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PDB ID	:	7AK5
EMDB ID	:	EMD-11810
Title	:	Cryo-EM structure of respiratory complex I in the deactive state from Mus musculus at 3.2 A
Authors	:	Yin, Z.; Bridges, H.R.; Grba, D.; Hirst, J.
Deposited on	:	2020-09-29
Resolution	:	3.17 Å(reported)
This i	s a l	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.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 3.17 Å.

Ramachandran outliers

Sidechain outliers

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		$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
	 Percentile relative Percentile relative 	ve to all structures	Deller
Sidechain outliers	Worse		Better
Ramachandran outliers			0.0%
Metric	;	Percentile Ranks	Value

154571

154315

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 $<\!\!=\!5\%$
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.

4023

3826

Mol	Chain	Length	Quality of chain	
1	А	115	• 78%	22%
2	В	224	6 9%	31%
3	С	263	• 78%	22%
4	D	463	• 90%	10%
5	Е	245	9%	14%
6	F	464	5% 92%	8%
7	G	715	5% 96%	
8	Н	318	• 97%	
9	Ι	212	• 84%	16%



 $Continued \ from \ previous \ page...$ Chain Length Quality of chain Mol 16% 10 J 17299% i Κ 11 9899% ÷ 12L 607 100% М 13459100% 14Ν 345100% 5% 15Ο 35590% 10% 7% Р 377 1677% 23% ÷ 17Q 17571% 29% R 18 11482% 18% 20% \mathbf{S} 991983% 17% 25% Т 2015647% 53% 9% U 2015656% 44% 8% 21V 11697% 8% 22W 13187% 13% 5% Х 1722399% •• 5% 24Υ 14398% • i Ζ 2514497% • i 6826 \mathbf{a} 100% 8% 27b 83 99% 5% 2876 \mathbf{c} 61% 39% ÷ 29 \mathbf{d} 12099% 30 106е 98% 12% 31 f 5788% 12% 5% 32g 15167% 33% 33 h 189 72% 28%



Mal	Choin	Longth	Quality of aboin	
IVIOI	Chain	Length	Quality of chain	
			6%	
34	i	127	76%	24%
			12%	
35	j	105	60%	40%
			13%	
36	k	104	74%	• 25%
			7%	
37	1	186	84%	16%
			9%	
38	m	129	97%	•
			10%	
39	n	179	98%	••
			17%	
40	0	137	83%	17%
			5%	
41	р	176	95%	5%
			_	
42	q	145	99%	•
			<u> </u>	
43	r	112	85%	• 14%
		104	.	
44	s	104	38% 6	52%



2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 65895 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.

• Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues		At	oms	AltConf	Trace		
1	А	90	Total 737	C 511	N 101	0 120	${S \atop 5}$	0	0

• Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	В	155	Total 1241	C 793	N 222	0 212	S 14	0	0

• Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	С	206	Total 1712	C 1105	N 294	O 310	${ m S} { m 3}$	0	0

• Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues		At	AltConf	Trace			
4	D	419	Total 3381	C 2163	N 578	0 616	$\begin{array}{c} \mathrm{S} \\ \mathrm{24} \end{array}$	0	0

• Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Е	210	Total 1639	C 1043	N 275	O 310	S 11	0	0

• Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.



Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	428	Total 3301	C 2080	N 590	O 609	S 22	0	0

• Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues		\mathbf{A}	AltConf	Trace			
7	G	687	Total 5287	C 3316	N 918	O 1012	S 41	0	0

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

Mol	Chain	Residues		At		AltConf	Trace		
8	Н	308	Total 2465	C 1659	N 373	0 411	S 22	0	0

• Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
9	Ι	178	Total 1408	C 885	N 243	0 268	S 12	0	0

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

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
10	J	171	Total 1277	C 857	N 185	O 220	S 15	0	0

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

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
11	K	98	Total 737	С 477	N 112	0 137	S 11	0	0

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

Mol	Chain	Residues		At	AltConf	Trace			
12	L	606	Total 4800	C 3182	N 746	0 827	S 45	0	0

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



Mol	Chain	Residues		At	AltConf	Trace			
13	М	459	Total 3632	C 2408	N 567	O 617	S 40	0	0

• Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues		At	AltConf	Trace			
14	Ν	344	Total 2696	C 1791	N 416	O 452	S 37	0	0

• Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues		At	AltConf	Trace			
15	О	320	Total 2607	C 1674	N 431	0 492	S 10	0	0

• Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
16	Р	290	Total 2297	C 1463	N 415	0 412	S 7	0	0

• Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues		At	oms		AltConf	Trace	
17	Q	125	Total 1015	C 642	N 179	O 190	${S \atop 4}$	0	0

• Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues		At	oms		AltConf	Trace	
18	R	94	Total 738	C 458	N 135	0 142	${ m S} { m 3}$	0	0

• Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues		At	oms	AltConf	Trace		
19	S	82	Total 659	C 413	N 125	0 118	${ m S} { m 3}$	0	0



• Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues		At	oms		AltConf	Trace	
20	Т	72	Total	С	Ν	0	\mathbf{S}	0	0
20	1	15	588	378	87	118	5	0	0
20	II	00	Total	С	Ν	0	S	0	0
20	U	00	706	453	104	144	5	0	0

• Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues		At	oms			AltConf	Trace
21	V	112	Total 915	C 596	N 152	0 164	${ m S} { m 3}$	0	0

• Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues		At	oms		AltConf	Trace	
22	W	114	Total 970	C 619	N 180	O 165	${ m S}{ m 6}$	0	0

• Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues		A	AltConf	Trace			
23	Х	171	Total 1396	C 889	N 250	O 247	S 10	0	0

• Molecule 24 is a protein called MCG5603.

Mol	Chain	Residues		At	oms	AltConf	Trace		
24	Y	140	Total 1037	C 662	N 175	0 192	S 8	0	0

• Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues		At	oms		AltConf	Trace	
25	Ζ	139	Total 1152	C 741	N 204	0 199	S 8	0	0

• Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.



Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
26	a	68	Total 556	C 360	N 99	O 93	$\frac{S}{4}$	0	0

• Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues		At	AltConf	Trace			
27	b	83	Total 651	$\begin{array}{c} \mathrm{C} \\ 427 \end{array}$	N 105	0 115	${f S}$ 4	0	0

• Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
28	с	46	Total 381	C 249	N 66	O 65	S 1	0	0

• Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues		At	oms	AltConf	Trace		
29	d	119	Total 985	C 645	N 167	0 164	S 9	0	0

• Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues		At	oms	AltConf	Trace		
30	е	104	Total 870	$\begin{array}{c} \mathrm{C} \\ 550 \end{array}$	N 161	0 151	${f S} 8$	0	0

• Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues		Atc	\mathbf{ms}			AltConf	Trace
31	f	50	Total 424	C 273	N 76	0 73	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
32	g	101	Total 850	$\begin{array}{c} \mathrm{C} \\ 549 \end{array}$	N 136	0 161	$\frac{S}{4}$	0	0



• Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
33	h	137	Total 1153	C 756	N 192	O 202	${ m S} { m 3}$	0	0

• Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues		At	oms			AltConf	Trace
34	i	96	Total 811	C 529	N 139	0 140	${ m S} { m 3}$	0	0

• Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues		Ato	\mathbf{ms}			AltConf	Trace
35	j	63	Total 542	C 358	N 89	0 94	S 1	0	0

• Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues		At	oms			AltConf	Trace
36	k	78	Total 630	C 416	N 107	O 105	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
37	1	156	Total 1312	C 846	N 219	O 236	S 11	0	0

• Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues		Ato	ms		AltConf	Trace
38	m	125	Total 1044	C 673	N 188	O 183	0	0

• Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.



Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
39	n	176	Total 1527	C 976	N 274	O 266	S 11	0	0

• Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues		At	oms	AltConf	Trace		
40	О	114	Total 984	C 620	N 185	0 171	S 8	0	0

• Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues		At	oms			AltConf	Trace
41	р	168	Total	С	N	0	S	0	0
			1424	896	256	264	8		

• Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues		At	oms			AltConf	Trace
42	q	143	Total 1192	C 766	N 212	0 210	${S \over 4}$	0	0

• Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace	
43	r	96	Total 776	C 490	N 145	0 138	${ m S} { m 3}$	0	0

• Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues		Aton	ıs		AltConf	Trace
44	S	39	Total 329	C 207	N 59	O 63	0	0

• Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).





Mol	Chain	Residues	Atoms	AltConf
45	В	1	Total Fe S 8 4 4	0
45	F	1	TotalFeS844	0
45	G	1	TotalFeS1688	0
45	G	1	TotalFeS1688	0
45	Ι	1	TotalFeS1688	0
45	Ι	1	TotalFeS1688	0

• Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).





