	SER	-	expression tag	UNP Q6SZW1
Е	-1	MET	_	initiating methionine	UNP Q6SZW1
Е	0	SER	_	expression tag	UNP Q6SZW1
Е	1	TYR	-	expression tag	UNP Q6SZW1
Е	2	HIS	_	expression tag	UNP Q6SZW1
Е	3	HIS	-	expression tag	UNP Q6SZW1
Е	4	HIS	-	expression tag	UNP Q6SZW1
Е	5	HIS	-	expression tag	UNP Q6SZW1
Е	6	HIS	-	expression tag	UNP Q6SZW1
Е	7	HIS	_	expression tag	UNP Q6SZW1
Е	8	ASP	_	expression tag	UNP Q6SZW1
Е	9	TYR	-	expression tag	UNP Q6SZW1
Е	10	ASP	-	expression tag	UNP Q6SZW1
Е	11	ILE	-	expression tag	UNP Q6SZW1
Е	12	PRO	-	expression tag	UNP Q6SZW1
Е	13	THR	-	expression tag	UNP Q6SZW1
Е	14	THR	-	expression tag	UNP Q6SZW1
Е	15	GLU	-	expression tag	UNP Q6SZW1
Е	16	ASN	-	expression tag	UNP Q6SZW1
Е	17	LEU	-	expression tag	UNP Q6SZW1



Chain	Residue	Modelled	Actual	Comment	Reference
Е	18	TYR	-	expression tag	UNP Q6SZW1
Е	19	PHE	_	expression tag	UNP Q6SZW1
Е	20	GLN	-	expression tag	UNP Q6SZW1
Е	21	GLY	-	expression tag	UNP Q6SZW1
Е	22	ALA	-	expression tag	UNP Q6SZW1
Е	23	MET	-	expression tag	UNP Q6SZW1
Е	24	GLY	-	expression tag	UNP Q6SZW1
Е	25	SER	-	expression tag	UNP Q6SZW1
F	-1	MET	-	initiating methionine	UNP Q6SZW1
F	0	SER	-	expression tag	UNP Q6SZW1
F	1	TYR	-	expression tag	UNP Q6SZW1
F	2	HIS	-	expression tag	UNP Q6SZW1
F	3	HIS	-	expression tag	UNP Q6SZW1
F	4	HIS	-	expression tag	UNP Q6SZW1
F	5	HIS	-	expression tag	UNP Q6SZW1
F	6	HIS	-	expression tag	UNP Q6SZW1
F	7	HIS	-	expression tag	UNP Q6SZW1
F	8	ASP	-	expression tag	UNP Q6SZW1
F	9	TYR	-	expression tag	UNP Q6SZW1
F	10	ASP	-	expression tag	UNP Q6SZW1
F	11	ILE	-	expression tag	UNP Q6SZW1
F	12	PRO	-	expression tag	UNP Q6SZW1
F	13	THR	-	expression tag	UNP Q6SZW1
F	14	THR	-	expression tag	UNP Q6SZW1
F	15	GLU	-	expression tag	UNP Q6SZW1
F	16	ASN	-	expression tag	UNP Q6SZW1
F	17	LEU	-	expression tag	UNP Q6SZW1
F	18	TYR	-	expression tag	UNP Q6SZW1
F	19	PHE	-	expression tag	UNP Q6SZW1
F	20	GLN	-	expression tag	UNP Q6SZW1
F	21	GLY	-	expression tag	UNP Q6SZW1
F	22	ALA	-	expression tag	UNP Q6SZW1
F	23	MET	-	expression tag	UNP Q6SZW1
F	24	GLY	-	expression tag	UNP Q6SZW1
F	25	SER	-	expression tag	UNP Q6SZW1
G	-1	MET	-	initiating methionine	UNP Q6SZW1
G	0	SER	-	expression tag	UNP Q6SZW1
G	1	TYR	-	expression tag	UNP Q6SZW1
G	2	HIS	-	expression tag	UNP Q6SZW1
G	3	HIS	-	expression tag	UNP Q6SZW1
G	4	HIS	-	expression tag	UNP Q6SZW1
G	5	HIS	-	expression tag	UNP Q6SZW1



