

wwPDB EM Validation Summary Report (i)

Dec 18, 2022 – 09:20 pm GMT

PDB ID	:	7B0N
EMDB ID	:	EMD-11969
Title	:	A 3.7-angstrom structure of Yarrowia lipolytica complex I with an R121M
		mutation in NUCM.
Authors	:	Hirst, J.; Grba, D.
Deposited on	:	2020-11-20
Resolution	:	3.70 Å(reported)
Based on initial model	:	6YJ4

This is a wwPDB EM Validation Summary 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.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
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)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 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	EM structures		
	(#Entries)	(#Entries)		
Clashscore	158937	4297		
Ramachandran outliers	154571	4023		
Sidechain outliers	154315	3826		

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

Mol	Chain	Length	Quality of chain	Quality of chain								
1	А	128	40% 65% 9%	27%								
2	В	210	16%	10% 16%								
3	С	293	16%	9% 17%								
4	D	466	84%	10% 6%								
5	Е	243	45% 79%	10% 11%								
6	F	488	42% 83%	11% 6%								
7	G	728	31%	8% 5%								
8	Н	341	<u>39%</u> 90%	10%								



Conti	nued fron	n previous j	page	
Mol	Chain	Length	Quality of chain	
_	_		17%	
9	I	193	88%	11% •
10	т	105	53%	
10	J	185	91%	9%
11	K	89	78%	22%
		00	34%	2270
12	L	655	86%	14%
			21%	
13	М	486	89%	11%
14	N	460	13%	1.00/
14	11	409	90%	10%
15	0	169	94%	5% •
			45%	
16	Р	355	93%	7%
	<u> </u>		20%	
17	Q	161	73% •	22%
10	D	110	26%	
18	n	118	90%	10%
19	S	87	84%	14%
10	~	01	96%	1470 00
20	Т	81	83%	17%
			83%	
21	U	88	89%	11%
- 22	V	144	36%	
	v	144	43%	6% 12%
23	W	124	94%	6% •
			45%	
24	Х	172	89%	10% •
~~	3.7	100	63%	
25	Y	180	98%	••
26	7	199	40%	70/
20		122	42%	1% •
27	a	86	98%	•
			56%	
28	b	78	100%	
		1.0.0	38%	
29	С	182	99%	•
20	A	72	30%	00/
- 30	u	10	92%	8%
31	е	89	76%	24%
			25%	
32	f	138	98%	••
			55%	
33	g	249	79%	20%



Mol	Chain	Length	Quality of chain	
34	h	139	30%	19%
35	i	90	96%	•
36	j	67	67%	21%
37	k	60	62% 78%	22%
38	1	149	83%	• 16%
39	m	93	99%	
40	n	109	98%	••
41	О	99	84%	16%
42	р	92	98%	••

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The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	FMN	F	501	-	Х	-	-
47	3PE	Н	6401	Х	-	-	-
47	3PE	Ι	501	X	-	-	-
47	3PE	М	502	Х	-	-	-
47	3PE	g	301	Х	-	-	-
51	EHZ	Т	201	Х	-	-	-
52	LMT	Y	1401	Х	-	-	-
52	LMT	Y	1402	Х	-	-	-



2 Entry composition (i)

There are 52 unique types of molecules in this entry. The entry contains 131131 atoms, of which 65779 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 NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	А	94	Total 1593	C 528	Н 827	N 111	O 125	${S \over 2}$	0	0

• Molecule 2 is a protein called Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
2	В	177	Total 2766	C 885	Н 1373	N 246	0 249	S 13	0	0

• Molecule 3 is a protein called NUGM protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	С	242	Total 3924	C 1285	Н 1925	N 339	0 371	$\frac{S}{4}$	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	282	ALA	-	expression tag	UNP Q9UUU0
С	283	ALA	-	expression tag	UNP Q9UUU0
С	284	ALA	-	expression tag	UNP Q9UUU0
С	285	ALA	-	expression tag	UNP Q9UUU0
С	286	ALA	-	expression tag	UNP Q9UUU0
С	287	ALA	-	expression tag	UNP Q9UUU0
С	288	HIS	-	expression tag	UNP Q9UUU0
С	289	HIS	-	expression tag	UNP Q9UUU0
С	290	HIS	-	expression tag	UNP Q9UUU0
С	291	HIS	-	expression tag	UNP Q9UUU0
С	292	HIS	-	expression tag	UNP Q9UUU0
С	293	HIS	-	expression tag	UNP Q9UUU0

• Molecule 4 is a protein called NUCM protein.



Mol	Chain	Residues	Atoms						AltConf	Trace
4	О	437	Total	С	Н	Ν	0	\mathbf{S}	0	0
1	D	101	6788	2181	3354	586	645	22		0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	121	MET	ARG	engineered mutation	UNP Q9UUU1

• Molecule 5 is a protein called Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues			Atom	s			AltConf	Trace
5	E	216	Total	С	Н	Ν	0	S	0	0
Ŭ	-	-10	3348	1060	1660	284	326	18		Ŭ

• Molecule 6 is a protein called Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues			Atom	s			AltConf	Trace
6	F	460	Total 7072	C 2248	Н 3513	N 629	O 658	S 24	0	0

• Molecule 7 is a protein called Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues			Atom	ıs			AltConf	Trace
7	G	694	Total	С	Н	Ν	0	\mathbf{S}	0	0
1	u	034	10447	3275	5173	928	1042	29	0	0

• Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
8	Н	341	Total 5463	C 1828	Н 2774	N 394	0 460	S 7	0	0

• Molecule 9 is a protein called Subunit NUIM of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues			Atom	ıs			AltConf	Trace
9	Ι	191	Total 2997	C 972	H 1471	N 255	O 289	S 10	0	0



• Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues			Atom		AltConf	Trace		
10	J	185	Total 3044	C 990	Н 1582	N 209	0 254	S 9	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	FME	-	initiating methionine	UNP S5U3X7

• Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues			Aton		AltConf	Trace		
11	K	89	Total 1446	C 465	Н 753	N 109	0 116	${ m S} { m 3}$	0	0

• Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues			Atom	s			AltConf	Trace
12	L	655	Total 10571	$\begin{array}{c} \mathrm{C} \\ 3485 \end{array}$	Н 5364	N 786	O 907	S 29	0	0

• Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues			Atom	s			AltConf	Trace
13	М	486	Total 7910	C 2601	Н 4053	N 586	O 655	${ m S}\ 15$	0	0

• Molecule 14 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues				AltConf	Trace			
14	Ν	469	Total 7780	C 2558	H 4004	N 550	O 656	S 12	0	0

• Molecule 15 is a protein called Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues				AltConf	Trace			
15	Ο	168	Total 2586	C 845	Н 1281	N 223	0 233	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0

• Molecule 16 is a protein called Epimerase domain-containing protein.