Mol	Chain	Residues	Atoms					AltConf		
46	В	1	Total	С	Ν	0	Р	0		
	D	L	51	41	1	8	1	0		
46	Т	т	Т	1	Total	С	Ν	0	Р	0
40	1	L	54	44	1	8	1	0		

• Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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



• Molecule 48 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
19	Б	1	Total	С	Ν	Ο	Р	0
40	Г	1	31	17	4	9	1	0

• Molecule 49 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues		AltConf				
40	п	1	Total	С	Ν	Ο	Р	0
49	49 H	1	51	41	1	8	1	U



Mol	Chain	Residues	Atoms	AltConf
40	т	1	Total C N O P	0
49	1	1	51 41 1 8 1	0
40	т	1	Total C N O P	0
49	49 L	1	51 41 1 8 1	0
40	49 M	1	Total C N O P	0
49		1	102 82 2 16 2	0
40	М	1	Total C N O P	0
49	111		102 82 2 16 2	0
40	N	1	Total C N O P	0
49	1 N	1	51 41 1 8 1	0
40	40 f	1	Total C N O P	0
49	1	1	39 29 1 8 1	0
40	i	1	Total C N O P	0
49	1		42 32 1 8 1	0

- Molecule 50 is CARDIOLIPIN (three-letter code: CDL) (formula: $\mathrm{C}_{81}\mathrm{H}_{156}\mathrm{O}_{17}\mathrm{P}_2).$



Mol	Chain	Residues	Atoms	AltConf
50	т	1	Total C O P	0
00	L	1	81 62 17 2	0 0 0 0
50	d	1	Total C O P	0
50	u	1	100 81 17 2	0
50	h	1	Total C O P	0
50	11	1	78 59 17 2	0
50	a	1	Total C O P	0
- 50	Ч	I	69 50 17 2	0



• Molecule 51 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
51	0	1	Total	С	Ν	Ο	Р	0
51	U	T	31	10	5	13	3	0

• Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					AltConf
52	Р	1	Total 48	C 21	N 7	0 17	Р 3	0



• Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Ator	\mathbf{ns}	AltConf
53	R	1	Total 1	Zn 1	0

• Molecule 54 is ${S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]ami no]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: <math>C_{25}H_{49}N_2O_9PS$).



Mol	Chain	Residues	Atoms					AltConf	
54	Т	1	Total	С	Ν	Ο	Р	\mathbf{S}	0
-04	T	1	37	25	2	8	1	1	0
54 U	1	Total	С	Ν	0	Р	S	0	
	U		37	25	2	8	1	1	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: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial
9% Chain E: 86% 14%
MET PHE SER LEU ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
83:88 A196 70:97 70:07 <
\bullet Molecule 6: NADH dehydrogenase [ubiquinone] flavo protein 1, mitochondrial
Chain F: 92% 8%
MET LIEU ALA ALA ALA ALA ALA ALA ALA ALA VAL ULEU VAL VAL ARG GLY VAL ARG CLY THR ALA ARG ARG FIE SER SER SER SER SER CLY CLS CLY CLS CLY CLS CLY CLS CLY CLS CLY CLS CLY CLS CLY CLS CLY CLS CLY CLS CLY CLS CLY CLS CLY CLS CLY CLS CLY CLS CLY CLS CLY CLY CLS CLY CLY CLS CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY
L276 K277 E278 C289 C289 C289 C289 C289 C289 C289 C28
\bullet Molecule 7: NADH-ubiquinone oxidore ductase 75 k Da subunit, mitochondrial
Chain G: 96% ·
MET LIEU LIEU LIEU LIEU LIEU LIEU LIEU LIEU
E512 K515 K515 K520 K530 K530 K530 K530 K530 K530 B566 K533 B617 K633 B6517 K653 R679 K679 R679 K679 B659 K679 R679 K679
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1
Chain H: 97% ·
Mei Hei Hei Hei Histor
\bullet Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial
Chain I: 84% 16%
MET TYR LEU SER SER SER SER ALA ALA ALA ALA ALA ALA ALA ALA ALA AL

• Molecule 10: NADH-ubiquinone oxidoreductase chain 6



	16%	
Chain J:	99% ·	
M1 Y78 P79 E80 W82	G83 884 N85 F91 F91 F91 F91 F94 695 F101 F101 F101 F101 F101 F101 F101 F10	
• Molecule 1	11: NADH-ubiquinone oxidoreductase chain 4L	
Chain K:	99% .	
• Molecule 1	12: NADH-ubiquinone oxidoreductase chain 5	
Chain L:	100%	
M1 K28 N206	L480 A390 A510 A510 K511 K515 L601 L606 GLU	
• Molecule 1	13: NADH-ubiquinone oxidoreductase chain 4	
Chain M:	100%	
M1 D187 M459		
• Molecule 1	14: NADH-ubiquinone oxidoreductase chain 2	
Chain N:	100%	
M1 K321		
• Molecule drial	15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex s	ubunit 10, mitochon-
Chain O:	90% 10%	
MET ALA ALA ARG LEU LEU LEU CEU VAL	PRO PRO ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	K223 E236
L241 K242 L249 D265		

• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial







• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



Chain a:	•
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex su	bunit 3
Chain b: 99%	
A1 I.4 MIO MIO MISI A1111 A111 A111 A111 A111 A111 A111 A111 A11	
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochor	ndrial
Chain c: 61% 39%	
MET ALA PALA PALA VAL VAL LEU LEU LEU LEU LEU LEU LEU PRO PRO AAC AAC ALA ALA ALA ALA AC CU VB PRO PRO PRO PRO PRO CU VB PRO CU VB CA CU VB CA CU VB CA CU VB CA CU VB CA CU VAL AC CU VAL AC CU VAL CU VAL CU VAL CU CU VAL CU VAL CU CU VAL CU CU CU CU CU CU CU CU CU CU CU CU CU	
\bullet Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2	
Chain d: 99%	
M1 G7 K104 E103 ARG	
\bullet Molecule 30: NADH dehydrogen ase [ubiquinone] iron-sulfur protein 5	
Chain e: 98%	
MET PI E100 E103 P103 PR0	
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex sub	ounit 1
Chain f: 88% 12%	
MET THR LEU GLM GLM B3 B3 B3 B4 B4 P4 9 49 F15 C	
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex drial	subunit 11, mitochon-
Chain g: 67% 33%	





• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:	10%		98%	••
MET A1 P5 N52 K52	K5 4 M5 6 M5 7 E6 5	R134	1148 1148 1148 1148 1178 1176 1176 1176 1176 1176 1178 1	

• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p: 95%							5%
MET PRO ASP SER W4	S14	P19	S24	N58	E165	A169 8170 6171 ALA ALA ALA	

• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:	99%	
MET E2 E2 R21 F142 F142 F144 LVS		
• Molecule 43:	NADH dehydrogenase [ubiquinone] 1 alpha subcomplex s	subunit 7



• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



Chain s:

38%

62%





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50184	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM $(4k \ge 4k)$	Depositor
Maximum map value	0.271	Depositor
Minimum map value	-0.107	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0355	Depositor
Map size (Å)	486.0, 486.0, 486.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^{\circ}$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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: 2MR, AYA, CDL, SAC, 3PE, ATP, PC1, NDP, SF4, FES, FME, FMN, ZN, EHZ

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	Bond	lengths	Bond angles		
WIOI	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.27	0/746	0.47	0/1019	
2	В	0.31	0/1272	0.46	0/1722	
3	С	0.29	0/1762	0.47	0/2401	
4	D	0.30	0/3452	0.46	0/4672	
5	Ε	0.26	0/1679	0.42	0/2288	
6	F	0.26	0/3376	0.45	0/4561	
7	G	0.28	0/5374	0.46	0/7281	
8	Н	0.28	0/2530	0.43	0/3458	
9	Ι	0.31	0/1438	0.47	0/1946	
10	J	0.28	0/1297	0.42	0/1765	
11	Κ	0.27	0/738	0.42	0/1002	
12	L	0.27	0/4913	0.43	0/6686	
13	М	0.27	0/3709	0.44	0/5052	
14	Ν	0.27	0/2748	0.43	0/3741	
15	0	0.27	0/2674	0.44	0/3626	
16	Р	0.27	0/2345	0.44	0/3166	
17	Q	0.27	0/1038	0.45	0/1401	
18	R	0.29	0/751	0.45	0/1011	
19	S	0.24	0/670	0.43	0/904	
20	Т	0.25	0/597	0.42	0/804	
20	U	0.27	0/718	0.40	0/970	
21	V	0.26	0/937	0.41	0/1270	
22	W	0.26	0/993	0.42	0/1335	
23	Х	0.27	0/1434	0.47	1/1937~(0.1%)	
24	Y	0.27	0/1061	0.43	0/1439	
25	Z	0.27	0/1183	0.42	0/1597	
26	a	0.28	0/569	0.41	0/766	
27	b	0.27	0/666	0.42	0/914	
28	с	0.25	0/392	0.39	0/533	
29	d	0.30	0/1017	0.40	0/1373	
30	е	0.27	0/892	0.43	0/1187	
31	f	0.26	0/434	0.43	0/584	



