

wwPDB EM Validation Summary Report (i)

Feb 1, 2023 – 07:34 pm GMT

PDB ID		7B41
EMDB ID	•	EMD-14251
Title	:	Bovine complex I in the presence of IM1761092, active class i (Composite map)
Authors	:	Bridges, H.R.; Blaza, J.N.; Yin, Z.; Chung, I.; Hirst, J.
Deposited on	:	2022-02-08
Resolution	:	2.30 Å(reported)

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)	:	2.32.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Motric	Whole archive	EM structures
IVIEUTIC	$(\# {\rm Entries})$	$(\# { m Entries})$
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 >=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.

Mol	Chain	Length	Quality of chain	
1	А	115	95%	5%
2	В	216	65% 6% ·	28%
3	С	266	74% •	22%
4	D	463	85%	8% 7%
5	Е	249	77% 9	% 14%
6	F	464	86%	7% 7%
7	G	727	• 88%	6% 5%
8	Н	318	90%	10% •



Mol	Chain	Length	Quality of chain	
9	Ι	212	80%	17%
10	J	175	• 90%	9% ••
11	К	98	• 89%	11%
12	L	606	• 88%	11% •
13	М	459	92%	8%
14	N	347	93%	7%
15	0	343	83%	10% • 7%
16	Р	380	83%	7% 10%
17	Q	175	• 67%	29%
18	R	124	• 73% •	23%
19	S	99	• 77% 8%	15%
20	Т	156	8%	
20	U	156	5 1% • 45%	
21	V	116	• 91%	6% •
22	W	128	▲	• 11%
23	X	172	• 94%	5% ••
24	Y	141	7%	11%
25	Z	144	83%	14%
26	2	70	•	1470
20	h	84	•	
21	0	76	9370	••
20	ر م	120	5% 5%	%
29	ů	120	93% 5%	• 6%
3U 01	e	100	89%	• 8%
31	t	57	88%	• 9%
32	g	154	59% 5% 36	%

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Mol	Chain	Length	Quality of chain	
33	h	189	72%	27%
34	i	127	6% 78% •	20%
35	j	108	58 % • 5	38%
36	k	98	• 80%	• 19%
37	1	186	82%	• 17%
38	m	129	96%	
39	n	179	95%	
40	О	137	84%	• 12%
41	р	176	96%	• •
42	q	145	99%	
43	r	113	81%	• 17%
44	s	109	40% 60%	

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2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 69138 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	Atoms					AltConf	Trace
1	А	115	Total 921	C 622	N 133	0 159	S 7	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 792	N 224	0 211	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	207	Total 1721	C 1111	N 296	0 311	${ m S} { m 3}$	0	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
4	D	430	Total 3459	C 2209	N 596	O 629	$\begin{array}{c} \mathrm{S} \\ \mathrm{25} \end{array}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

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



Mol	Chain	Residues	Atoms					AltConf	Trace
5	Е	213	Total 1655	C 1057	N 277	0 311	S 10	0	0

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

Mol	Chain	Residues		At	AltConf	Trace			
6	F	430	Total 3310	C 2086	N 591	O 613	S 20	0	0

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

Mol	Chain	Residues		At	AltConf	Trace			
7	G	688	Total 5279	C 3307	N 920	O 1013	S 39	0	0

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

Mol	Chain	Residues		At	AltConf	Trace			
8	Н	318	Total 2509	C 1681	N 385	0 420	S 23	0	0

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

Mol	Chain	Residues		A	AltConf	Trace			
9	Ι	176	Total 1414	C 889	N 243	0 270	S 12	0	0

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

Mol	Chain	Residues		\mathbf{A}	AltConf	Trace			
10	J	174	Total 1337	C 902	N 189	0 234	S 12	0	0

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

Mol	Chain	Residues		A	AltConf	Trace			
11	K	98	Total 745	C 486	N 112	0 131	S 16	0	0

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



Mol	Chain	Residues		At	AltConf	Trace			
12	L	606	Total 4791	C 3186	N 736	O 826	S 43	0	0

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

Mol	Chain	Residues		At	AltConf	Trace			
13	М	459	Total 3654	C 2436	N 570	O 609	S 39	0	0