Chain	Residue	Modelled	Actual	Comment	Reference
G	6	HIS	-	expression tag	UNP Q6SZW1
G	7	HIS	-	expression tag	UNP Q6SZW1
G	8	ASP	-	expression tag	UNP Q6SZW1
G	9	TYR	-	expression tag	UNP Q6SZW1
G	10	ASP	-	expression tag	UNP Q6SZW1
G	11	ILE	-	expression tag	UNP Q6SZW1
G	12	PRO	-	expression tag	UNP Q6SZW1
G	13	THR	-	expression tag	UNP Q6SZW1
G	14	THR	-	expression tag	UNP Q6SZW1
G	15	GLU	-	expression tag	UNP Q6SZW1
G	16	ASN	-	expression tag	UNP Q6SZW1
G	17	LEU	-	expression tag	UNP Q6SZW1
G	18	TYR	-	expression tag	UNP Q6SZW1
G	19	PHE	-	expression tag	UNP Q6SZW1
G	20	GLN	-	expression tag	UNP Q6SZW1
G	21	GLY	-	expression tag	UNP Q6SZW1
G	22	ALA	-	expression tag	UNP Q6SZW1
G	23	MET	-	expression tag	UNP Q6SZW1
G	24	GLY	-	expression tag	UNP Q6SZW1
G	25	SER	-	expression tag	UNP Q6SZW1
Н	-1	MET	-	initiating methionine	UNP Q6SZW1
Н	0	SER	-	expression tag	UNP Q6SZW1
Н	1	TYR	-	expression tag	UNP Q6SZW1
Н	2	HIS	-	expression tag	UNP Q6SZW1
Н	3	HIS	-	expression tag	UNP Q6SZW1
Н	4	HIS	-	expression tag	UNP Q6SZW1
Н	5	HIS	-	expression tag	UNP Q6SZW1
Н	6	HIS	-	expression tag	UNP Q6SZW1
Н	7	HIS	-	expression tag	UNP Q6SZW1
Н	8	ASP	-	expression tag	UNP Q6SZW1
Н	9	TYR	-	expression tag	UNP Q6SZW1
Н	10	ASP	-	expression tag	UNP Q6SZW1
Н	11	ILE	-	expression tag	UNP Q6SZW1
Н	12	PRO	-	expression tag	UNP Q6SZW1
Н	13	THR	-	expression tag	UNP Q6SZW1
H	14	THR	-	expression tag	UNP Q6SZW1
H	15	GLU	_	expression tag	UNP Q6SZW1
H	16	ASN	-	expression tag	UNP Q6SZW1
H	17	LEU	_	expression tag	UNP $Q6SZW1$
H	18	TYR	_	expression tag	UNP Q6SZW1
Н	19	PHE	-	expression tag	UNP Q6SZW1
Н	20	GLN	-	expression tag	UNP Q6SZW1



Chain	Residue	Modelled	Actual	Comment	Reference
Н	21	GLY	-	expression tag	UNP Q6SZW1
Н	22	ALA	-	expression tag	UNP Q6SZW1
Н	23	MET	-	expression tag	UNP Q6SZW1
Н	24	GLY	-	expression tag	UNP Q6SZW1
Н	25	SER	-	expression tag	UNP Q6SZW1
J	145	MET	_	initiating methionine	UNP Q6SZW1
J	146	SER	-	expression tag	UNP Q6SZW1
J	147	TYR	-	expression tag	UNP Q6SZW1
J	148	HIS	-	expression tag	UNP Q6SZW1
J	149	HIS	-	expression tag	UNP Q6SZW1
J	150	HIS	-	expression tag	UNP Q6SZW1
J	151	HIS	-	expression tag	UNP Q6SZW1
J	152	HIS	-	expression tag	UNP Q6SZW1
J	153	HIS	-	expression tag	UNP Q6SZW1
J	154	ASP	-	expression tag	UNP Q6SZW1
J	155	TYR	-	expression tag	UNP Q6SZW1
J	156	ASP	-	expression tag	UNP Q6SZW1
J	157	ILE	-	expression tag	UNP Q6SZW1
J	158	PRO	-	expression tag	UNP Q6SZW1
J	159	THR	-	expression tag	UNP Q6SZW1
J	160	THR	-	expression tag	UNP Q6SZW1
J	161	GLU	-	expression tag	UNP Q6SZW1
J	162	ASN	-	expression tag	UNP Q6SZW1
J	163	LEU	-	expression tag	UNP Q6SZW1
J	164	TYR	-	expression tag	UNP Q6SZW1
J	165	PHE	-	expression tag	UNP Q6SZW1
J	166	GLN	-	expression tag	UNP Q6SZW1
J	167	GLY	-	expression tag	UNP Q6SZW1
J	168	ALA	-	expression tag	UNP Q6SZW1
J	169	MET	-	expression tag	UNP Q6SZW1
J	170	GLY	-	expression tag	UNP Q6SZW1
J	171	SER	-	expression tag	UNP Q6SZW1
Ι	145	MET	-	initiating methionine	UNP Q6SZW1
Ι	146	SER	-	expression tag	UNP Q6SZW1
I	147	TYR	-	expression tag	UNP Q6SZW1
I	148	HIS	-	expression tag	UNP Q6SZW1
Ι	149	HIS	-	expression tag	UNP Q6SZW1
Ι	150	HIS	-	expression tag	UNP Q6SZW1
I	151	HIS	-	expression tag	UNP Q6SZW1
Ι	152	HIS	-	expression tag	UNP Q6SZW1
I	153	HIS	-	expression tag	UNP Q6SZW1
I	154	ASP	-	expression tag	UNP Q6SZW1