Mol	Chain	Residues			AltConf	Trace				
16	Р	355	Total 5575	C 1785	Н 2763	N 493	0 524	S 10	0	0

• Molecule 17 is a protein called Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues			Aton	ns			AltConf	Trace
17	Q	125	Total 2031	$\begin{array}{c} \mathrm{C} \\ 659 \end{array}$	Н 994	N 190	O 186	${ m S} { m 2}$	0	0

• Molecule 18 is a protein called zf-CHCC domain-containing protein.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
18	R	118	Total 1798	C 574	Н 876	N 166	0 177	${ m S}{ m 5}$	0	0

• Molecule 19 is a protein called Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues			ns			AltConf	Trace	
19	S	86	Total 1351	C 418	H 684	N 126	0 122	S 1	0	0

• Molecule 20 is a protein called Acyl carrier protein.

Mol	Chain	Residues		A	toms			AltConf	Trace
20	Т	81	Total 1234	C 391	Н 614	N 98	O 131	0	0

• Molecule 21 is a protein called Acyl carrier protein.

Mol	Chain	Residues			Aton	ıs			AltConf	Trace
21	U	88	Total 1322	C 416	Н 655	N 106	0 143	${ m S} { m 2}$	0	0

• Molecule 22 is a protein called Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues			Atom	IS			AltConf	Trace
22	V	126	Total 2049	C 653	Н 1021	N 173	O 200	${ m S} { m 2}$	0	0



• Molecule 23 is a protein called Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues			Atom	IS			AltConf	Trace
23	W	123	Total 2054	C 667	Н 1018	N 182	0 185	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 24 is a protein called Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues			AltConf	Trace				
24	Х	171	Total 2678	C 847	H 1333	N 236	0 252	S 10	0	0

• Molecule 25 is a protein called Complex I-B14.7.

Mol	Chain	Residues			Atom	S			AltConf	Trace
25	v	170	Total	С	Η	Ν	Ο	\mathbf{S}	0	0
20	I	113	2638	842	1311	240	240	5	0	0

• Molecule 26 is a protein called GRIM-19.

Mol	Chain	Residues				AltConf	Trace			
26	Ζ	122	Total 1983	C 629	Н 1000	N 180	O 169	${f S}{5}$	0	0

• Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues			AltConf	Trace				
27	a	86	Total 1353	C 432	Н 672	N 127	O 119	${ m S} { m 3}$	0	0

• Molecule 28 is a protein called subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues			Aton	ns			AltConf	Trace
28	b	78	Total 1257	C 418	Н 618	N 115	O 105	${ m S}$ 1	0	0

• Molecule 29 is a protein called Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I).



Mol	Chain	Residues			Atom	IS			AltConf	Trace
29	с	182	Total 2804	C 898	Н 1407	N 241	O 256	${ m S} { m 2}$	0	0

• Molecule 30 is a protein called subunit NEBM of protein NADH:Ubiquinone Oxidoreductase (Complex I) [Yarrowia lipolytica].

Mol	Chain	Residues		At	oms			AltConf	Trace
30	d	67	Total 1042	C 339	H 532	N 86	0 85	0	0

• Molecule 31 is a protein called Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues			Aton	ns			AltConf	Trace
31	е	68	Total 1082	C 336	Н 536	N 102	O 102	S 6	0	0

• Molecule 32 is a protein called Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues			Atom	S			AltConf	Trace
32	f	137	Total 2225	C 730	Н 1089	N 194	0 210	${ m S}\ 2$	0	0

• Molecule 33 is a protein called Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues			Atom	5			AltConf	Trace
33	g	198	Total 3188	C 1019	Н 1603	N 273	0 291	${S \over 2}$	0	0

• Molecule 34 is a protein called subunit NUNM of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues			Atom	ıs			AltConf	Trace
34	h	113	Total 1786	C 585	Н 877	N 153	0 170	${f S}$ 1	0	0

• Molecule 35 is a protein called Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I).



Mol	Chain	Residues			Aton	ns			AltConf	Trace
35	i	86	Total 1300	C 420	Н 641	N 120	0 118	S 1	0	0

• Molecule 36 is a protein called Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues		ŀ	Atom	s			AltConf	Trace
36	j	53	Total 884	C 299	Н 439	N 77	O 66	${ m S} { m 3}$	0	0

• Molecule 37 is a protein called Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues		At	oms	AltConf	Trace		
37	k	47	Total 734	C 242	Н 361	N 70	O 61	0	0

• Molecule 38 is a protein called Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues			Aton	ıs			AltConf	Trace
38	1	125	Total 2012	C 674	Н 973	N 166	0 197	${ m S} { m 2}$	0	0

• Molecule 39 is a protein called Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues		Α	toms			AltConf	Trace
39	m	92	Total 1453	$\begin{array}{c} \mathrm{C} \\ 472 \end{array}$	Н 718	N 134	O 129	0	0

• Molecule 40 is a protein called Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues			Atom	ıs			AltConf	Trace
40	n	108	Total 1804	C 571	Н 904	N 172	0 154	${ m S} { m 3}$	0	0

• Molecule 41 is a protein called Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I).



Mol	Chain	Residues	Atoms					AltConf	Trace	
41	О	83	Total 1366	C 431	Н 685	N 123	0 119	S 8	0	0

• Molecule 42 is a protein called Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace	
42	р	91	Total 1492	C 475	Н 726	N 138	O 150	${ m S} { m 3}$	0	0

• Molecule 43 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$).



Mol	Chain	Residues	A	toms			AltConf
/3	Л	1	Total C	H N	Ο	Р	0
40	D	I	61 17	34 1	8	1	0
/3	Ц	1	Total C	H N	Ο	Р	0
40	11	1	64 18	36 1	8	1	0
/3	Т	1	Total C	H N	Ο	Р	0
40	L	1	188 56	112 2	16	2	0
/3	т	1	Total C	H N	Ο	Р	0
40	L	1	188 56	112 2	16	2	0
/3	Ν	1	Total C	H N	Ο	Р	0
40	IN	1	106 32	64 1	8	1	0
/13	d	1	Total C	H N	0	Р	0
40	u	L	61 17	34 1	8	1	0



• Molecule 44 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	AltConf
44	Е	1	TotalFeS422	0
44	G	1	TotalFeS422	0

• Molecule 45 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf	
45	Б	1	Total	С	Η	Ν	0	Р	0
40	Г	1	49	17	18	4	9	1	0



• Molecule 46 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
46	F	1	Total Fe S	0
10	1	Ŧ	8 4 4	0
46	С	1	Total Fe S	0
40	G	1	16 8 8	0
46	С	1	Total Fe S	0
40	G	1	16 8 8	0
46	Т	1	Total Fe S	0
40	1	1	16 8 8	0
46	т	1	Total Fe S	0
40	1	L	16 8 8	0

• Molecule 47 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).