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

Mol	Chain	Residues		At	AltConf	Trace			
14	Ν	347	Total 2733	C 1817	N 416	0 457	S 43	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 2589	C 1662	N 429	0 488	S 10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	255	LYS	ASN	variant	UNP P34942

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

Mol	Chain	Residues		Ate	AltConf	Trace			
16	Р	341	Total 2747	C 1777	N 486	O 479	${ m S}{ m 5}$	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 1016	C 641	N 181	0 191	${ m S} { m 3}$	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	95	Total 730	C 448	N 137	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		
10	C	81	Total	С	Ν	Ο	\mathbf{S}	0	0
19	G	04	677	425	126	124	2	0	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
20	Т	76	Total	С	Ν	Ο	S	0	0
20	T	10	612	393	90	124	5	0	0
20	II	86	Total	С	Ν	Ο	\mathbf{S}	0	0
20	U	80	693	447	102	139	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 911	C 589	N 154	0 165	${ m S} { m 3}$	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 971	C 622	N 180	0 165	${S \atop 4}$	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 1402	C 887	N 253	O 252	S 10	0	0

• Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.



Mol	Chain	Residues		At	oms	AltConf	Trace		
24	Y	140	Total 1030	$\begin{array}{c} \mathrm{C} \\ 657 \end{array}$	N 176	0 191	S 6	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
25	7	140	Total	С	Ν	0	\mathbf{S}	0	0
20		140	1146	737	200	200	9	0	0

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

Mol	Chain	Residues		Ate	oms			AltConf	Trace
26	a	70	Total 569	C 365	N 104	O 95	${ m S}{ m 5}$	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
27	b	82	Total 646	C 422	N 108	0 114	${ m S} { m 2}$	0	0

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

Mol	Chain	Residues		Aton	ns		AltConf	Trace
28	с	48	Total	С	N	0	0	0
			405	268	69	68		

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

Mol	Chain	Residues		At	oms			AltConf	Trace
29	d	113	Total 945	C 619	N 161	0 162	${ m S} { m 3}$	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
30	е	97	Total 819	C 518	N 156	0 139	S 6	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	52	Total 451	C 296	N 79	O 75	S 1	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	98	Total 824	C 529	N 137	0 154	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	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	138	Total 1154	C 759	N 196	0 197	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	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	102	Total 879	$\begin{array}{c} \mathrm{C} \\ 579 \end{array}$	N 150	O 149	S 1	0	0

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

Mol	Chain	Residues		At	\mathbf{oms}	AltConf	Trace		
35	j	67	Total 580	C 381	N 95	O 103	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	79	Total 638	C 418	N 107	0 111	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

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



Mol	Chain	Residues		At	oms			AltConf	Trace
37	1	155	Total 1304	C 844	N 213	O 239	S 8	0	0

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

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
20	m	197	Total	С	N	Ō	0	0
- 30	111	121	1061	681	187	193	0	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
39	n	172	Total 1492	C 955	N 273	O 257	S 7	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	120	Total 1035	C 645	N 199	0 183	S 8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	р	171	Total 1443	C 904	N 266	O 265	S 8	0	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
42	q	145	Total 1209	C 778	N 216	0 210	${f S}{5}$	0	0

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



Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	94	Total 767	C 485	N 143	O 136	${ m S} { m 3}$	0	0

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

Mol	Chain	Residues		Atc	\mathbf{ms}			AltConf	Trace
44	g	44	Total	С	Ν	Ο	S	0	0
44	a		371	233	66	71	1	0	0

• Molecule 45 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $\rm C_{24}H_{46}O_{11}).$



Mol	Chain	Residues	Atoms	AltConf
45	А	1	Total C O 35 24 11	0
45	А	1	$\begin{array}{rrrr} \text{Total} & \text{C} & \text{O} \\ 35 & 24 & 11 \end{array}$	0
45	J	1	$\begin{array}{rrrr} \text{Total} & \text{C} & \text{O} \\ 35 & 24 & 11 \end{array}$	0
45	L	1	Total C O 35 24 11	0
45	L	1	Total C O 35 24 11	0
45	L	1	Total C O 35 24 11	0
45	М	1	Total C O 35 24 11	0