Mal	Mol Chain		lengths	Bond angles		
1VIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
32	g	0.27	0/878	0.40	0/1196	
33	h	0.28	0/1188	0.43	0/1610	
34	i	0.26	0/828	0.42	0/1125	
35	j	0.24	0/566	0.43	0/775	
36	k	0.26	0/650	0.41	0/878	
37	1	0.27	0/1367	0.42	0/1866	
38	m	0.27	0/1073	0.42	0/1455	
39	n	0.26	0/1581	0.41	0/2140	
40	0	0.28	0/1009	0.43	0/1355	
41	р	0.27	0/1457	0.42	0/1969	
42	q	0.28	0/1234	0.45	0/1681	
43	r	0.28	0/786	0.43	0/1062	
44	s	0.26	0/338	0.42	0/458	
All	All	0.27	0/66360	0.44	1/89981~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
23	Х	55	CYS	CA-CB-SG	7.78	128.00	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	86/115~(75%)	83~(96%)	3 (4%)	0	100	100
2	В	153/224~(68%)	142 (93%)	10 (6%)	1 (1%)	22	60
3	С	204/263~(78%)	193 (95%)	11 (5%)	0	100	100
4	D	412/463~(89%)	386 (94%)	26 (6%)	0	100	100
5	Е	208/245~(85%)	194 (93%)	14 (7%)	0	100	100
6	F	426/464 (92%)	401 (94%)	25 (6%)	0	100	100
7	G	685/715~(96%)	649 (95%)	36 (5%)	0	100	100
8	Н	304/318~(96%)	279 (92%)	25 (8%)	0	100	100
9	Ι	176/212~(83%)	168 (96%)	8 (4%)	0	100	100
10	J	169/172~(98%)	164 (97%)	5 (3%)	0	100	100
11	K	96/98~(98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/607~(100%)	562 (93%)	42 (7%)	0	100	100
13	М	457/459~(100%)	430 (94%)	27 (6%)	0	100	100
14	Ν	342/345~(99%)	325 (95%)	17 (5%)	0	100	100
15	Ο	318/355~(90%)	293 (92%)	25 (8%)	0	100	100
16	Р	282/377~(75%)	265 (94%)	17 (6%)	0	100	100
17	Q	123/175~(70%)	119 (97%)	4 (3%)	0	100	100
18	R	92/114 (81%)	90 (98%)	2 (2%)	0	100	100
19	S	80/99~(81%)	73 (91%)	7 (9%)	0	100	100
20	Т	71/156~(46%)	63 (89%)	8 (11%)	0	100	100
20	U	86/156~(55%)	82 (95%)	4 (5%)	0	100	100
21	V	110/116~(95%)	102 (93%)	8 (7%)	0	100	100
22	W	112/131~(86%)	101 (90%)	11 (10%)	0	100	100
23	Х	169/172~(98%)	157 (93%)	12 (7%)	0	100	100
24	Y	138/143~(96%)	131 (95%)	7 (5%)	0	100	100
25	Z	137/144~(95%)	129 (94%)	8 (6%)	0	100	100
26	a	66/68~(97%)	65 (98%)	1 (2%)	0	100	100
27	b	81/83~(98%)	74 (91%)	7 (9%)	0	100	100
28	с	44/76~(58%)	43 (98%)	1 (2%)	0	100	100
29	d	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
30	e	102/106~(96%)	91 (89%)	11 (11%)	0	100	100
31	f	48/57~(84%)	44 (92%)	4 (8%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
32	g	99/151~(66%)	96~(97%)	3 (3%)	0	100	100
33	h	135/189~(71%)	130 (96%)	5 (4%)	0	100	100
34	i	92/127~(72%)	81 (88%)	11 (12%)	0	100	100
35	j	61/105~(58%)	59~(97%)	2 (3%)	0	100	100
36	k	76/104 (73%)	74 (97%)	2 (3%)	0	100	100
37	1	154/186~(83%)	144 (94%)	10 (6%)	0	100	100
38	m	123/129~(95%)	117 (95%)	6 (5%)	0	100	100
39	n	174/179~(97%)	167 (96%)	7 (4%)	0	100	100
40	0	112/137~(82%)	103 (92%)	9 (8%)	0	100	100
41	р	166/176~(94%)	156 (94%)	10 (6%)	0	100	100
42	q	141/145~(97%)	132 (94%)	9 (6%)	0	100	100
43	r	92/112~(82%)	84 (91%)	8 (9%)	0	100	100
44	S	37/104~(36%)	35~(95%)	2(5%)	0	100	100
All	All	7960/9192 (87%)	7484 (94%)	475 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	64	CYS

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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	81/103~(79%)	81 (100%)	0	100	100
2	В	131/185~(71%)	130 (99%)	1 (1%)	81	92
3	С	188/227~(83%)	188 (100%)	0	100	100
4	D	362/394~(92%)	362 (100%)	0	100	100
5	Е	183/205~(89%)	183 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
6	F	343/370~(93%)	343~(100%)	0	100	100
7	G	579/601~(96%)	577 (100%)	2 (0%)	92	97
8	Н	270/279~(97%)	270 (100%)	0	100	100
9	Ι	145/178 (82%)	145 (100%)	0	100	100
10	J	131/137~(96%)	131 (100%)	0	100	100
11	K	87/87~(100%)	87 (100%)	0	100	100
12	L	548/549~(100%)	548 (100%)	0	100	100
13	М	414/414 (100%)	414 (100%)	0	100	100
14	Ν	306/307~(100%)	306 (100%)	0	100	100
15	О	284/309~(92%)	284 (100%)	0	100	100
16	Р	251/325~(77%)	250 (100%)	1 (0%)	91	96
17	Q	112/153~(73%)	112 (100%)	0	100	100
18	R	79/94~(84%)	79 (100%)	0	100	100
19	S	73/80~(91%)	73 (100%)	0	100	100
20	Т	67/135~(50%)	67 (100%)	0	100	100
20	U	81/135~(60%)	81 (100%)	0	100	100
21	V	100/102~(98%)	100 (100%)	0	100	100
22	W	108/114 (95%)	108 (100%)	0	100	100
23	Х	153/154 (99%)	153 (100%)	0	100	100
24	Y	105/107~(98%)	105 (100%)	0	100	100
25	Ζ	120/123~(98%)	120 (100%)	0	100	100
26	a	58/58~(100%)	58 (100%)	0	100	100
27	b	72/72~(100%)	72 (100%)	0	100	100
28	с	40/67~(60%)	40 (100%)	0	100	100
29	d	106/107~(99%)	106 (100%)	0	100	100
30	е	92/94~(98%)	92 (100%)	0	100	100
31	f	46/53~(87%)	46 (100%)	0	100	100
32	g	92/129~(71%)	92 (100%)	0	100	100
33	h	122/162~(75%)	122 (100%)	0	100	100
34	i	90/118~(76%)	90 (100%)	0	100	100
35	j	58/87~(67%)	58 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
36	k	60/78~(77%)	59~(98%)	1 (2%)	60	82
37	1	141/161~(88%)	141 (100%)	0	100	100
38	m	111/114~(97%)	111 (100%)	0	100	100
39	n	161/164~(98%)	160 (99%)	1 (1%)	86	94
40	0	106/121~(88%)	106 (100%)	0	100	100
41	р	153/158~(97%)	153 (100%)	0	100	100
42	q	129/131~(98%)	129 (100%)	0	100	100
43	r	86/95~(90%)	86 (100%)	0	100	100
44	s	38/95~(40%)	38 (100%)	0	100	100
All	All	7062/7931 (89%)	7056 (100%)	6 (0%)	93	98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	64	CYS
7	G	495	ARG
7	G	679	ARG
16	Р	177	ARG
36	k	25	ARG
39	n	174	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
2	В	172	GLN
3	С	39	GLN
3	С	87	GLN
3	С	200	ASN
4	D	114	ASN
4	D	149	ASN
4	D	313	GLN
4	D	398	HIS
5	Е	55	GLN
6	F	113	HIS
6	F	257	ASN
7	G	475	GLN
7	G	546	GLN
8	Н	5	ASN



Mol	Chain	Res	Type
8	Н	97	ASN
8	Н	169	GLN
9	Ι	172	GLN
11	Κ	92	ASN
12	L	29	HIS
12	L	209	ASN
12	L	230	HIS
12	L	320	ASN
12	L	594	ASN
12	L	605	ASN
13	М	92	GLN
13	М	169	ASN
13	М	175	ASN
13	М	374	ASN
14	N	172	GLN
14	N	174	GLN
14	N	222	ASN
15	0	180	GLN
16	Р	93	ASN
16	Р	131	HIS
17	Q	46	GLN
21	V	36	HIS
22	W	101	GLN
23	Х	34	GLN
26	a	58	ASN
30	е	97	HIS
32	g	109	ASN
33	h	108	GLN
34	i	12	GLN
35	j	42	HIS
35	j	58	GLN
37	1	2	HIS
37	1	77	HIS
37	1	154	HIS
42	q	13	GLN
42	q	87	HIS
42	q	113	HIS
43	r	46	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)

11 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	Type	Chain	Dog	Link	Bo	ond leng	$_{\rm ths}$	Bond angles			
MOI	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
4	2MR	D	85	4	$10,\!12,\!13$	2.46	2 (20%)	5,13,15	1.42	1 (20%)	
1	FME	А	1	1	8,9,10	0.96	0	7,9,11	0.84	0	
10	FME	J	1	10	8,9,10	0.93	0	7,9,11	0.94	0	
13	FME	М	1	13	8,9,10	0.96	0	7,9,11	0.66	0	
34	SAC	i	1	34	7,8,9	1.00	0	8,9,11	0.73	0	
43	AYA	r	1	43	6,7,8	1.28	1 (16%)	5,8,10	1.10	1 (20%)	
27	AYA	b	1	27	6,7,8	1.24	1 (16%)	$5,\!8,\!10$	1.40	1 (20%)	
8	FME	Н	1	8	$8,\!9,\!10$	0.91	0	7,9,11	1.39	1 (14%)	
14	FME	Ν	1	14	8,9,10	0.90	0	7,9,11	0.93	0	
12	FME	L	1	12	8,9,10	0.94	0	7,9,11	1.07	1 (14%)	
11	FME	К	1	11	8,9,10	0.92	0	7,9,11	1.14	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
4	2MR	D	85	4	-	3/10/13/15	-
1	FME	А	1	1	-	3/7/9/11	-
10	FME	J	1	10	-	4/7/9/11	-
13	FME	М	1	13	-	0/7/9/11	-
34	SAC	i	1	34	-	2/7/8/10	-
43	AYA	r	1	43	-	0/4/6/8	-
27	AYA	b	1	27	-	1/4/6/8	-
8	FME	Н	1	8	-	5/7/9/11	-
14	FME	N	1	14	-	3/7/9/11	-
12	FME	L	1	12	-	4/7/9/11	-



Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	FME	К	1	11	-	2/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
4	D	85	2MR	CZ-NE	5.38	1.45	1.34
4	D	85	2MR	CZ-NH2	4.91	1.44	1.33
43	r	1	AYA	CA-N	-2.47	1.44	1.46
27	b	1	AYA	CA-N	-2.33	1.44	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
8	Н	1	FME	C-CA-N	3.05	115.24	109.73
27	b	1	AYA	CB-CA-N	2.87	112.81	109.61
4	D	85	2MR	CD-NE-CZ	2.50	128.08	123.41
11	Κ	1	FME	C-CA-N	2.42	114.11	109.73
12	L	1	FME	C-CA-N	2.20	113.70	109.73
43	r	1	AYA	CB-CA-N	2.12	111.97	109.61

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
1	А	1	FME	O-C-CA-CB
4	D	85	2MR	O-C-CA-CB
8	Н	1	FME	O-C-CA-CB
8	Н	1	FME	CA-CB-CG-SD
10	J	1	FME	CB-CA-N-CN
10	J	1	FME	C-CA-CB-CG
11	Κ	1	FME	C-CA-CB-CG
12	L	1	FME	O-C-CA-CB
14	Ν	1	FME	CB-CA-N-CN
14	Ν	1	FME	N-CA-CB-CG
34	i	1	SAC	C-CA-N-C1A
34	i	1	SAC	CB-CA-N-C1A
4	D	85	2MR	NE-CD-CG-CB
1	А	1	FME	N-CA-CB-CG
1	А	1	FME	CB-CG-SD-CE
10	J	1	FME	CA-CB-CG-SD
11	K	1	FME	N-CA-CB-CG


Mol	Chain	Res	Type	Atoms
4	D	85	2MR	CA-CB-CG-CD
8	Н	1	FME	CB-CG-SD-CE
27	b	1	AYA	C-CA-N-CT
10	J	1	FME	CB-CG-SD-CE
14	Ν	1	FME	C-CA-CB-CG
12	L	1	FME	CB-CG-SD-CE
12	L	1	FME	CA-CB-CG-SD
8	Н	1	FME	C-CA-CB-CG
8	Н	1	FME	CB-CA-N-CN
12	L	1	FME	CB-CA-N-CN

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 28 ligands modelled in this entry, 1 is monoatomic - leaving 27 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	ol Type Chain Res		Dec	Tink	Bo	Bond lengths			Bond angles		
IVIOI	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
50	CDL	d	201	-	99,99,99	0.88	7 (7%)	105,111,111	1.03	4 (3%)	
49	3PE	Ι	202	-	50,50,50	0.86	4 (8%)	$53,\!55,\!55$	1.01	2 (3%)	
50	CDL	L	702	-	80,80,99	0.98	8 (10%)	86,92,111	1.08	4 (4%)	
47	FES	G	803	7	0,4,4	-	-	-		<u> </u>	
45	SF4	G	801	7	0,12,12	-	-	-			
45	SF4	Ι	204	9	0,12,12	-	-	-			
49	3PE	Н	401	-	50,50,50	0.86	4 (8%)	$53,\!55,\!55$	1.09	2 (3%)	
50	CDL	h	201	_	77,77,99	0.98	7 (9%)	83,89,111	1.10	4 (4%)	



Mal	Tune	Chain	Dog	Tink	Bo	ond leng	ths	Bo	nd angle	s
IVIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
47	FES	Е	301	5	0,4,4	-	-	-		
52	NDP	Р	501	-	45,52,52	2.29	6 (13%)	53,80,80	1.70	9 (16%)
45	SF4	В	201	2	0,12,12	-	-	-		
45	SF4	Ι	203	9	0,12,12	-	-	-		
49	3PE	L	701	-	50, 50, 50	0.85	4 (8%)	53,55,55	1.03	2 (3%)
46	PC1	В	202	-	50,50,53	0.98	4 (8%)	56,58,61	1.00	2 (3%)
48	FMN	F	501	-	33,33,33	1.09	2 (6%)	48,50,50	1.32	8 (16%)
54	EHZ	U	201	20	29,36,37	1.68	5 (17%)	35,44,47	1.45	4 (11%)
49	3PE	f	101	-	38,38,50	0.99	4 (10%)	41,43,55	1.00	2 (4%)
49	3PE	М	502	-	50,50,50	0.86	4 (8%)	53,55,55	1.08	2(3%)
45	SF4	G	802	7	0,12,12	-	-	-		
49	3PE	Ν	401	-	50,50,50	0.87	4 (8%)	53,55,55	1.03	2 (3%)
51	ATP	0	401	-	26,33,33	0.92	1 (3%)	31,52,52	1.59	6 (19%)
50	CDL	q	201	-	68,68,99	1.05	7 (10%)	74,80,111	1.10	4 (5%)
54	EHZ	Т	201	20	29,36,37	1.68	5 (17%)	35,44,47	1.55	5 (14%)
49	3PE	М	501	-	50,50,50	0.87	4 (8%)	53,55,55	0.96	2(3%)
46	PC1	Ι	201	-	53,53,53	0.94	4 (7%)	59,61,61	0.99	2 (3%)
45	SF4	F	502	6	0,12,12	-	-	-		
49	3PE	i	201	-	41,41,50	0.95	4 (9%)	44,46,55	1.09	2 (4%)

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
50	CDL	d	201	-	-	60/110/110/110	-
49	3PE	Ι	202	-	-	15/54/54/54	-
50	CDL	L	702	-	-	41/91/91/110	-
47	FES	G	803	7	-	-	0/1/1/1
45	SF4	G	801	7	-	-	0/6/5/5
45	SF4	Ι	204	9	-	-	0/6/5/5
49	3PE	Н	401	-	-	21/54/54/54	-
50	CDL	h	201	-	-	41/88/88/110	-
47	FES	Е	301	5	-	-	0/1/1/1
52	NDP	Р	501	-	-	10/30/77/77	0/5/5/5
45	SF4	В	201	2	-	-	0/6/5/5
45	SF4	Ι	203	9	-	-	0/6/5/5



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	3PE	L	701	-	-	18/54/54/54	-
46	PC1	В	202	-	-	21/54/54/57	-
48	FMN	F	501	-	-	8/18/18/18	0/3/3/3
54	EHZ	U	201	20	-	11/42/44/45	-
49	3PE	f	101	-	-	13/42/42/54	-
49	3PE	М	502	-	-	18/54/54/54	-
45	SF4	G	802	7	-	-	0/6/5/5
51	ATP	0	401	-	-	7/18/38/38	0/3/3/3
49	3PE	Ν	401	-	-	24/54/54/54	-
50	CDL	q	201	-	-	37/79/79/110	-
54	EHZ	Т	201	20	-	16/42/44/45	-
49	3PE	М	501	-	-	25/54/54/54	-
46	PC1	Ι	201	-	-	22/57/57/57	-
45	SF4	F	502	6	-	-	0/6/5/5
49	3PE	i	201	-	-	17/45/45/54	-

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
52	Р	501	NDP	P2B-O2B	12.55	1.83	1.59
54	Т	201	EHZ	C15-N2	5.49	1.45	1.33
54	U	201	EHZ	C15-N2	5.42	1.45	1.33
54	U	201	EHZ	C12-N1	5.23	1.45	1.33
54	Т	201	EHZ	C12-N1	5.19	1.45	1.33
52	Р	501	NDP	PN-O5D	4.04	1.75	1.59
48	F	501	FMN	C4A-N5	3.50	1.37	1.30
52	Р	501	NDP	O2B-C2B	-3.11	1.32	1.44
50	L	702	CDL	OA6-CA4	-2.65	1.40	1.46
50	q	201	CDL	OB6-CB4	-2.63	1.40	1.46
50	h	201	CDL	OA6-CA4	-2.62	1.40	1.46
50	d	201	CDL	OA6-CA4	-2.61	1.40	1.46
52	Р	501	NDP	O4B-C4B	-2.61	1.39	1.45
49	Н	401	3PE	O21-C2	-2.59	1.40	1.46
48	F	501	FMN	C10-N1	2.59	1.38	1.33
50	L	702	CDL	OA8-CA7	2.58	1.40	1.33
49	М	501	3PE	O21-C2	-2.57	1.40	1.46
49	Ι	202	3PE	O21-C2	-2.56	1.40	1.46
46	Ι	201	PC1	O21-C2	-2.55	1.40	1.46
50	L	702	CDL	OB6-CB4	-2.55	1.40	1.46