Mol	Chain	Residues	Atoms	AltConf
47	TT	1	Total C H N O P	0
41	П	1	162 48 94 2 16 2	0
47	тт	1	Total C H N O P	0
47	п	1	162 48 94 2 16 2	0
47	т	1	Total C H N O P	0
41	1	1	74 22 42 1 8 1	0
47	т	1	Total C H N O P	0
41	L	1	399 123 246 3 24 3	0
47	т	1	Total C H N O P	0
41	L	1	399 123 246 3 24 3	0
47	т	1	Total C H N O P	0
41	L	I	399 123 246 3 24 3	0
17	М	1	Total C H N O P	0
-11	111	1	69 20 39 1 8 1	0
17	Ν	1	Total C H N O P	0
71	11	1	133 41 82 1 8 1	0
17	V	1	Total C H N O P	0
71	I	1	79 23 46 1 8 1	0
17	Z	1	Total C H N O P	0
41		1	109 33 66 1 8 1	0
17	h	1	Total C H N O P	0
11	D	1	109 33 66 1 8 1	0
47	d	1	Total C H N O P	0
11	u	1	52 14 28 1 8 1	U
47	σ	1	Total C H N O P	0
- 11	б	L	68 20 38 1 8 1	

• Molecule 48 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).





Mol	Chain	Residues	Atoms	AltConf
19	М	1	Total C H O P	0
40	111	1	205 64 122 17 2	0
18	0	1	Total C H O P	0
40	0	1	145 44 82 17 2	0
18	7	1	Total C H O P	0
40		1	123 38 66 17 2	0
18	9	1	Total C H O P	0
40	a	T	108 33 56 17 2	0
18	h	1	Total C H O P	0
10	U	1	100 29 52 17 2	

• Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).





Mol	Chain	Residues	Atoms					AltConf	
40	р	1	Total	С	Η	Ν	Ο	Р	0
49	Г	1	74	21	26	7	17	3	0

• Molecule 50 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
50	R	1	Total Zn 1 1	0

• Molecule 51 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]ami no]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).





Mol	Chain	Residues		Atoms										
51	Т	1	Total	С	Η	Ν	Ο	Р	S	0				
	1	L	75	22	40	2	9	1	1	0				
51	T	1	Total	С	Η	Ν	Ο	Р	S	0				
51	U	T	77	23	41	2	9	1	1	0				

• Molecule 52 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $\rm C_{24}H_{46}O_{11}).$



Mol	Chain	Residues	Atoms	AltConf
59	V	1	Total C H O	0
52	1	L	162 48 92 22	0
50	V	1	Total C H O	0
52	1	L	162 48 92 22	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NADH-ubiquinone oxidoreductase chain 3





• Molecule 5: Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I)



• Molecule 6: Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I)







• Molecule 8: NADH-ubiquinone oxidoreductase chain 1





• Molecule 9: Subunit NUIM of protein NADH:Ubiquinone Oxidoreductase (Complex I)



1357 K358 7356 7356 7365 7365 7365 7365 7365 7365 7376 8377 8377 8377 8377 8377 8377 8377 8377 8377 8377 8377 8377 8377 8420 8420 8420

• Molecule 10: NADH-ubiquinone oxidoreductase chain 6





 \bullet Molecule 11: NADH-ubiquinone oxidore
ductase chain 4L







• Molecule 12: NADH-ubiquinone oxidoreductase chain 5





PROTEIN DATA BANK



• Molecule 17: Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I)





• Molecule 22: Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I)



• Molecule 23: Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I)



• Molecule 24: Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I)



• Molecule 26: GRIM-19





NET 12 A3 A1 A27 A27 A31 C28 A31 A31 A31 A35 A31 A35 A35 A35 A35 A35 A35 A35 A35 A35 A35	K62 R58 F58 F59 F50 F50 K67 K67 K67 K68 K68 K68 K68 K68 K68 K68 K68 K68 K68	PRO PRO VAL VAL VAL VAL VAL ILE VAL ALA ALA ALA ALA ALA CUU CUU
• Molecule 32: Subunit N7BM o	f NADH:Ubiquinone Oxidored	uctase (Complex I)
Chain f:	98%	
MET S2 W13 E14 H18 W21 W21 W21 M21 M24 M24 M24 M29 M20 M20 M20 M20 M20 M20 M20 M20 M20 M20	R59 R65 R65 R65 R66 R66 R98 R98 R94 R93 R94 R93 R93 R93 R93 R93 R93 R93 R93 R93 R93	A.9 C 1297 1298 11998 11998 11998 11998 11998 11998 11998 11999 11995 11907 11
• Molecule 33: Subunit NESM o	f NADH:Ubiquinone Oxidored	luctase (Complex I)
Chain g:	79%	20%
MET LLEU LLEU LLEU LTYR TTYR ASR ASR ASR ASR ALA ASR TTHR TTHR TTHR TTHR TTHR TTHR TTHR TT	ALA VAL CYS CYS CYS CYS LYS ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	A47 L48 A50 Y 51 N55 E53 E55 E55 E55 E55 K60 K60
461 862 863 864 864 965 966 967 968 969 963 964 965 965 963 964 965 965 963 963 964 965 965 963 970 971 973 974 975 976 977 978 978 978 978 979 970 970 970 970 971 970 971 970 971 970 970 970 970 970 970 970 970 970 970 970 970 970 970 970 970 970 970 970 <	P80 R81 P82 P83 P83 A83 E85 A85 E87 A86 E93 E93 E93 A95 E93 A95 A95	 197 Y98 Y100 P100 P100 R102 P105 P105 P105 P105 P106 P111 P111 P111 P111 P111 P111 P112 P111 P121 P121 P121
K1.27 D1.28 L1.37 L1.37 L1.37 D1.38 K1.43 V1.42 K1.43 D1.44 K1.43 C1.44 K1.44 K1.44 K1.45 C1.48 K1.44 K1.44	1151 1154 1155 1155 1155 1155 1155 1155	P174 P178 1178 1178 1178 1188 1188 1188 1188 1188 1200 1200 1200 1210 1210 1211 1215
D219 A220 L221 E224 R2255 V231 D230 V233 V233 L234 A234 C238 K239 K239 K240 K241 K241		
• Molecule 34: subunit NUNM o	f protein NADH:Ubiquinone (Oxidoreductase (Complex I)
Chain h:	81%	19%
MET LEU LEU ARG HIS HIS THR ARG ALA ALA ALA ARG GLN ALA ASN ASN ASN ASN ASN ASN ASN ASN ASN AS	HIS 017 738 138 141 741 743 744 744 745 747 948 948 948 948	S58 L59 G60 L61 V62 V62 A63 A63 A63 A63 A63 A63 A73 C69 C76 C76 H77 T78 T78
E81 K87 E90 E90 E91 E95 E95 E108 E114 E115 E115 E115 E119 E119 E119 E1120	D133 4 6138 6 6139 5 5140 5 5144 6 8148 6 8148 6 8148 6 8148 6	
• Molecule 35: Subunit NUUM o	of NADH:Ubiquinone Oxidored	ductase (Complex I)
Chain i:	96%	
MET G2 G3 G4 K5 K5 K10 D11 D11 M15 W26 W26 W26 W26 W26 W26 W26 W26	F32 136 A37 A37 C39 C39 C40 C44 C44 C44 C44 C44 C44 C44 C44 C44	R55 657 158 657 158 860 860 865 865 865 865 865 865 865 865 865 865