Chain	Residue	Modelled	Actual	Comment	Reference
Ι	155	TYR	-	expression tag	UNP Q6SZW1
Ι	156	ASP	_	expression tag	UNP Q6SZW1
Ι	157	ILE	-	expression tag	UNP Q6SZW1
Ι	158	PRO	-	expression tag	UNP Q6SZW1
Ι	159	THR	-	expression tag	UNP Q6SZW1
Ι	160	THR	-	expression tag	UNP Q6SZW1
Ι	161	GLU	-	expression tag	UNP Q6SZW1
Ι	162	ASN	-	expression tag	UNP Q6SZW1
Ι	163	LEU	-	expression tag	UNP Q6SZW1
Ι	164	TYR	-	expression tag	UNP Q6SZW1
Ι	165	PHE	-	expression tag	UNP Q6SZW1
Ι	166	GLN	-	expression tag	UNP Q6SZW1
Ι	167	GLY	-	expression tag	UNP Q6SZW1
Ι	168	ALA	-	expression tag	UNP Q6SZW1
Ι	169	MET	-	expression tag	UNP Q6SZW1
Ι	170	GLY	-	expression tag	UNP Q6SZW1
Ι	171	SER	-	expression tag	UNP Q6SZW1
K	145	MET	-	initiating methionine	UNP Q6SZW1
K	146	SER	-	expression tag	UNP Q6SZW1
K	147	TYR	-	expression tag	UNP Q6SZW1
K	148	HIS	-	expression tag	UNP Q6SZW1
K	149	HIS	-	expression tag	UNP Q6SZW1
K	150	HIS	-	expression tag	UNP Q6SZW1
K	151	HIS	-	expression tag	UNP Q6SZW1
K	152	HIS	-	expression tag	UNP Q6SZW1
K	153	HIS	-	expression tag	UNP Q6SZW1
K	154	ASP	-	expression tag	UNP Q6SZW1
K	155	TYR	-	expression tag	UNP Q6SZW1
K	156	ASP	-	expression tag	UNP Q6SZW1
K	157	ILE	-	expression tag	UNP Q6SZW1
K	158	PRO	-	expression tag	UNP Q6SZW1
K	159	THR	-	expression tag	UNP Q6SZW1
K	160	THR	-	expression tag	UNP Q6SZW1
K	161	GLU	-	expression tag	UNP Q6SZW1
K	162	ASN	-	expression tag	UNP Q6SZW1
K	163	LEU	-	expression tag	UNP Q6SZW1
K	164	TYR	-	expression tag	UNP Q6SZW1
K	165	PHE	-	expression tag	UNP Q6SZW1
K	166	GLN	-	expression tag	UNP Q6SZW1
K	167	GLY	-	expression tag	UNP Q6SZW1
K	168	ALA	-	expression tag	UNP Q6SZW1
K	169	MET	-	expression tag	UNP Q6SZW1