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	d	201	CDL	OA8-CA7	2.55	1.40	1.33
50	q	201	CDL	OB8-CB7	2.53	1.40	1.33
50	h	201	CDL	OA8-CA7	2.53	1.40	1.33
49	М	502	3PE	O21-C2	-2.52	1.40	1.46
46	В	202	PC1	O21-C2	-2.50	1.40	1.46
49	N	401	3PE	O21-C2	-2.50	1.40	1.46
50	L	702	CDL	OB8-CB7	2.49	1.40	1.33
50	h	201	CDL	OB8-CB7	2.48	1.40	1.33
49	L	701	3PE	O31-C31	2.47	1.40	1.33
50	d	201	CDL	OB8-CB7	2.46	1.40	1.33
49	М	501	3PE	O31-C31	2.46	1.40	1.33
49	f	101	3PE	O31-C31	2.46	1.40	1.33
49	i	201	3PE	O21-C2	-2.44	1.40	1.46
50	q	201	CDL	OA8-CA7	2.43	1.40	1.33
49	Н	401	3PE	O31-C31	2.43	1.40	1.33
49	Ι	202	3PE	O31-C31	2.42	1.40	1.33
46	Ι	201	PC1	O31-C31	2.42	1.40	1.33
46	В	202	PC1	O31-C31	2.38	1.40	1.33
54	U	201	EHZ	C9-S1	2.37	1.81	1.76
49	f	101	3PE	O21-C2	-2.36	1.40	1.46
49	i	201	3PE	O31-C31	2.36	1.40	1.33
50	d	201	CDL	OB6-CB4	-2.36	1.40	1.46
49	М	502	3PE	O31-C31	2.34	1.40	1.33
51	0	401	ATP	C5-C4	2.33	1.47	1.40
50	q	201	CDL	OA6-CA4	-2.33	1.40	1.46
54	Т	201	EHZ	C9-S1	2.32	1.81	1.76
50	q	201	CDL	OA6-CA5	2.32	1.40	1.34
49	Ν	401	3PE	O31-C31	2.31	1.40	1.33
49	f	101	3PE	O21-C21	2.31	1.40	1.34
50	h	201	CDL	OB6-CB4	-2.28	1.40	1.46
50	h	201	CDL	OB6-CB5	2.28	1.40	1.34
49	Ν	401	3PE	O31-C3	-2.27	1.40	1.45
54	U	201	EHZ	O4-C15	-2.27	1.18	1.23
54	Т	201	EHZ	O4-C15	-2.23	1.19	1.23
49	L	701	3PE	021-C2	-2.23	1.41	1.46
49	i	201	3PE	O21-C21	2.21	1.40	1.34
54	Т	201	EHZ	O3-C12	-2.20	1.18	1.23
49	М	502	3PE	O31-C3	-2.19	1.40	1.45
49	i	201	3PE	O31-C3	-2.19	1.40	1.45
50	L	702	CDL	OB6-CB5	2.18	1.40	1.34
46	В	202	PC1	O21-C21	2.17	1.40	1.34
50	d	201		OA6-CA5	2.17	1.40	1.34



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	L	701	3PE	O21-C21	2.16	1.40	1.34
52	Р	501	NDP	C2A-N1A	2.15	1.37	1.33
46	В	202	PC1	O31-C3	-2.15	1.40	1.45
50	q	201	CDL	OA8-CA6	-2.14	1.40	1.45
50	d	201	CDL	OB8-CB6	-2.13	1.40	1.45
54	U	201	EHZ	O3-C12	-2.13	1.18	1.23
50	d	201	CDL	OB6-CB5	2.13	1.40	1.34
50	q	201	CDL	OB6-CB5	2.12	1.40	1.34
46	Ι	201	PC1	O31-C3	-2.12	1.40	1.45
49	L	701	3PE	O31-C3	-2.11	1.40	1.45
49	Ν	401	3PE	O21-C21	2.10	1.40	1.34
49	Ι	202	3PE	O31-C3	-2.10	1.40	1.45
49	М	502	3PE	O21-C21	2.10	1.40	1.34
49	Н	401	3PE	O31-C3	-2.09	1.40	1.45
52	Р	501	NDP	O5D-C5D	-2.09	1.36	1.44
46	Ι	201	PC1	O21-C21	2.09	1.40	1.34
49	М	501	3PE	O21-C21	2.09	1.40	1.34
49	f	101	3PE	O31-C3	-2.09	1.40	1.45
50	h	201	CDL	OA6-CA5	2.08	1.40	1.34
49	Ι	202	3PE	O21-C21	2.08	1.40	1.34
50	L	702	CDL	OA8-CA6	-2.06	1.40	1.45
50	L	702	CDL	OA6-CA5	2.05	1.40	1.34
49	Н	401	3PE	O21-C21	2.05	1.40	1.34
49	М	501	3PE	O31-C3	-2.04	1.40	1.45
50	h	201	CDL	OB8-CB6	-2.03	1.40	1.45
50	L	702	CDL	OB8-CB6	-2.03	1.40	1.45

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
52	Р	501	NDP	PN-O3-PA	-7.22	108.06	132.83
54	Т	201	EHZ	C8-C9-S1	5.36	120.27	113.63
54	U	201	EHZ	C8-C9-S1	5.18	120.03	113.63
50	d	201	CDL	OB6-CB5-C51	4.18	120.50	111.50
50	L	702	CDL	OB6-CB5-C51	4.12	120.38	111.50
49	i	201	3PE	O21-C21-C22	4.09	120.31	111.50
49	М	502	3PE	O21-C21-C22	4.08	120.30	111.50
50	h	201	CDL	OA6-CA5-C11	4.08	120.30	111.50
46	В	202	PC1	O21-C21-C22	4.00	120.13	111.50
50	q	201	CDL	OB6-CB5-C51	4.00	120.12	111.50
49	Н	401	3PE	O21-C21-C22	3.92	119.94	111.50
50	L	702	CDL	OA6-CA5-C11	3.89	119.89	111.50



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
50	d	201	CDL	OA6-CA5-C11	3.84	119.78	111.50
49	L	701	3PE	O21-C21-C22	3.83	119.76	111.50
49	N	401	3PE	O21-C21-C22	3.77	119.64	111.50
49	Ι	202	3PE	O21-C21-C22	3.71	119.51	111.50
46	Ι	201	PC1	O21-C21-C22	3.71	119.49	111.50
51	0	401	ATP	PB-O3B-PG	-3.71	120.11	132.83
49	f	101	3PE	O21-C21-C22	3.69	119.46	111.50
49	М	501	3PE	O21-C21-C22	3.68	119.42	111.50
51	0	401	ATP	N3-C2-N1	-3.67	122.95	128.68
50	q	201	CDL	OA6-CA5-C11	3.66	119.39	111.50
50	h	201	CDL	OB6-CB5-C51	3.57	119.19	111.50
48	F	501	FMN	C4-N3-C2	-3.50	119.17	125.64
51	0	401	ATP	PA-O3A-PB	-3.41	121.12	132.83
52	Р	501	NDP	O2B-P2B-O1X	-3.21	96.99	109.39
52	Р	501	NDP	PA-O5B-C5B	-3.08	103.64	121.68
48	F	501	FMN	C4A-C10-N1	-2.98	117.81	124.73
48	F	501	FMN	C4A-C4-N3	2.88	120.51	113.19
50	h	201	CDL	OA8-CA7-C31	2.84	120.83	111.91
50	d	201	CDL	OB8-CB7-C71	2.84	120.81	111.91
51	0	401	ATP	C4-C5-N7	-2.81	106.47	109.40
52	Р	501	NDP	PN-O5D-C5D	-2.77	105.42	121.68
48	F	501	FMN	C4A-C10-N10	2.77	120.53	116.48
49	М	502	3PE	O31-C31-C32	2.67	120.27	111.91
46	Ι	201	PC1	O31-C31-C32	2.64	120.19	111.91
49	L	701	3PE	O31-C31-C32	2.62	120.14	111.91
49	i	201	3PE	O31-C31-C32	2.62	120.12	111.91
49	Н	401	3PE	O31-C31-C32	2.61	120.10	111.91
48	F	501	FMN	O4-C4-C4A	-2.60	119.70	126.60
52	Р	501	NDP	O3X-P2B-O2X	2.55	117.39	107.64
49	Ν	401	3PE	O31-C31-C32	2.53	119.84	111.91
50	q	201	CDL	OB8-CB7-C71	2.51	119.79	111.91
50	q	201	CDL	OA8-CA7-C31	2.48	119.69	111.91
49	Ι	202	3PE	O31-C31-C32	2.46	119.64	111.91
50	d	201	CDL	OA8-CA7-C31	2.46	119.63	111.91
50	h	201	CDL	OB8-CB7-C71	2.43	119.54	111.91
50	L	702	CDL	OA8-CA7-C31	2.43	119.53	111.91
49	f	101	3PE	O31-C31-C32	2.41	119.48	111.91
46	В	202	PC1	O31-C31-C32	2.40	119.43	111.91
49	М	501	3PE	O31-C31-C32	2.39	119.42	111.91
50	L	702	CDL	OB8-CB7-C71	2.39	119.41	111.91
51	0	401	ATP	C3'-C2'-C1'	2.39	104.57	100.98
48	F	501	FMN	C10-N1-C2	2.35	121.60	116.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
54	Т	201	EHZ	C13-C12-N1	2.34	120.37	116.42
48	F	501	FMN	C4-C4A-C10	2.34	120.72	116.79
52	Р	501	NDP	C2A-N1A-C6A	-2.32	114.78	118.75
54	Т	201	EHZ	C7-C8-C9	-2.30	108.64	113.89
54	U	201	EHZ	C14-C13-C12	-2.29	108.55	112.36
52	Р	501	NDP	O2N-PN-O1N	2.28	123.51	112.24
54	U	201	EHZ	C10-S1-C9	2.27	108.95	101.87
54	Т	201	EHZ	O2-C9-S1	-2.22	119.73	122.61
48	F	501	FMN	C10-C4A-N5	-2.12	120.35	124.86
52	Р	501	NDP	O5D-PN-O1N	-2.12	100.79	109.07
54	U	201	EHZ	C13-C12-N1	2.11	119.98	116.42
51	0	401	ATP	C2-N1-C6	2.06	122.28	118.75
54	Т	201	EHZ	C5-C6-C7	-2.06	108.94	114.85
52	P	501	NDP	C5B-C4B-C3B	-2.02	107.59	115.18

There are no chirality outliers.