K80 181 183 A86 A85 A85 A85 A85 A A A A A A A A A A A A
• Molecule 36: Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I)
67% Chain j: 79% 21%
MET ALA ALA ALA THR YE YE YE YE VIJ HIS VIJ HIS VIJ HIS VIJ HIS VIJ HIS VIJ HIS VIJ HIS VIJ HIS VIJ HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS
GLY LYS VAL GLU HIS
• Molecule 37: Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I)
62% Chain k: 78% 22%
MET A2 P3 P3 P3 P3 P3 P3 P3 P3 P3 P3 P4 P3 P3 P3 P3 P3 P3 P3 P3 P3 P3 P3 P3 P3
• Molecule 38: Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I)
56% Chain I: 83% 16%
MET LEU SER ARG ARG ARG ARG ARG ARG ARG ARG CAN ARG ARG CAN AR
B67 E68 M72 D74 D75 D74 D74 D75 D75 D76 D77 D76 D76 D770
C136 C137 S140 S146 A142 S146 A142 S146 S148 S148 <t< td=""></t<>
• Molecule 39: Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I)
Chain m: 99%
MET MET 110 110 49 1110 411 412 48 412 48 412 48 412 48 412 48 412 48 412 48 412 48 48 48 48 48 48 48 48 48 48 48 48 48
688 288 292 293 293 293 293 294 293 294 295 294 295 295 295 295 295 295 295 295 295 295
• Molecule 40: Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I)
57% Chain n: 98%



• Molecule 41: Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I)

													_	_		65	%																																
С	hŧ	ai	n	0:															84	1%															1	6%													
	•	•	•	•	•	•	••	•					>	>			•	•	-	••	•	•		•	•	•	•	•	•			•	•	••	••			••	-	••	•	••	٠	٠	•	•	•	••	••
MET	A2	E3	F4	P5	P6	L7	L8	S9	q 10	E11	D12	M13	K14 124 E	d I N H I G	01U	Ĭ	L20	A21	1 CL	R25	C26	A27		L30	V31 P32	L33	N34	E35	K39	C 7 M	M43	A46	C47	G48	H49	E50	R51	E53	Y54	M56	C57	E58	V59 A60	D61	го2 063	R64	R65	V66 V67	A68
٠	•	•	•	•	•	•	•	•	••	••	••	••	••	•																																			
M69	D70	K71	1.72	K73	A74	E75	K76	177	E78	Q79	A 80	K81	A82	A83	A84 AT A	ALA	ALA	ALA	ALA	ALA	ALA	ASP	GLU	GLU	LYS																								

• Molecule 42: Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I)

										32%	6																									
C	ha	ai	n	р	: -													ç	8%	6																•••
4		•		•	•	•	•	•	•	•	•	•	•	•	•	٠		٠	٠		•	•	•	•	•	٠			٠	_		٠		••	٠	
MET	S2	ß	H4	q5	R6 P7	E8	FJ	D13	D14	115	N16	Y17	N18	D19	E28	L38	K46	E53	E54		H59	F60	E61	D62	C63	K64	020	D/ 2	Q 80	R87	N88	D89	06d	S91	K92	



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21013	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	48	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-2700	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.278	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	472.49997, 472.49997, 472.49997	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FES, LMT, CDL, ZN, NDP, FME, EHZ, 3PE, FMN, PLC

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).

Mal	Chain	Bo	ond lengths	B	ond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.75	0/773	0.68	0/1054
2	В	1.01	4/1432~(0.3%)	0.72	2/1948~(0.1%)
3	С	0.97	0/2062	0.70	1/2813~(0.0%)
4	D	0.92	1/3513~(0.0%)	0.73	2/4763~(0.0%)
5	Ε	0.73	0/1725	0.67	1/2343~(0.0%)
6	F	0.72	1/3638~(0.0%)	0.67	1/4910~(0.0%)
7	G	0.85	3/5368~(0.1%)	0.71	3/7285~(0.0%)
8	Н	0.76	1/2751~(0.0%)	0.66	1/3758~(0.0%)
9	Ι	1.12	4/1564~(0.3%)	0.74	1/2121~(0.0%)
10	J	0.66	0/1477	0.62	0/2015
11	Κ	0.76	0/692	0.71	0/937
12	L	0.74	0/5327	0.63	1/7273~(0.0%)
13	М	0.86	0/3941	0.65	1/5382~(0.0%)
14	Ν	0.93	0/3846	0.62	1/5242~(0.0%)
15	0	0.75	0/1344	0.63	0/1822
16	Р	0.73	0/2873	0.67	1/3894~(0.0%)
17	\mathbf{Q}	0.90	1/1067~(0.1%)	0.71	1/1442~(0.1%)
18	R	0.84	0/946	0.60	0/1283
19	S	0.64	0/677	0.67	1/907~(0.1%)
20	Т	0.49	0/628	0.65	1/854~(0.1%)
21	U	0.53	0/673	0.60	0/916
22	V	0.68	0/1049	0.59	0/1420
23	W	0.79	0/1061	0.65	0/1427
24	Х	0.71	0/1374	0.70	3/1856~(0.2%)
25	Y	0.66	0/1359	0.63	0/1851
26	Ζ	0.80	0/1007	0.72	1/1357~(0.1%)
27	a	0.68	0/697	0.72	2/940~(0.2%)
28	b	0.72	0/665	0.62	0/909
29	с	0.78	0/1438	0.65	1/1965~(0.1%)
30	d	0.75	0/523	0.58	0/707
31	е	0.67	0/555	0.61	0/740
32	f	0.94	1/1174~(0.1%)	0.67	1/1597~(0.1%)