Chain	Residue	Modelled	Actual	Comment	Reference
K	170	GLY	-	expression tag	UNP Q6SZW1
K	171	SER	-	expression tag	UNP Q6SZW1
L	145	MET	-	initiating methionine	UNP Q6SZW1
L	146	SER	-	expression tag	UNP Q6SZW1
L	147	TYR	-	expression tag	UNP Q6SZW1
L	148	HIS	-	expression tag	UNP Q6SZW1
L	149	HIS	-	expression tag	UNP Q6SZW1
L	150	HIS	-	expression tag	UNP Q6SZW1
L	151	HIS	-	expression tag	UNP Q6SZW1
L	152	HIS	-	expression tag	UNP Q6SZW1
L	153	HIS	-	expression tag	UNP Q6SZW1
L	154	ASP	-	expression tag	UNP Q6SZW1
L	155	TYR	-	expression tag	UNP Q6SZW1
L	156	ASP	-	expression tag	UNP Q6SZW1
L	157	ILE	-	expression tag	UNP Q6SZW1
L	158	PRO	-	expression tag	UNP Q6SZW1
L	159	THR	-	expression tag	UNP Q6SZW1
L	160	THR	-	expression tag	UNP Q6SZW1
L	161	GLU	-	expression tag	UNP Q6SZW1
L	162	ASN	-	expression tag	UNP Q6SZW1
L	163	LEU	-	expression tag	UNP Q6SZW1
L	164	TYR	-	expression tag	UNP Q6SZW1
L	165	PHE	-	expression tag	UNP Q6SZW1
L	166	GLN	-	expression tag	UNP Q6SZW1
L	167	GLY	-	expression tag	UNP Q6SZW1
L	168	ALA	-	expression tag	UNP Q6SZW1
L	169	MET	-	expression tag	UNP Q6SZW1
L	170	GLY	-	expression tag	UNP Q6SZW1
L	171	SER	-	expression tag	UNP Q6SZW1
М	145	MET	-	initiating methionine	UNP Q6SZW1
М	146	SER	-	expression tag	UNP Q6SZW1
М	147	TYR	-	expression tag	UNP Q6SZW1
М	148	HIS	-	expression tag	UNP Q6SZW1
М	149	HIS	-	expression tag	UNP Q6SZW1
М	150	HIS	-	expression tag	UNP Q6SZW1
М	151	HIS	-	expression tag	UNP Q6SZW1
Μ	152	HIS	-	expression tag	UNP Q6SZW1
M	153	HIS	-	expression tag	UNP Q6SZW1
М	154	ASP	-	expression tag	UNP Q6SZW1
M	155	TYR	-	expression tag	UNP Q6SZW1
М	156	ASP	-	expression tag	UNP Q6SZW1
М	157	ILE	-	expression tag	UNP Q6SZW1



Chain	Residue	Modelled	Actual	Comment	Reference
М	158	PRO	-	expression tag	UNP Q6SZW1
М	159	THR	-	expression tag	UNP Q6SZW1
М	160	THR	-	expression tag	UNP Q6SZW1
М	161	GLU	-	expression tag	UNP Q6SZW1
М	162	ASN	_	expression tag	UNP Q6SZW1
М	163	LEU	-	expression tag	UNP Q6SZW1
М	164	TYR	-	expression tag	UNP Q6SZW1
М	165	PHE	-	expression tag	UNP Q6SZW1
М	166	GLN	-	expression tag	UNP Q6SZW1
М	167	GLY	-	expression tag	UNP Q6SZW1
М	168	ALA	-	expression tag	UNP Q6SZW1
М	169	MET	-	expression tag	UNP Q6SZW1
М	170	GLY	-	expression tag	UNP Q6SZW1
М	171	SER	-	expression tag	UNP Q6SZW1
N	145	MET	-	initiating methionine	UNP Q6SZW1
N	146	SER	-	expression tag	UNP Q6SZW1
N	147	TYR	-	expression tag	UNP Q6SZW1
N	148	HIS	-	expression tag	UNP Q6SZW1
N	149	HIS	-	expression tag	UNP Q6SZW1
N	150	HIS	-	expression tag	UNP Q6SZW1
N	151	HIS	-	expression tag	UNP Q6SZW1
N	152	HIS	-	expression tag	UNP Q6SZW1
N	153	HIS	-	expression tag	UNP Q6SZW1
N	154	ASP	-	expression tag	UNP Q6SZW1
N	155	TYR	-	expression tag	UNP Q6SZW1
N	156	ASP	-	expression tag	UNP Q6SZW1
N	157	ILE	-	expression tag	UNP Q6SZW1
N	158	PRO	-	expression tag	UNP Q6SZW1
N	159	THR	-	expression tag	UNP Q6SZW1
N	160	THR	-	expression tag	UNP Q6SZW1
N	161	GLU	-	expression tag	UNP Q6SZW1
N	162	ASN	-	expression tag	UNP Q6SZW1
N	163	LEU	-	expression tag	UNP Q6SZW1
N	164	TYR	-	expression tag	UNP Q6SZW1
N	165	PHE	-	expression tag	UNP Q6SZW1
N	166	GLN	-	expression tag	UNP Q6SZW1
N	167	GLY	_	expression tag	UNP Q6SZW1
N	168	ALA	-	expression tag	UNP Q6SZW1
N	169	MET	-	expression tag	UNP Q6SZW1
N	170	GLY	-	expression tag	UNP Q6SZW1
N	171	SER	-	expression tag	UNP Q6SZW1
0	145	MET	-	initiating methionine	UNP Q6SZW1