All	(425)) torsion	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms
46	В	202	PC1	O22-C21-O21-C2
46	В	202	PC1	C22-C21-O21-C2
46	Ι	201	PC1	C11-O13-P-O14
46	Ι	201	PC1	C1-O11-P-O12
48	F	501	FMN	C2'-C1'-N10-C10
48	F	501	FMN	N10-C1'-C2'-O2'
48	F	501	FMN	N10-C1'-C2'-C3'
48	F	501	FMN	C3'-C4'-C5'-O5'
48	F	501	FMN	O4'-C4'-C5'-O5'
48	F	501	FMN	C5'-O5'-P-O2P
48	F	501	FMN	C5'-O5'-P-O3P
49	Н	401	3PE	C11-O13-P-O14
49	Н	401	3PE	O13-C11-C12-N
49	Н	401	3PE	O22-C21-O21-C2
49	Ι	202	3PE	O13-C11-C12-N
49	L	701	3PE	C11-O13-P-O12
49	L	701	3PE	C11-O13-P-O14
49	L	701	3PE	C22-C21-O21-C2
49	М	501	3PE	C1-O11-P-O12
49	М	501	3PE	C1-O11-P-O13
49	М	501	3PE	C1-O11-P-O14
49	N	401	3PE	C11-O13-P-O11
49	Ν	401	3PE	C11-O13-P-O12



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Mol	Chain	Res	Type	Atoms
49	N	401	3PE	C11-O13-P-O14
49	N	401	3PE	O13-C11-C12-N
49	N	401	3PE	O21-C2-C3-O31
49	i	201	3PE	O13-C11-C12-N
49	i	201	3PE	C22-C21-O21-C2
50	L	702	CDL	CA2-OA2-PA1-OA3
50	L	702	CDL	CA3-OA5-PA1-OA4
50	L	702	CDL	OB7-CB5-OB6-CB4
50	d	201	CDL	CB2-C1-CA2-OA2
50	d	201	CDL	C1-CA2-OA2-PA1
50	d	201	CDL	CA2-OA2-PA1-OA3
50	d	201	CDL	CA2-OA2-PA1-OA4
50	d	201	CDL	CB2-OB2-PB2-OB3
50	d	201	CDL	CB2-OB2-PB2-OB4
50	d	201	CDL	C51-CB5-OB6-CB4
50	h	201	CDL	CA3-OA5-PA1-OA3
50	h	201	CDL	CA3-OA5-PA1-OA4
50	h	201	CDL	CB2-OB2-PB2-OB4
50	h	201	CDL	CB3-OB5-PB2-OB3
50	q	201	CDL	CA3-OA5-PA1-OA3
50	q	201	CDL	CB3-OB5-PB2-OB3
50	q	201	CDL	C51-CB5-OB6-CB4
51	0	401	ATP	C5'-O5'-PA-O1A
51	0	401	ATP	C5'-O5'-PA-O2A
52	Р	501	NDP	C5B-O5B-PA-O1A
52	Р	501	NDP	C5B-O5B-PA-O3
52	Р	501	NDP	C2N-C3N-C7N-N7N
54	Т	201	EHZ	C6-C7-C8-C9
54	Т	201	EHZ	S1-C10-C11-N1
54	Т	201	EHZ	C12-C13-C14-N2
54	Т	201	EHZ	N2-C15-C16-O5
54	Т	201	EHZ	O4-C15-C16-O5
54	Т	201	EHZ	C16-C17-C20-O6
54	U	201	EHZ	O1-C7-C8-C9
54	U	201	EHZ	C6-C7-C8-C9
46	Ι	201	PC1	O32-C31-O31-C3
50	d	201	CDL	OB9-CB7-OB8-CB6
50	d	201	CDL	C71-CB7-OB8-CB6
50	h	201	CDL	OA9-CA7-OA8-CA6
49	L	701	3PE	O22-C21-O21-C2
49	i	201	3PE	O22-C21-O21-C2
50	d	201	CDL	OB7-CB5-OB6-CB4



Mol	Chain	Res	Type	Atoms
50	q	201	CDL	OB7-CB5-OB6-CB4
46	B	202	PC1	C32-C31-O31-C3
46	Ι	201	PC1	C32-C31-O31-C3
50	h	201	CDL	C31-CA7-OA8-CA6
49	Н	401	3PE	C22-C21-O21-C2
50	L	702	CDL	C51-CB5-OB6-CB4
49	М	502	3PE	C32-C31-O31-C3
46	В	202	PC1	O32-C31-O31-C3
50	d	201	CDL	O1-C1-CA2-OA2
49	N	401	3PE	C32-C31-O31-C3
49	N	401	3PE	O32-C31-O31-C3
52	Р	501	NDP	O4B-C4B-C5B-O5B
52	Р	501	NDP	O4D-C4D-C5D-O5D
54	Т	201	EHZ	C21-C22-C23-C24
49	М	502	3PE	O32-C31-O31-C3
50	q	201	CDL	CA2-C1-CB2-OB2
49	Н	401	3PE	C32-C31-O31-C3
52	Р	501	NDP	O4D-C1D-N1N-C6N
50	q	201	CDL	O1-C1-CB2-OB2
49	М	501	3PE	O21-C2-C3-O31
46	Ι	201	PC1	C22-C21-O21-C2
49	М	502	3PE	C22-C21-O21-C2
46	В	202	PC1	C21-C22-C23-C24
50	q	201	CDL	CA5-C11-C12-C13
50	L	702	CDL	CB5-C51-C52-C53
49	М	501	3PE	C32-C31-O31-C3
50	d	201	CDL	CB7-C71-C72-C73
46	Ι	201	PC1	O22-C21-O21-C2
49	Н	401	3PE	O32-C31-O31-C3
49	f	101	3PE	C31-C32-C33-C34
49	М	501	3PE	O32-C31-O31-C3
50	L	702	CDL	C11-CA5-OA6-CA4
46	Ι	201	PC1	C1-O11-P-O13
49	Н	401	3PE	C11-O13-P-O11
49	Ι	202	3PE	C11-O13-P-O11
49	L	701	3PE	C11-O13-P-O11
49	М	501	3PE	C11-O13-P-O11
50	L	702	CDL	CA3-OA5-PA1-OA2
50	d	201	CDL	CA2-OA2-PA1-OA5
50	d	201	CDL	CB2-OB2-PB2-OB5
50	h	201	CDL	CA3-OA5-PA1-OA2
50	q	201	CDL	C31-CA7-OA8-CA6



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Mol	Chain	Res	Type	Atoms	
49	М	502	3PE	O22-C21-O21-C2	
50	L	702	CDL	OA7-CA5-OA6-CA4	
49	М	502	3PE	C35-C36-C37-C38	
49	М	502	3PE	C21-C22-C23-C24	
50	q	201	CDL	C40-C41-C42-C43	
50	h	201	CDL	C11-CA5-OA6-CA4	
46	В	202	PC1	C36-C37-C38-C39	
49	f	101	3PE	C3A-C3B-C3C-C3D	
50	L	702	CDL	C12-C13-C14-C15	
50	d	201	CDL	C33-C34-C35-C36	
50	d	201	CDL	C40-C41-C42-C43	
50	h	201	CDL	C74-C75-C76-C77	
50	q	201	CDL	C38-C39-C40-C41	
54	Т	201	EHZ	C18-C17-C20-O6	
54	Т	201	EHZ	C19-C17-C20-O6	
49	L	701	3PE	C36-C37-C38-C39	
49	f	101	3PE	C32-C33-C34-C35	
49	L	701	3PE	C3-C2-O21-C21	
50	h	201	CDL	OA7-CA5-OA6-CA4	
49	Ι	202	3PE	C38-C39-C3A-C3B	
50	d	201	CDL	C57-C58-C59-C60	
50	h	201	CDL	C32-C33-C34-C35	
50	q	201	CDL	C12-C13-C14-C15	
46	Ι	201	PC1	C25-C26-C27-C28	
50	d	201	CDL	C16-C17-C18-C19	
49	М	502	3PE	C3E-C3F-C3G-C3H	
46	В	202	PC1	C3A-C3B-C3C-C3D	
49	Ι	202	3PE	C3D-C3E-C3F-C3G	
50	d	201	CDL	C71-C72-C73-C74	
50	d	201	CDL	C79-C80-C81-C82	
49	Н	401	3PE	C37-C38-C39-C3A	
50	L	702	CDL	CB7-C71-C72-C73	
46	В	202	PC1	C39-C3A-C3B-C3C	
49	М	501	3PE	C2B-C2C-C2D-C2E	
49	N	401	3PE	C39-C3A-C3B-C3C	
50	h	201	CDL	C18-C19-C20-C21	
46	В	202	PC1	C26-C27-C28-C29	
46	В	202	PC1	C28-C29-C2A-C2B	
49	N	401	3PE	C22-C23-C24-C25	
49	f	101	3PE	C22-C23-C24-C25	
50	d	201	CDL	C15-C16-C17-C18	
50	a	201	CDL	C34-C35-C36-C37	