Mal	Chain	Bo	ond lengths	B	ond angles
IVIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
33	g	0.61	0/1614	0.66	0/2182
34	h	0.70	0/937	0.63	0/1270
35	i	0.66	0/679	0.66	0/924
36	j	0.60	0/465	0.64	0/630
37	k	0.58	0/385	0.71	0/522
38	l	0.67	0/1073	0.60	0/1451
39	m	0.70	0/756	0.66	0/1021
40	n	0.63	0/926	0.67	0/1253
41	0	0.59	0/695	0.62	0/930
42	р	0.78	0/782	0.69	1/1051~(0.1%)
All	All	0.80	16/65531~(0.0%)	0.67	28/88965~(0.0%)

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Ι	366	CYS	CB-SG	-7.20	1.70	1.82
17	Q	58	VAL	CB-CG2	-6.42	1.39	1.52
9	Ι	330	CYS	CB-SG	-6.34	1.71	1.82
7	G	229	VAL	CB-CG1	-6.27	1.39	1.52
8	Н	194	VAL	CB-CG1	-5.84	1.40	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
14	N	2685	ARG	NE-CZ-NH1	-6.29	117.15	120.30
7	G	191	ARG	NE-CZ-NH1	5.97	123.28	120.30
6	F	400	ARG	NE-CZ-NH2	5.96	123.28	120.30
24	Х	112	ARG	NE-CZ-NH1	5.89	123.25	120.30
42	р	87	ARG	NE-CZ-NH1	5.86	123.23	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	766	827	826	8	0
2	В	1393	1373	1373	10	0
3	С	1999	1925	1925	16	0
4	D	3434	3354	3354	34	0
5	Е	1688	1660	1660	19	0
6	F	3559	3513	3513	33	0
7	G	5274	5173	5173	34	0
8	Н	2689	2774	2774	22	0
9	Ι	1526	1471	1471	14	0
10	J	1462	1582	1582	13	0
11	Κ	693	753	753	18	0
12	L	5207	5364	5364	61	0
13	М	3857	4053	4053	37	0
14	Ν	3776	4004	4004	33	0
15	0	1305	1281	1281	6	0
16	Р	2812	2763	2763	18	0
17	Q	1037	994	994	5	0
18	R	922	876	876	8	0
19	S	667	684	684	7	0
20	Т	620	614	614	7	0
21	U	667	655	655	5	0
22	V	1028	1021	1021	5	0
23	W	1036	1018	1018	5	0
24	Х	1345	1333	1333	10	0
25	Y	1327	1311	1310	2	0
26	Ζ	983	1000	1000	8	0
27	a	681	672	671	0	0
28	b	639	618	620	0	0
29	с	1397	1407	1407	0	0
30	d	510	532	532	0	0
31	е	546	536	536	0	0
32	f	1136	1089	1089	0	0
33	g	1585	1603	1603	0	0
34	h	909	877	877	0	0
35	i	659	641	641	0	0
36	j	445	439	439	0	0
37	k	373	361	361	0	0
38	1	1039	973	973	0	0
39	m	735	718	718	0	0
40	n	900	904	904	0	0
41	0	681	685	685	0	0
42	р	766	726	726	0	0
43	D	27	34	28	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	Н	28	36	27	0	0
43	L	76	112	106	3	0
43	N	42	64	64	0	0
43	d	27	34	28	0	0
44	Е	4	0	0	1	0
44	G	4	0	0	0	0
45	F	31	18	18	1	0
46	F	8	0	0	0	0
46	G	16	0	0	0	0
46	Ι	16	0	0	1	0
47	Н	68	94	87	1	0
47	Ι	32	42	38	0	0
47	L	153	246	246	3	0
47	М	30	39	34	0	0
47	N	51	82	82	3	0
47	Y	33	46	40	1	0
47	Z	43	66	60	0	0
47	b	43	66	63	0	0
47	d	24	28	22	0	0
47	g	30	38	34	0	0
48	М	83	122	113	0	0
48	0	63	82	73	1	0
48	Z	57	66	58	1	0
48	a	52	56	48	0	0
48	b	48	52	40	0	0
49	Р	48	26	26	2	0
50	R	1	0	0	0	0
51	Т	35	40	0	3	0
51	U	36	41	0	0	0
52	Y	70	92	92	0	0
All	All	65352	65779	65583	386	0

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The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 386 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
14:N:2539:ILE:HD11	14:N:2638:ILE:HG22	1.44	0.97	
3:C:216:LEU:HD11	4:D:126:LEU:HD23	1.58	0.84	
51:T:201:EHZ:N2	51:T:201:EHZ:O3	2.12	0.81	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
16:P:131:ARG:NH2	49:P:401:NDP:O2X	2.15	0.80	
16:P:247:ARG:NH1	16:P:334:ASP:O	2.16	0.79	

Continued from previous page...

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	ved Outliers H		Percentiles	
1	А	90/128~(70%)	85~(94%)	5 (6%)	0	100	100	
2	В	175/210~(83%)	168 (96%)	7 (4%)	0	100	100	
3	С	240/293~(82%)	221 (92%)	18 (8%)	1 (0%)	34	69	
4	D	435/466~(93%)	410 (94%)	25~(6%)	0	100	100	
5	Е	214/243~(88%)	199 (93%)	14 (6%)	1 (0%)	29	66	
6	F	458/488 (94%)	425 (93%)	33 (7%)	0	100	100	
7	G	692/728~(95%)	639 (92%)	53 (8%)	0	100	100	
8	Н	339/341~(99%)	321 (95%)	18 (5%)	0	100	100	
9	Ι	189/193~(98%)	181 (96%)	8 (4%)	0	100	100	
10	J	183/185~(99%)	174 (95%)	9 (5%)	0	100	100	
11	К	87/89~(98%)	83 (95%)	4 (5%)	0	100	100	
12	L	653/655~(100%)	616 (94%)	36 (6%)	1 (0%)	47	78	
13	М	484/486 (100%)	464 (96%)	20 (4%)	0	100	100	
14	Ν	467/469~(100%)	452 (97%)	15 (3%)	0	100	100	
15	Ο	166/169~(98%)	156 (94%)	10 (6%)	0	100	100	
16	Р	353/355~(99%)	337 (96%)	16 (4%)	0	100	100	
17	Q	123/161 (76%)	118 (96%)	5 (4%)	0	100	100	
18	R	116/118~(98%)	106 (91%)	9 (8%)	1 (1%)	17	54	