Chain	Residue	Modelled	Actual Comment		Reference
0	146	SER	-	expression tag	UNP Q6SZW1
0	147	TYR	-	expression tag	UNP Q6SZW1
0	148	HIS	-	expression tag	UNP Q6SZW1
0	149	HIS	-	expression tag	UNP Q6SZW1
0	150	HIS	-	expression tag	UNP Q6SZW1
0	151	HIS	-	expression tag	UNP Q6SZW1
0	152	HIS	-	expression tag	UNP Q6SZW1
0	153	HIS	-	expression tag	UNP Q6SZW1
0	154	ASP	-	expression tag	UNP Q6SZW1
0	155	TYR	-	expression tag	UNP Q6SZW1
0	156	ASP	-	expression tag	UNP Q6SZW1
0	157	ILE	-	expression tag	UNP Q6SZW1
0	158	PRO	-	expression tag	UNP Q6SZW1
0	159	THR	-	expression tag	UNP Q6SZW1
0	160	THR	-	expression tag	UNP Q6SZW1
0	161	GLU	-	expression tag	UNP Q6SZW1
0	162	ASN	-	expression tag	UNP Q6SZW1
0	163	LEU	-	expression tag	UNP Q6SZW1
0	164	TYR	-	expression tag	UNP Q6SZW1
0	165	PHE	-	expression tag	UNP Q6SZW1
0	166	GLN	-	expression tag	UNP Q6SZW1
0	167	GLY	-	expression tag	UNP Q6SZW1
0	168	ALA	-	expression tag	UNP Q6SZW1
0	169	MET	-	expression tag	UNP Q6SZW1
0	170	GLY	-	expression tag	UNP Q6SZW1
0	171	SER	-	expression tag	UNP Q6SZW1
Р	145	MET	-	initiating methionine	UNP Q6SZW1
Р	146	SER	-	expression tag	UNP Q6SZW1
Р	147	TYR	-	expression tag	UNP Q6SZW1
Р	148	HIS	-	expression tag	UNP Q6SZW1
Р	149	HIS	-	expression tag	UNP Q6SZW1
Р	150	HIS	-	expression tag	UNP Q6SZW1
Р	151	HIS	-	expression tag	UNP Q6SZW1
Р	152	HIS	-	expression tag	UNP Q6SZW1
Р	153	HIS	-	expression tag	UNP Q6SZW1
Р	154	ASP	-	expression tag	UNP Q6SZW1
Р	155	TYR	-	expression tag	UNP Q6SZW1
Р	156	ASP	-	expression tag	UNP Q6SZW1
P	157	ILE	-	expression tag	UNP Q6SZW1
P	158	PRO	-	expression tag	UNP Q6SZW1
Р	159	THR	-	expression tag	UNP Q6SZW1
Р	160	THR	-	expression tag	UNP Q6SZW1