Mol	Chain	Residues	Atoms	AltConf
45	М	1	Total C O 35 24 11	0
45	М	1	Total C O 35 24 11	0
45	Ν	1	Total C O 35 24 11	0
45	Y	1	Total C O 35 24 11	0
45	Y	1	Total C O 35 24 11	0
45	Y	1	Total C O 35 24 11	0
45	h	1	Total C O 35 24 11	0
45	j	1	Total C O 35 24 11	0
45	1	1	Total C O 35 24 11	0

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



Mol	Chain	Residues		Ato	oms			AltConf
46	Δ	1	Total	С	Ν	Ο	Р	0
40 A	1	21	11	1	8	1	0	
46	В	1	Total	С	Ν	Ο	Р	0
40	D	1	54	44	1	8	1	U



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Mol	Chain	Residues		Ato	oms			AltConf
46	Р	1	Total	С	Ν	0	Р	0
40 D	D	L	35	25	1	8	1	0
46	т	1	Total	С	Ν	0	Р	0
40	L		49	39	1	8	1	U



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

• Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).





Mol	Chain	Residues	Atoms	AltConf
18	F	1	Total Fe S	0
40	Ľ	T	4 2 2	0
18	С	1	Total Fe S	0
40	G		4 2 2	0

• Molecule 49 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
40	F	1	Total	С	Ν	0	Р	0
49	Г	T	31	17	4	9	1	0

 $\bullet\,$ Molecule 50 is POTASSIUM ION (three-letter code: K) (formula: K).



Mol	Chain	Residues	Atoms		AltConf
50	G	1	Total 1	K 1	0

• Molecule 51 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues		Ato	oms			AltConf
51	Ц	1	Total	С	Ν	0	Р	0
51	11	1	44	34	1	8	1	0
51	н	1	Total	С	Ν	Ο	Р	0
51	11	1	34	24	1	8	1	0
51	Т	1	Total	\mathbf{C}	Ν	Ο	Р	0
01	I	I	51	41	1	8	1	0
51	T.	1	Total	\mathbf{C}	Ν	Ο	Р	0
- 51	Ľ	I	49	39	1	8	1	0
51	T.	1	Total	С	Ν	Ο	Р	0
	Ц	Ĩ	45	35	1	8	1	0
51	М	1	Total	С	Ν	Ο	Р	0
01	101	1	46	36	1	8	1	0
51	М	1	Total	С	Ν	Ο	Р	0
01	101	Ŧ	51	41	1	8	1	0
51	Ν	1	Total	С	Ν	Ο	Р	0
01	11	Ŧ	51	41	1	8	1	0
51	Ν	1	Total	С	Ν	Ο	Р	0
	11	1	41	31	1	8	1	0
51	Ν	1	Total	С	Ν	Ο	Р	0
	11	*	29	19	1	8	1	Ŭ



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Mol	Chain	Residues	Atoms					AltConf	
51 P	1	Total	С	Ν	0	Р	0		
	L	37	27	1	8	1	0		
51	51 X	1	Total	С	Ν	0	Р	0	
51		1	51	41	1	8	1	0	
51	V	V	V 1	Total	С	Ν	0	Р	0
51	1	T	35	25	1	8	1	0	
51 d	1	Total	С	N	0	Р	0		
	a 1	51	41	1	8	1	0		

• Molecule 52 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
52	Т	1	Total	С	Ο	Р	0
52	J	1	62	43	17	2	0
52	K	1	Total	С	Ο	Р	0
52	Т	1	71	52	17	2	0
52	т	1	Total	С	Ο	Р	0
52	L		69	50	17	2	0
52	h	1	Total	С	Ο	Р	0
52	11	T	67	48	17	2	0
52	G	1	Total	С	0	Р	0
52	Ч	1	76	57	17	2	0

• Molecule 53 is 1-carbamimidoyl-3-[2-(3-chloranyl-4-iodanyl-phenyl)ethyl]guanidine (three-letter code: I49) (formula: $C_{10}H_{13}CIIN_5$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					AltConf
53	Ν	1	Total 17	C 10	Cl 1	I 1	N 5	0

• Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
54	0	1	Total	С	Ν	Ο	Р	0
	0	1	32	10	5	14	3	0

• Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).