Mol	Chain	Analysed	Favoured Allowed		Outliers Perce		ntiles
19	S	84/87~(97%)	78~(93%)	6~(7%)	0	100	100
20	Т	79/81~(98%)	73~(92%)	5~(6%)	1 (1%)	12	47
21	U	86/88~(98%)	78 (91%)	8 (9%)	0	100	100
22	V	124/144~(86%)	119 (96%)	5 (4%)	0	100	100
23	W	121/124 (98%)	112 (93%)	9(7%)	0	100	100
24	Х	169/172~(98%)	160 (95%)	9(5%)	0	100	100
25	Y	177/180~(98%)	171 (97%)	6 (3%)	0	100	100
26	Ζ	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
27	a	84/86~(98%)	82 (98%)	2 (2%)	0	100	100
28	b	76/78~(97%)	67 (88%)	9 (12%)	0	100	100
29	с	180/182~(99%)	166 (92%)	14 (8%)	0	100	100
30	d	65/73~(89%)	65 (100%)	0	0	100	100
31	е	66/89~(74%)	65~(98%)	1 (2%)	0	100	100
32	f	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
33	g	196/249~(79%)	187 (95%)	9(5%)	0	100	100
34	h	111/139 (80%)	106 (96%)	5 (4%)	0	100	100
35	i	84/90~(93%)	82 (98%)	2 (2%)	0	100	100
36	j	51/67~(76%)	50 (98%)	1 (2%)	0	100	100
37	k	45/60~(75%)	41 (91%)	4 (9%)	0	100	100
38	1	123/149~(83%)	112 (91%)	9(7%)	2(2%)	9	43
39	m	90/93~(97%)	84 (93%)	6 (7%)	0	100	100
40	n	106/109~(97%)	99~(93%)	6 (6%)	1 (1%)	17	54
41	0	81/99~(82%)	78~(96%)	3 (4%)	0	100	100
42	р	89/92~(97%)	84 (94%)	5 (6%)	0	100	100
All	All	8006/8568~(93%)	7557 (94%)	441 (6%)	8 (0%)	54	83

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	1260	VAL
5	Е	217	ASP
38	1	148	SER
40	n	90	TYR
3	С	254	PRO



5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	86/113~(76%)	86 (100%)	0	100	100	
2	В	152/180~(84%)	152 (100%)	0	100	100	
3	С	218/251 (87%)	218 (100%)	0	100	100	
4	D	367/394~(93%)	367 (100%)	0	100	100	
5	Е	191/212~(90%)	191 (100%)	0	100	100	
6	F	367/389~(94%)	367 (100%)	0	100	100	
7	G	566/595~(95%)	565~(100%)	1 (0%)	93	97	
8	Н	293/301~(97%)	293 (100%)	0	100	100	
9	Ι	157/158~(99%)	157 (100%)	0	100	100	
10	J	166/166~(100%)	166 (100%)	0	100	100	
11	K	76/76~(100%)	76 (100%)	0	100	100	
12	L	579/579~(100%)	578 (100%)	1 (0%)	93	97	
13	М	433/433~(100%)	433 (100%)	0	100	100	
14	Ν	432/432~(100%)	431 (100%)	1 (0%)	93	97	
15	Ο	132/133~(99%)	132~(100%)	0	100	100	
16	Р	299/311~(96%)	299 (100%)	0	100	100	
17	Q	107/140~(76%)	107 (100%)	0	100	100	
18	R	98/98~(100%)	98 (100%)	0	100	100	
19	S	72/73~(99%)	72 (100%)	0	100	100	
20	Т	68/68~(100%)	68 (100%)	0	100	100	
21	U	75/75~(100%)	74 (99%)	1 (1%)	69	83	
22	V	113/129 (88%)	111 (98%)	2(2%)	59	77	
23	W	109/110 (99%)	109 (100%)	0	100	100	
24	X	147/148 (99%)	147 (100%)	0	100	100	
25	Y	130/131~(99%)	130 (100%)	0	100	100	
26	Ζ	$101/101 \ (100\%)$	101 (100%)	0	100	100	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
27	a	68/68~(100%)	68~(100%)	0	100	100	
28	b	65/65~(100%)	65~(100%)	0	100	100	
29	с	148/148~(100%)	148 (100%)	0	100	100	
30	d	52/58~(90%)	52 (100%)	0	100	100	
31	е	59/76~(78%)	59~(100%)	0	100	100	
32	f	122/123~(99%)	122 (100%)	0	100	100	
33	g	161/211~(76%)	160 (99%)	1 (1%)	86	93	
34	h	98/119~(82%)	98 (100%)	0	100	100	
35	i	64/68~(94%)	64 (100%)	0	100	100	
36	j	45/55~(82%)	45 (100%)	0	100	100	
37	k	32/45~(71%)	32~(100%)	0	100	100	
38	1	109/129~(84%)	109 (100%)	0	100	100	
39	m	72/73~(99%)	72 (100%)	0	100	100	
40	n	99/100~(99%)	99 (100%)	0	100	100	
41	0	70/76~(92%)	70 (100%)	0	100	100	
42	р	84/85~(99%)	84 (100%)	0	100	100	
All	All	6882/7295~(94%)	6875 (100%)	7 (0%)	93	98	

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
21	U	73	LYS
22	V	25	MET
33	g	62	ARG
22	V	27	GLU
14	N	2488	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	185	ASN
14	Ν	2706	ASN
16	Р	234	ASN
41	0	16	HIS



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues 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 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).