Chain	Residue	Modelled	Actual	Comment	Reference
Р	161	GLU	-	expression tag	UNP Q6SZW1
Р	162	ASN	-	expression tag	UNP Q6SZW1
Р	163	LEU	-	expression tag	UNP Q6SZW1
Р	164	TYR	-	expression tag	UNP Q6SZW1
Р	165	PHE	-	expression tag	UNP Q6SZW1
Р	166	GLN	-	expression tag	UNP Q6SZW1
Р	167	GLY	-	expression tag	UNP Q6SZW1
Р	168	ALA	-	expression tag	UNP Q6SZW1
Р	169	MET	-	expression tag	UNP Q6SZW1
Р	170	GLY	-	expression tag	UNP Q6SZW1
Р	171	SER	-	expression tag	UNP Q6SZW1

• Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Ate	oms			AltConf
2	Λ	1	Total	С	Ν	Ο	Р	0
2		T	44	21	7	14	2	0
2	B	1	Total	С	Ν	Ο	Р	0
2	D	1	44	21	7	14	2	0
2	С	1	Total	С	Ν	Ο	Р	0
	U	1	44	21	7	14	2	0
0	Л	1	Total	С	Ν	Ο	Р	0
	D	1	44	21	7	14	2	0
2	F	1	Total	С	Ν	Ο	Р	0
			44	21	7	14	2	0



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contentaca	<i>J</i> · <i>O</i> · · · <i>O</i>	proceed ac	pagom

Mol	Chain	Residues	Atoms				AltConf	
9	Б	1	Total	С	Ν	Ο	Р	0
	Г	1	44	21	7	14	2	0
9	С	1	Total	С	Ν	Ο	Р	0
	G		44	21	7	14	2	0
9	Ц	1	Total	С	Ν	Ο	Р	0
	11		44	21	7	14	2	0

MolProbity failed to run properly - this section is therefore empty.



3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136346	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	41.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 ($6k \ge 4k$)	Depositor
Maximum map value	0.908	Depositor
Minimum map value	-0.420	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	251.99998, 251.99998, 251.99998	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor



4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond



Mal	Trune	Chain	Dec	Tinle	Bond lengths			Bond angles		
IVIOI	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	В	901	-	42,48,48	0.60	0	50,73,73	0.77	3 (6%)
2	NAD	G	901	-	42,48,48	0.60	0	50,73,73	0.76	3 (6%)
2	NAD	С	901	-	42,48,48	0.60	0	50,73,73	0.76	3 (6%)
2	NAD	D	901	-	42,48,48	0.60	0	50,73,73	0.77	3 (6%)
2	NAD	Н	901	-	42,48,48	0.60	0	50,73,73	0.77	3 (6%)
2	NAD	Е	901	-	42,48,48	0.60	0	50,73,73	0.76	3 (6%)
2	NAD	А	901	-	42,48,48	0.61	0	50,73,73	0.77	3 (6%)
2	NAD	F	901	-	42,48,48	0.60	0	50,73,73	0.77	3 (6%)

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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	В	901	-	-	1/26/62/62	0/5/5/5
2	NAD	G	901	-	-	1/26/62/62	0/5/5/5
2	NAD	С	901	-	-	1/26/62/62	0/5/5/5
2	NAD	D	901	-	-	1/26/62/62	0/5/5/5
2	NAD	Н	901	-	-	1/26/62/62	0/5/5/5
2	NAD	Е	901	-	-	1/26/62/62	0/5/5/5
2	NAD	А	901	-	-	2/26/62/62	0/5/5/5
2	NAD	F	901	-	-	1/26/62/62	0/5/5/5

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	D	901	NAD	C6N-N1N-C2N	-2.62	119.59	121.97
2	В	901	NAD	C6N-N1N-C2N	-2.61	119.59	121.97
2	Е	901	NAD	C6N-N1N-C2N	-2.58	119.62	121.97
2	F	901	NAD	C6N-N1N-C2N	-2.58	119.62	121.97
2	С	901	NAD	C6N-N1N-C2N	-2.57	119.63	121.97
2	Н	901	NAD	C6N-N1N-C2N	-2.57	119.63	121.97
2	А	901	NAD	C6N-N1N-C2N	-2.55	119.65	121.97
2	G	901	NAD	C6N-N1N-C2N	-2.53	119.67	121.97