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Mol	Chain	Res	Type	Atoms	
49	Ι	202	3PE	C34-C35-C36-C37	
50	d	201	CDL	C73-C74-C75-C76	
49	f	101	3PE	O13-C11-C12-N	
50	L	702	CDL	CA7-C31-C32-C33	
46	В	202	PC1	C38-C39-C3A-C3B	
49	М	501	3PE	C38-C39-C3A-C3B	
49	М	501	3PE	C3A-C3B-C3C-C3D	
50	h	201	CDL	C56-C57-C58-C59	
49	N	401	3PE	C31-C32-C33-C34	
50	q	201	CDL	OA9-CA7-OA8-CA6	
54	Т	201	EHZ	C13-C14-N2-C15	
50	q	201	CDL	C43-C44-C45-C46	
50	L	702	CDL	CB3-CB4-CB6-OB8	
50	d	201	CDL	C14-C15-C16-C17	
49	М	502	3PE	C28-C29-C2A-C2B	
50	q	201	CDL	C53-C54-C55-C56	
50	h	201	CDL	C51-CB5-OB6-CB4	
49	Н	401	3PE	C2E-C2F-C2G-C2H	
49	f	101	3PE	C38-C39-C3A-C3B	
46	Ι	201	PC1	C37-C38-C39-C3A	
49	Н	401	3PE	C3E-C3F-C3G-C3H	
50	d	201	CDL	C62-C63-C64-C65	
54	U	201	EHZ	C21-C22-C23-C24	
50	L	702	CDL	O1-C1-CB2-OB2	
52	Р	501	NDP	C3B-C4B-C5B-O5B	
50	L	702	CDL	CB2-C1-CA2-OA2	
50	h	201	CDL	OB7-CB5-OB6-CB4	
49	М	501	3PE	C33-C34-C35-C36	
49	М	501	3PE	C39-C3A-C3B-C3C	
50	h	201	CDL	CA4-CA3-OA5-PA1	
46	B	$20\overline{2}$	PC1	C25-C26-C27-C28	
50	d	201	CDL	C59-C60-C61-C62	
49	М	502	3PE	C3C-C3D-C3E-C3F	
46	В	202	PC1	C2C-C2D-C2E-C2F	
49	Ν	401	3PE	C36-C37-C38-C39	
49	L	701	3PE	C28-C29-C2A-C2B	
49	I	202	3PE	C22-C21-O21-C2	
50	q	201	CDL	C11-CA5-OA6-CA4	
50	q	201	CDL	OB5-CB3-CB4-OB6	
50	d	201	CDL	C23-C24-C25-C26	
49	L	701	3PE	C37-C38-C39-C3A	
50	a	201	CDL	O1-C1-CA2-OA2	



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Mol	Chain	\mathbf{Res}	Type	Atoms	
49	Ι	202	3 PE	O22-C21-O21-C2	
50	L	702	CDL	C52-C53-C54-C55	
50	d	201	CDL	C34-C35-C36-C37	
50	d	201	CDL	C58-C59-C60-C61	
51	0	401	ATP	O4'-C4'-C5'-O5'	
49	i	201	3PE	C2A-C2B-C2C-C2D	
50	L	702	CDL	C19-C20-C21-C22	
49	N	401	3PE	C26-C27-C28-C29	
46	В	202	PC1	C29-C2A-C2B-C2C	
50	q	201	CDL	OA7-CA5-OA6-CA4	
50	d	201	CDL	C21-C22-C23-C24	
50	L	702	CDL	CA2-OA2-PA1-OA5	
50	q	201	CDL	CA3-OA5-PA1-OA2	
50	q	201	CDL	C37-C38-C39-C40	
49	i	201	3PE	C24-C25-C26-C27	
49	Ι	202	3PE	C21-C22-C23-C24	
49	Н	401	3PE	C22-C23-C24-C25	
50	L	702	CDL	CA2-C1-CB2-OB2	
49	Н	401	3PE	C28-C29-C2A-C2B	
50	d	201	CDL	C31-C32-C33-C34	
49	Н	401	3PE	C1-C2-C3-O31	
49	L	701	3PE	C22-C23-C24-C25	
49	М	501	3PE	C1-C2-C3-O31	
49	N	401	3PE	C1-C2-C3-O31	
49	i	201	3PE	C1-C2-C3-O31	
46	В	202	PC1	C2F-C2G-C2H-C2I	
49	Н	401	3PE	C3A-C3B-C3C-C3D	
50	L	702	CDL	C84-C85-C86-C87	
50	q	201	CDL	C72-C73-C74-C75	
49	М	502	3PE	C38-C39-C3A-C3B	
49	М	501	3PE	C22-C21-O21-C2	
52	Р	501	NDP	C3D-C4D-C5D-O5D	
54	U	201	EHZ	C5-C6-C7-O1	
50	d	201	CDL	C37-C38-C39-C40	
49	L	701	3PE	C2F-C2G-C2H-C2I	
49	f	101	3PE	C3E-C3F-C3G-C3H	
50	q	201	CDL	C14-C15-C16-C17	
50	d	201	CDL	C18-C19-C20-C21	
50	h	201	CDL	C71-C72-C73-C74	
49	N	401	3PE	C3B-C3C-C3D-C3E	
50	d	201	CDL	C77-C78-C79-C80	
48	F	501	FMN	C5'-O5'-P-O1P	

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Mol	Chain	Res	Type	Atoms
49	i	201	3PE	C26-C27-C28-C29
50	d	201	CDL	C17-C18-C19-C20
50	q	201	CDL	OA5-CA3-CA4-OA6
50	h	201	CDL	C11-C12-C13-C14
50	d	201	CDL	C51-C52-C53-C54
50	d	201	CDL	C84-C85-C86-C87
54	U	201	EHZ	C2-C3-C4-C5
49	М	502	3PE	C26-C27-C28-C29
50	h	201	CDL	C36-C37-C38-C39
49	N	401	3PE	C22-C21-O21-C2
49	М	501	3PE	C36-C37-C38-C39
50	q	201	CDL	OB5-CB3-CB4-CB6
49	Ι	202	3PE	C3F-C3G-C3H-C3I
49	i	201	3PE	C22-C23-C24-C25
50	d	201	CDL	CB5-C51-C52-C53
49	N	401	3PE	C33-C34-C35-C36
49	N	401	3PE	C3F-C3G-C3H-C3I
50	h	201	CDL	C51-C52-C53-C54
49	f	101	3PE	C1-C2-C3-O31
50	d	201	CDL	CA3-CA4-CA6-OA8
49	Н	401	3PE	C35-C36-C37-C38
46	Ι	201	PC1	C11-O13-P-O11
50	h	201	CDL	CB2-OB2-PB2-OB5
50	q	201	CDL	CB3-OB5-PB2-OB2
46	Ι	201	PC1	C32-C33-C34-C35
46	В	202	PC1	O11-C1-C2-O21
50	h	201	CDL	OB5-CB3-CB4-OB6
50	L	702	CDL	C34-C35-C36-C37
49	Ι	202	3 PE	C2F-C2G-C2H-C2I
49	Н	401	3 PE	O21-C2-C3-O31
50	d	201	CDL	OA6-CA4-CA6-OA8
50	d	201	CDL	OB6-CB4-CB6-OB8
49	М	502	3 PE	C39-C3A-C3B-C3C
50	d	201	CDL	C11-CA5-OA6-CA4
49	М	502	3PE	C3D-C3E-C3F-C3G
49	М	501	3PE	O22-C21-O21-C2
49	М	502	3PE	C2B-C2C-C2D-C2E
54	Т	201	EHZ	O2-C9-S1-C10
54	U	201	EHZ	O2-C9-S1-C10
49	N	401	3PE	O22-C21-O21-C2
50	d	201	\overline{CDL}	OA7-CA5-OA6-CA4
49	i	201	3PE	C36-C37-C38-C39



Mol	Chain	Res	Type	Atoms	
46	В	202	PC1	O11-C1-C2-C3	
49	N	401	3PE	O11-C1-C2-C3	
50	L	702	CDL	O1-C1-CA2-OA2	
54	U	201	EHZ	C2-C1-C21-C22	
49	Н	401	3PE	C24-C25-C26-C27	
49	L	701	3PE	C3A-C3B-C3C-C3D	
54	U	201	EHZ	C19-C17-C20-O6	
49	i	201	3PE	C3-C2-O21-C21	
50	d	201	CDL	CB3-CB4-OB6-CB5	
54	Т	201	EHZ	C8-C9-S1-C10	
54	U	201	EHZ	C8-C9-S1-C10	
50	d	201	CDL	C11-C12-C13-C14	
50	L	702	CDL	CA3-CA4-CA6-OA8	
49	М	501	3PE	C35-C36-C37-C38	
54	Т	201	EHZ	O1-C7-C8-C9	
50	L	702	CDL	OB6-CB4-CB6-OB8	
50	h	201	CDL	C34-C35-C36-C37	
46	Ι	201	PC1	C39-C3A-C3B-C3C	
51	0	401	ATP	PG-O3B-PB-O1B	
50	d	201	CDL	C43-C44-C45-C46	
50	d	201	CDL	CB3-OB5-PB2-OB2	
50	h	201	CDL	CB3-OB5-PB2-OB2	
50	q	201	CDL	CB2-OB2-PB2-OB5	
49	М	501	3PE	C27-C28-C29-C2A	
49	М	502	3PE	C2F-C2G-C2H-C2I	
50	h	201	CDL	C14-C15-C16-C17	
46	Ι	201	PC1	C1-O11-P-O14	
49	Н	401	3PE	C1-O11-P-O12	
49	Ι	202	3PE	C11-O13-P-O12	
49	М	501	3PE	C11-O13-P-O12	
49	М	501	3PE	C11-O13-P-O14	
49	N	401	3PE	C1-O11-P-O14	
50	L	702	CDL	CA2-OA2-PA1-OA4	
50	d	201	CDL	CB3-OB5-PB2-OB3	
50	h	201	CDL	CB2-OB2-PB2-OB3	
52	Р	501	NDP	C5B-O5B-PA-O2A	
50	d	201	CDL	C74-C75-C76-C77	
50	L	702	CDL	C54-C55-C56-C57	
49	i	201	3PE	C32-C33-C34-C35	
49	М	501	3PE	C12-C11-O13-P	
49	М	502	3PE	C12-C11-O13-P	
49	N	401	3PE	C12-C11-O13-P	