Mal	Turne	Chain	Dec	Link	B	ond leng	$_{ m gths}$	Bond angles		
		Unain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
13	FME	М	503	13	8,9,10	0.88	0	7,9,11	1.07	1 (14%)
11	FME	K	1	11	8,9,10	1.03	1 (12%)	7,9,11	1.23	1 (14%)
8	FME	Н	1	8	8,9,10	1.17	1 (12%)	7,9,11	1.07	0
14	FME	N	2403	14	8,9,10	1.45	1 (12%)	7,9,11	0.55	0
12	FME	L	706	12	8,9,10	1.01	1 (12%)	7,9,11	1.04	0
1	FME	А	1	1	8,9,10	1.07	1 (12%)	7,9,11	1.27	1 (14%)
10	FME	J	1	10	8,9,10	0.97	0	7,9,11	1.02	1 (14%)

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
13	FME	М	503	13	-	0/7/9/11	-
11	FME	К	1	11	-	2/7/9/11	-
8	FME	Н	1	8	-	1/7/9/11	-
14	FME	Ν	2403	14	-	2/7/9/11	-
12	FME	L	706	12	-	2/7/9/11	-
1	FME	А	1	1	-	3/7/9/11	-
10	FME	J	1	10	-	2/7/9/11	-

All (5) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
14	Ν	2403	FME	CA-N	-3.69	1.41	1.46
8	Н	1	FME	CA-N	-2.42	1.42	1.46
11	Κ	1	FME	CA-N	-2.17	1.43	1.46
1	А	1	FME	CA-N	-2.16	1.43	1.46
12	L	706	FME	CN-N	2.05	1.40	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	1	FME	C-CA-N	2.75	114.70	109.73
11	Κ	1	FME	C-CA-N	2.32	113.92	109.73
10	J	1	FME	CE-SD-CG	2.25	108.13	100.40
13	М	503	FME	C-CA-N	2.11	113.55	109.73

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	А	1	FME	C-CA-CB-CG
1	А	1	FME	O-C-CA-CB
8	Н	1	FME	O1-CN-N-CA
11	Κ	1	FME	N-CA-CB-CG
10	J	1	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 1 is monoatomic - leaving 37 for Mogul analysis.

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 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).



Mal	Turne	Chain	Dec	Tink	B	ond leng	gths	Bond angles			
	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
44	FES	G	803	7	0,4,4	-	-	-			
47	3PE	g	301	-	29,29,50	1.21	3 (10%)	32,34,55	1.30	5 (15%)	
46	SF4	Ι	503	9	0,12,12	-	-	-			
48	CDL	М	501	-	82,82,99	1.33	8 (9%)	88,94,111	1.11	5 (5%)	
43	PLC	L	701	-	41,41,41	1.30	6 (14%)	$47,\!49,\!49$	1.14	4 (8%)	
46	SF4	G	802	7	0,12,12	-	-	-			
47	3PE	\mathbf{L}	704	-	$50,\!50,\!50$	0.87	4 (8%)	$53,\!55,\!55$	1.09	3 (5%)	
47	3PE	М	502	-	29,29,50	1.20	4 (13%)	$32,\!34,\!55$	1.21	4 (12%)	
46	SF4	Ι	502	9	0,12,12	-	-	-			
46	SF4	F	502	6	0,12,12	-	-	-			
48	CDL	b	401	-	47,47,99	1.33	7 (14%)	53,59,111	1.35	6 (11%)	
47	3PE	Η	6403	-	$45,\!45,\!50$	1.19	3 (6%)	$48,\!50,\!55$	1.10	3 (6%)	
49	NDP	Р	401	-	$45,\!52,\!52$	2.54	9 (20%)	53,80,80	1.76	11 (20%)	
43	PLC	D	501	-	26,26,41	1.48	6 (23%)	32,34,49	1.15	3 (9%)	
51	EHZ	U	201	21	31,35,37	2.12	7 (22%)	41,45,47	1.40	4 (9%)	
43	PLC	Ν	2401	-	41,41,41	1.12	5 (12%)	47,49,49	1.08	3 (6%)	
48	CDL	0	601	-	62,62,99	1.19	7 (11%)	68,74,111	1.20	7 (10%)	
47	3PE	d	502	-	23,23,50	1.33	3 (13%)	26,28,55	1.26	3 (11%)	
43	PLC	L	702	-	33,33,41	1.36	2 (6%)	39,41,49	1.10	2(5%)	
51	EHZ	Т	201	20	30,34,37	2.15	8 (26%)	40,44,47	1.51	8 (20%)	
47	3PE	Y	1403	-	32,32,50	1.16	5 (15%)	35,37,55	1.11	3 (8%)	
48	CDL	Ζ	201	-	56,56,99	1.20	7 (12%)	62,68,111	1.21	7 (11%)	
45	FMN	F	501	-	33,33,33	3.26	13 (39%)	48,50,50	2.57	21 (43%)	
47	3PE	L	705	-	50,50,50	0.89	4 (8%)	53,55,55	1.30	3 (5%)	
43	PLC	d	501	-	26,26,41	1.46	5 (19%)	32,34,49	1.30	6 (18%)	
44	FES	Е	301	5	0,4,4	-	-	-			
47	3PE	b	402	-	42,42,50	1.21	6 (14%)	45,47,55	1.12	3 (6%)	
46	SF4	G	801	7	0,12,12	-	-	-			
52	LMT	Υ	1401	-	36,36,36	0.92	2 (5%)	47,47,47	1.11	2 (4%)	
52	LMT	Y	1402	-	36,36,36	0.89	0	47,47,47	1.18	6 (12%)	
48	CDL	a	101	-	51,51,99	1.27	9 (17%)	57,63,111	1.45	6 (10%)	
43	PLC	Н	6402	-	26,26,41	1.48	5 (19%)	30,32,49	1.88	4 (13%)	
47	3PE	L	703	-	50,50,50	0.86	4 (8%)	$53,\!55,\!55$	1.02	2 (3%)	
47	3PE	Н	6401	-	21,21,50	1.28	2 (9%)	24,26,55	1.18	2 (8%)	
47	3PE	Ν	2402	-	50,50,50	0.90	2 (4%)	53,55,55	1.09	2 (3%)	
47	3PE	Ι	501	-	31,31,50	1.14	<mark>3 (9%)</mark>	34,36,55	1.21	3 (8%)	



Mol Typ	Type	Chain	Dog	Tink	B	ond leng	gths	B	ond ang	les
	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
47	3PE	Ζ	202	-	42,42,50	0.97	3 (7%)	45,47,55	1.03	3 (6%)