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	В	901	NAD	C3D-C2D-C1D	2.47	104.70	100.98
2	D	901	NAD	C3D-C2D-C1D	2.46	104.68	100.98
2	Н	901	NAD	C3D-C2D-C1D	2.45	104.67	100.98
2	F	901	NAD	C3D-C2D-C1D	2.45	104.66	100.98
2	G	901	NAD	C3D-C2D-C1D	2.37	104.54	100.98
2	С	901	NAD	C3D-C2D-C1D	2.33	104.49	100.98
2	А	901	NAD	C3D-C2D-C1D	2.33	104.48	100.98
2	Е	901	NAD	C3D-C2D-C1D	2.30	104.44	100.98
2	G	901	NAD	C5A-C6A-N6A	2.28	123.82	120.35
2	Н	901	NAD	C5A-C6A-N6A	2.28	123.82	120.35
2	С	901	NAD	C5A-C6A-N6A	2.28	123.82	120.35
2	А	901	NAD	C5A-C6A-N6A	2.27	123.81	120.35
2	F	901	NAD	C5A-C6A-N6A	2.27	123.80	120.35
2	Е	901	NAD	C5A-C6A-N6A	2.25	123.78	120.35
2	D	901	NAD	C5A-C6A-N6A	2.25	123.78	120.35
2	В	901	NAD	C5A-C6A-N6A	2.24	123.76	120.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	901	NAD	O4B-C4B-C5B-O5B
2	В	901	NAD	O4B-C4B-C5B-O5B
2	F	901	NAD	O4B-C4B-C5B-O5B
2	Н	901	NAD	O4B-C4B-C5B-O5B
2	С	901	NAD	O4B-C4B-C5B-O5B
2	D	901	NAD	O4B-C4B-C5B-O5B
2	Ε	901	NAD	O4B-C4B-C5B-O5B
2	G	901	NAD	O4B-C4B-C5B-O5B
2	А	901	NAD	C3B-C4B-C5B-O5B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the



average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.































4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



$\mathbf{5}$ Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-17369. 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.

Orthogonal projections (i) 5.1

5.1.1**Primary** map



Х





Ζ

5.1.2Raw map



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



5.2 Central slices (i)

5.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

5.2.2 Raw map



X Index: 150

Y Index: 150

Z Index: 150

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



5.3 Largest variance slices (i)

5.3.1 Primary map



X Index: 111





Z Index: 144

5.3.2 Raw map



X Index: 122

Y Index: 122



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



5.4 Orthogonal standard-deviation projections (False-color) (i)

5.4.1 Primary map



5.4.2 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.



5.5 Orthogonal surface views (i)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 Raw map



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

5.6 Mask visualisation (i)

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



6 Map analysis (i)

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

6.1 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.



6.2 Volume estimate (i)



The volume at the recommended contour level is 185 nm^3 ; this corresponds to an approximate mass of 167 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.



6.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.373 ${\rm \AA^{-1}}$



7 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.

7.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.373 ${\rm \AA^{-1}}$



7.2 Resolution estimates (i)

$\mathbf{Bosolution} \text{ ostimato } (\mathbf{\hat{\lambda}})$	Estim	Estimation criterion (FSC cut-off)				
Resolution estimate (A)	0.143	0.5	Half-bit			
Reported by author	2.68	-	-			
Author-provided FSC curve	2.68	3.00	2.76			
Unmasked-calculated*	3.21	3.53	3.24			

*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 3.21 differs from the reported value 2.68 by more than 10 %



8 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-17369 and PDB model 8P2L. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.16 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.



8.2 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.

8.3 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 (0.16).



8.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.



8.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.5960	0.4460	
А	0.7200	0.4830	
В	0.7200	0.4830	— 10
C	0.7190	0.4820	1.0
D	0.7200	0.4820	
Е	0.7200	0.4810	
F	0.7200	0.4820	
G	0.7190	0.4820	
Н	0.7200	0.4830	
I	0.2010	0.3270	
J	0.2010	0.3270	
K	0.2010	0.3260	0.0
L	0.2010	0.3250	<0.0
М	0.2010	0.3280	
N	0.2010	0.3290	
0	0.2010	0.3280	
Р	0.2020	0.3300	