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Mol	Chain	\mathbf{Res}	Type	Atoms
49	i	201	3PE	C12-C11-O13-P
46	В	202	PC1	C31-C32-C33-C34
50	q	201	CDL	C71-C72-C73-C74
50	L	702	CDL	C71-CB7-OB8-CB6
49	f	101	3PE	O11-C1-C2-O21
46	В	202	PC1	C2B-C2C-C2D-C2E
46	Ι	201	PC1	O13-C11-C12-N
49	i	201	3PE	O21-C2-C3-O31
49	L	701	3PE	C2B-C2C-C2D-C2E
50	L	702	CDL	C23-C24-C25-C26
49	Н	401	3PE	C25-C26-C27-C28
50	L	702	CDL	OB9-CB7-OB8-CB6
54	U	201	EHZ	C18-C17-C20-O6
49	f	101	3PE	O11-C1-C2-C3
50	q	201	CDL	OA5-CA3-CA4-CA6
50	d	201	CDL	C80-C81-C82-C83
49	М	501	3PE	C31-C32-C33-C34
49	Ι	202	3PE	C32-C33-C34-C35
50	L	702	CDL	C22-C23-C24-C25
49	Ν	401	3PE	O11-C1-C2-O21
49	i	201	3PE	C2B-C2C-C2D-C2E
50	h	201	CDL	C17-C18-C19-C20
50	q	201	CDL	C51-C52-C53-C54
50	d	201	CDL	CB3-CB4-CB6-OB8
50	h	201	CDL	CA3-CA4-CA6-OA8
50	q	201	CDL	C31-C32-C33-C34
49	L	701	3PE	C33-C34-C35-C36
50	q	201	CDL	C42-C43-C44-C45
49	N	401	3PE	C35-C36-C37-C38
51	0	401	ATP	PG-O3B-PB-O2B
52	Р	501	NDP	PN-O3-PA-O2A
46	Ι	201	PC1	C34-C35-C36-C37
49	М	501	3PE	C3D-C3E-C3F-C3G
54	Т	201	EHZ	C1-C2-C3-C4
46	Ι	201	PC1	C27-C28-C29-C2A
49	М	502	3PE	C2D-C2E-C2F-C2G
49	f	101	3PE	C37-C38-C39-C3A
49	i	201	3PE	C27-C28-C29-C2A
50	d	201	CDL	CA5-C11-C12-C13
49	L	701	3PE	C34-C35-C36-C37
46	Ι	201	PC1	O21-C2-C3-O31
50	h	201	CDL	C19-C20-C21-C22



Mol	Chain	Res	Type	Atoms
50	L	702	CDL	C32-C33-C34-C35
50	L	702	CDL	C77-C78-C79-C80
49	L	701	3PE	C2A-C2B-C2C-C2D
54	U	201	EHZ	C7-C8-C9-O2
50	h	201	CDL	CA3-CA4-OA6-CA5
50	h	201	CDL	CA6-CA4-OA6-CA5
50	h	201	CDL	CB6-CB4-OB6-CB5
50	q	201	CDL	CA3-CA4-OA6-CA5
50	d	201	CDL	C52-C53-C54-C55
49	Ι	202	3PE	C24-C25-C26-C27
49	Ι	202	3PE	C2E-C2F-C2G-C2H
50	L	702	CDL	C13-C14-C15-C16
51	0	401	ATP	C3'-C4'-C5'-O5'
49	Ι	202	3PE	C29-C2A-C2B-C2C
54	Т	201	EHZ	C11-C10-S1-C9
50	q	201	CDL	C35-C36-C37-C38
49	f	101	3PE	O21-C2-C3-O31
50	L	702	CDL	OA6-CA4-CA6-OA8
50	L	702	CDL	C78-C79-C80-C81
50	L	702	CDL	C82-C83-C84-C85
46	Ι	201	PC1	C1-C2-C3-O31
50	q	201	CDL	CA3-CA4-CA6-OA8
49	М	502	3PE	C2E-C2F-C2G-C2H
50	h	201	CDL	OB5-CB3-CB4-CB6
46	В	202	PC1	C24-C25-C26-C27
49	Н	401	3PE	C32-C33-C34-C35
50	d	201	CDL	OA9-CA7-OA8-CA6
46	Ι	201	PC1	C24-C25-C26-C27
54	Т	201	EHZ	C3-C4-C5-C6
50	h	201	CDL	C13-C14-C15-C16
50	d	201	CDL	C61-C62-C63-C64
50	L	702	CDL	C52-C51-CB5-OB6
50	h	201	CDL	CB3-CB4-OB6-CB5
50	q	201	CDL	CA6-CA4-OA6-CA5
50	h	201	CDL	C72-C73-C74-C75
49	М	501	3PE	C26-C27-C28-C29
50	h	201	CDL	C52-C51-CB5-OB6
49	Н	401	3PE	C34-C35-C36-C37
49	N	401	3PE	C25-C26-C27-C28
46	Ι	201	PC1	O11-C1-C2-O21
50	h	201	CDL	C22-C23-C24-C25
50	q	201	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
51	0	401	ATP	C5'-O5'-PA-O3A
50	d	201	CDL	C31-CA7-OA8-CA6
50	L	702	CDL	C12-C11-CA5-OA6
49	L	701	3PE	C3F-C3G-C3H-C3I
50	L	702	CDL	C52-C51-CB5-OB7
49	М	501	3PE	C3C-C3D-C3E-C3F
46	Ι	201	PC1	C36-C37-C38-C39
49	i	201	3PE	C11-O13-P-O14
50	L	702	CDL	CB2-OB2-PB2-OB3
50	d	201	CDL	CB3-OB5-PB2-OB4
50	L	702	CDL	C74-C75-C76-C77
50	h	201	CDL	C52-C51-CB5-OB7
50	L	702	CDL	C80-C81-C82-C83
49	f	101	3PE	C35-C36-C37-C38
49	L	701	3PE	C2C-C2D-C2E-C2F
50	d	201	CDL	C42-C43-C44-C45
46	Ι	201	PC1	C12-C11-O13-P
50	d	201	CDL	C41-C42-C43-C44
50	h	201	CDL	C1-CB2-OB2-PB2
50	h	201	CDL	CA7-C31-C32-C33
49	i	201	3PE	C33-C34-C35-C36
50	d	201	CDL	C72-C71-CB7-OB8
46	В	202	PC1	O31-C31-C32-C33
50	d	201	CDL	C32-C31-CA7-OA8

Continued from previous page...

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.





































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-11810. 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: 180



Y Index: 180



Z Index: 180

6.2.2 Raw map



X Index: 180

Y Index: 180



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: 178





Z Index: 219

6.3.2 Raw map



X Index: 179

Y Index: 172



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 0.0355. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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



6.5 Mask visualisation (i)

This section 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

6.5.1 emd_11810_msk_1.map (i)





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 352 nm^3 ; this corresponds to an approximate mass of 318 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 0.315 $\mathrm{\AA^{-1}}$



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 0.315 $\mathrm{\AA^{-1}}$



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	3.17	-	-	
Author-provided FSC curve	3.17	3.64	3.21	
Unmasked-calculated*	4.02	7.42	4.14	

*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 4.02 differs from the reported value 3.17 by more than 10 %


9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11810 and PDB model 7AK5. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.0355 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 (0.0355).



9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 73% 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 (0.0355) and Q-score for the entire model and for each chain.

\mathbf{Chain}	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.7324	0.5420
А	0.7305	0.5410
В	0.8159	0.5700
С	0.8223	0.5850
D	0.8194	0.5800
Е	0.6665	0.5120
F	0.7070	0.5260
G	0.7418	0.5450
Н	0.7701	0.5520
Ι	0.8184	0.5820
J	0.6667	0.5220
K	0.7776	0.5560
L	0.7296	0.5360
М	0.7905	0.5650
Ν	0.8009	0.5660
О	0.7315	0.5430
Р	0.6991	0.5190
Q	0.7636	0.5600
R	0.7697	0.5720
S	0.5859	0.4850
Т	0.3855	0.3940
U	0.6147	0.4920
V	0.6785	0.5190
W	0.6897	0.5260
Х	0.7430	0.5490
Y	0.6863	0.5240
Z	0.7448	0.5480
a	0.8101	0.5600
b	0.7078	0.5220
с	0.6622	0.5130
d	0.7342	0.5520
е	0.7476	0.5520
f	0.6756	0.5200
g	0.7322	0.5410
h	0.7448	0.5580

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Chain	Atom inclusion	Q-score
i	0.6513	0.5040
j	0.6281	0.5000
k	0.5971	0.4830
1	0.7153	0.5420
m	0.7035	0.5280
n	0.6864	0.5330
0	0.5753	0.4700
р	0.7049	0.5290
q	0.7923	0.5700
r	0.7520	0.5560
S	0.6719	0.5200