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
44	FES	G	803	7	-	-	0/1/1/1
47	3PE	g	301	-	1/1/4/4	9/33/33/54	-
48	CDL	М	501	-	-	45/93/93/110	-
46	SF4	Ι	503	9	-	-	0/6/5/5
43	PLC	L	701	-	-	23/45/45/45	-
47	3PE	М	502	-	1/1/4/4	18/33/33/54	-
47	3PE	L	704	-	-	21/54/54/54	-
46	SF4	G	802	7	-	-	0/6/5/5
46	SF4	Ι	502	9	-	-	0/6/5/5
48	CDL	b	401	-	-	20/58/58/110	-
46	SF4	F	502	6	-	-	0/6/5/5
47	3PE	Н	6403	-	-	18/49/49/54	-
49	NDP	Р	401	-	-	11/30/77/77	0/5/5/5
43	PLC	D	501	-	-	11/30/30/45	-
51	EHZ	U	201	21	-	8/43/43/45	-
43	PLC	Ν	2401	-	-	17/45/45/45	-
48	CDL	Ο	601	-	-	28/73/73/110	-
47	3PE	d	502	-	-	14/27/27/54	-
43	PLC	L	702	-	-	18/37/37/45	-
51	EHZ	Т	201	20	1/1/9/9	15/42/42/45	-
47	3PE	Y	1403	-	-	16/36/36/54	-
48	CDL	Ζ	201	-	-	38/67/67/110	-
45	FMN	F	501	-	-	12/18/18/18	0/3/3/3
47	3PE	L	705	-	-	22/54/54/54	-
43	PLC	d	501	-	-	11/30/30/45	-
47	3PE	b	402	-	-	15/46/46/54	-
44	FES	Е	301	5	-	-	0/1/1/1
46	SF4	G	801	7	-	_	0/6/5/5
52	LMT	Y	1401	-	4/4/10/10	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	LMT	Y	1402	-	4/4/10/10	11/21/61/61	0/2/2/2
48	CDL	а	101	-	-	23/62/62/110	-
43	PLC	Н	6402	-	-	13/30/30/45	-
47	3PE	L	703	-	-	23/54/54/54	-
47	3PE	Н	6401	-	1/1/4/4	12/24/24/54	-
47	3PE	Ν	2402	-	-	23/54/54/54	-
47	3PE	Ι	501	-	1/1/4/4	21/35/35/54	-
47	3PE	Z	202	-	-	12/46/46/54	-

The worst 5 of 152 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	Р	401	NDP	P2B-O2B	14.28	1.86	1.59
45	F	501	FMN	O3'-C3'	-10.24	1.18	1.43
45	F	501	FMN	O2-C2	8.34	1.39	1.24
45	F	501	FMN	O4-C4	8.24	1.39	1.23
51	Т	201	EHZ	C15-N2	6.41	1.47	1.33

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
45	F	501	FMN	C9-C9A-N10	7.99	132.64	121.84
43	Н	6402	PLC	C7-N-C6	-7.08	91.43	109.73
47	L	705	3PE	O21-C21-C22	6.85	126.27	111.50
49	Р	401	NDP	PN-O3-PA	-6.70	109.82	132.83
45	F	501	FMN	C10-N1-C2	6.25	129.40	116.90

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
47	Н	6401	3PE	C2
47	Ι	501	3PE	C2
47	М	502	3PE	C2
47	g	301	3PE	C2
51	Т	201	EHZ	C16

5 of 537 torsion outliers are listed below:

43 D 501 PLC C1-O3P-P-O2P	Mol	Chain	Res	Type	Atoms
	43	D	501	PLC	C1-O3P-P-O2P

Continued on next page...



Mol	Chain	Res	Type	Atoms
43	Н	6402	PLC	O3P-C1-C2-O2
43	Н	6402	PLC	C4-O4P-P-O1P
43	Н	6402	PLC	C4-O4P-P-O2P
43	L	701	PLC	O4P-C4-C5-N

There are no ring outliers.

13 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	Ι	503	SF4	1	0
43	L	701	PLC	2	0
47	Н	6403	3PE	1	0
49	Р	401	NDP	2	0
48	0	601	CDL	1	0
43	L	702	PLC	1	0
51	Т	201	EHZ	3	0
47	Y	1403	3PE	1	0
48	Ζ	201	CDL	1	0
45	F	501	FMN	1	0
47	L	705	3PE	3	0
44	Е	301	FES	1	0
47	N	2402	3PE	3	0

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.







































































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-11969. 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



6.1.2 Raw map



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



6.2 Central slices (i)

6.2.1 Primary map



X Index: 225



Y Index: 225



Z Index: 225

6.2.2 Raw map



X Index: 225

Y Index: 225



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



6.3 Largest variance slices (i)

Primary map 6.3.1



X Index: 241



Y Index: 231



Z Index: 286

Raw map 6.3.2



X Index: 240

Y Index: 232



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



6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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



Mask visualisation (i) 6.5

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

emd_11969_msk_1.map (i) 6.5.1





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 176 $\rm nm^3;$ this corresponds to an approximate mass of 159 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.270 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.270 ${\rm \AA^{-1}}$


8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion (FSC cut-off)		
resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.72	4.36	3.79
Unmasked-calculated*	6.35	8.71	6.73

*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 6.35 differs from the reported value 3.7 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11969 and PDB model 7B0N. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).



9.4 Atom inclusion (i)



At the recommended contour level, 46% of all backbone atoms, 46% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

\mathbf{Chain}	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.4596	0.4670
А	0.3676	0.4450
В	0.5880	0.5110
С	0.5965	0.5190
D	0.5486	0.4970
Е	0.4058	0.4400
F	0.4406	0.4530
G	0.5205	0.4860
Н	0.4430	0.4580
Ι	0.6294	0.5180
J	0.3720	0.4470
K	0.4603	0.4680
L	0.4683	0.4730
Μ	0.5430	0.4950
Ν	0.5775	0.5130
О	0.4175	0.4500
Р	0.4425	0.4580
Q	0.5525	0.5010
R	0.5485	0.5010
S	0.3115	0.3990
Т	0.0877	0.3100
U	0.1943	0.3840
V	0.4314	0.4720
W	0.4526	0.4540
X	0.4269	0.4400
Y	0.3188	0.4390
Z	0.4452	0.4680
a	0.4266	0.4650
b	0.3597	0.4570
c	0.4792	0.4840
d	0.4180	0.4600
e	0.4569	0.4530
f	0.5467	0.4960
g	0.2852	0.3810
h	0.4508	0.4660

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Chain	Atom inclusion	Q-score
i	0.3772	0.4280
j	0.2396	0.3850
k	0.2813	0.3820
1	0.3392	0.4380
m	0.3862	0.4420
n	0.3780	0.4180
0	0.2756	0.3770
р	0.5308	0.4730