Mol	Chain	Residues	Aton	AltConf	
55	О	1	Total 1	Mg 1	0

• Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					AltConf
56	D	1	Total	С	Ν	Ο	Р	0
50	1	1	48	21	7	17	3	U

• Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

• Molecule 58 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					AltConf	
59	т	1	Total	С	Ν	0	Р	\mathbf{S}	0
36 1	1	37	25	2	8	1	1	0	
59	TT	II 1	Total	С	Ν	0	Р	S	0
58 0	U	L	37	25	2	8	1	1	U



Mol	Chain	Residues	Atoms	AltConf
59	О	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 5 1 \end{array}$	0

• Molecule 60 is water.



Mol	Chain	Residues	Atoms	AltConf
60	А	21	Total O	0
		21	21 21	0
60	В	62	Total O	0
		_	62 62	
60	С	83	Total O	0
			$\begin{array}{ccc} 83 & 83 \\ \hline T_{otal} & O \end{array}$	
60	D	155	155 155	0
			Total O	
60	E	13	13 13	0
<u> </u>	Б	50	Total O	0
60	F	59	$59 ext{ }59$	0
60	G	183	Total O	0
00		105	183 183	0
60	Н	61	Total O	0
			61 61	
60	Ι	91	Total O	0
			91 91 Tutul O	
60	J	21	Total U	0
			21 21 Total O	
60	Κ	15	15 15	0
			Total O	
60	L	31	31 31	0
<u> </u>	ъл	40	Total O	0
60	M	49	49 49	0
60	Ν	40	Total O	0
00	11	43	49 49	0
60	0	21	Total O	0
			21 21	
60	Р	58	Total O	0
			58 58	
60	Q	59	50 50	0
			Total O	
60	R	39	39 39	0
	~	2	Total O	
60	S	2	2 2	0
60	V	1 5	Total O	0
00	V	15	15 15	U
60	W.	10	Total O	Ο
	vv	10	10 10	0
60	x	23	Total O	0
	~ 1	20	23 23	



α \cdot \cdot \cdot	C		
Continued	trom	nremons	naae
Continucu	110110	preduous	pagem
		1	1 0

Mol	Chain	Residues	Atoms	AltConf
60	Y	3	Total O 3 3	0
60	Z	24	Total O 24 24	0
60	a	11	Total O 11 11	0
60	b	7	Total O 7 7	0
60	d	9	Total O 9 9	0
60	е	15	Total O 15 15	0
60	f	1	Total O 1 1	0
60	g	4	Total O 4 4	0
60	h	15	Total O 15 15	0
60	i	2	$\begin{array}{cc} \text{Total} & \text{O} \\ 2 & 2 \end{array}$	0
60	j	1	Total O 1 1	0
60	k	2	$\begin{array}{cc} \text{Total} & \text{O} \\ 2 & 2 \end{array}$	0
60	l	3	Total O 3 3	0
60	m	7	Total O 7 7	0
60	n	9	Total O 9 9	0
60	р	10	Total O 10 10	0
60	q	35	Total O 35 35	0
60	r	25	Total O 25 25	0
60	s	4	$\begin{array}{c c} Total & O \\ 4 & 4 \end{array}$	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 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B:		65%	6% •	28%
MET MLA MLA MLA MLA MLA	LEU LEU PRO PRO PRO VAL ARG SER SER SER SER SER SER SER SER	ALA ALA SILN CLEU ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	SER THR PRO PRO VAL SER	ALA ARG VAL VAL PRO PRO PRO ALA ALA ALA ALA

• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:	74%	·	22%	-
MET ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	GLN GLN VAL VAL VAL ARG SER ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	ARG GLU SER SER ALA ALA ASP ASP	158 P59 T62 D66 D112	T115 Y155 E158



• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



• Molecule 5: NA	ADH dehydrogenase [ubiquinone]	flavoprotein 2, mitochondrial
Chain E:	77%	9% 14%
MET PHE LEU LEU SER SER ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	LEU ALA ALA ALA ALA ALA CLY CLY CLY ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	A5 112 113 113 1104 1104 1105 1105 1105 1138
N150 E162 1169 1181 1181 7182 8183 8192 8192 8192		
• Molecule 6: NA	ADH dehydrogenase [ubiquinone]	flavoprotein 1, mitochondrial
Chain F:	86%	7% 7%
MET LEU ALA ALA ARG ARG ARG LEU CLEU GLY SER SER PRO PRO PRO	ALL ARG VAL SER VAL VAL VAL ARG ARG ASP PRO ASP AG A A A A A A A A A A A A A A A A A A	P86 886 886 886 886 193 194 118 118 113 118 113 1192 1192 1192 1192 1192 1192 1192
E248 N291 N302 1306 E313 E313 E313 T327 T327	1350 1355 1355 1355 1355 1355 1355 1355	
• Molecule 7: NA	ADH-ubiquinone oxidoreductase	75 kDa subunit, mitochondrial
Chain G:	88%	6% 5%
MET LEU LEU ARG ARG PRO PRO ARG LEU CEU CEU LEU LEU	SER SER SER SER SER SER SER SER SER THR THR THR THR THR THR THR THR THR TH	R39 V73 E84 E84 E84 E109 C133 C133 C133 C133 C133 C133 C133 C13
W262 D265 D265 E231 E231 E231 E232 F292	D324 D324 D375 U376 U376 U377 U377 1452 D462 D462 S481 S481 S481 S482 €482	N483 11484 6455 6455 6512 6526 0536 0546 0546 0546 0546 1568 1568 1568 1568 1568 1568 1587 1588
1656 1657 1665 8831 8831 8831 617 883 617 ALA ALA ALA	ALA VAL GLU GLU FRO FRO FRO CTS	
• Molecule 8: NA	ADH-ubiquinone oxidoreductase	chain 1
Chain H:	90%	10% ·
M1 F2 16 16 18 18 121 121 121 121 132 1332	R34 B1 B1 B1 B2 B8 A122 C103 C133 C133 C133 C133 C133 C133 C133	M183 R195 S209 S209 F23 F236 F236 F236 F236 F236 F236 F236
1289 N302		
• Molecule 9: NA	ADH dehydrogenase [ubiquinone]	iron-sulfur protein 8, mitochondrial

Chain I:

80%

17%

•





• Molecule 14: NADH-ubiquinone oxidoreductase chain 2





 \bullet Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:	83%	10% • 7%	
MET ALA ALA ALA ARG ARG ARG PRO PRO ARG VAL PRO GIT VAL PRO GIT TILE	HIS THR SER VAL CLN DHE L1 M18 K21 K21 K21 142 H50 H50	Y83 888 888 888 97 97 97 110 4111 4111 1110 4111 1110 1111 1135 1135 1135 1131 1135 1135	
Y152 Y176 P177 P177 P177 P179 Q189 Q189 Q184 Q184 Q184 Q184 Q184 Q184 X197 X197	1202 1203 1206 1206 1226 1226 1226 1226 1226 1226		
• Molecule 16: NAL drial)H dehydrogenase [ubiquin	none] 1 alpha subcomplex subunit	9, mitochon-
Chain P:	83%	7% 10%	
MET ALA ALA ALA ALA ALA ALA PLS VAL ARC ARC ARC PRO PRO PRO MET SER	ARG SER SER SER VAL PRO ALA ALA ALA ALA SER PRO GLN GLN GLN	L1 A26 V47 C51 C51 B97 B97 B145 D146 D176 D176 D176 D176 C208 Y236 K212 K212	
P259 H260 P261 P261 P263 V263 N265 N265 N266 E285 R266 H287 H287 H288 H288	P265 P265 E306 E330 E330 E333 1333 V33 V333	PRO	
• Molecule 17: NADI	I dehydrogenase [ubiquino	ne] iron-sulfur protein 4, mitochond	lrial
Chain Q:	67%	• 29%	
MET ALA ALA VAL VAL SER MET SER SER ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	ARG VAL VAL ALA ALA VAL VAL VAL VAL SER VAL SER SER SER SER SER SER SER SER SER SER	SER THR SER SER SER SER ARG ARG ASP ASP ASP ASP ASP THR ASP T13 CIN CIN CIN CIN CIN CIN CIN CIN CIN CIN	
132 842 446 1133 1133			
• Molecule 18: NADE	I dehydrogenase [ubiquino	ne] iron-sulfur protein 6, mitochond	lrial
Chain R:	73%	• 23%	
MET ALA ALA ALA ALA LLEU THR PHE LLEU LLEU CLEU CLY ALA ALA ALA ALA ALA ALA	VAL THR ARG GLY PLEU CL2 CL2 CL2 CL2 CL2 CL2 CL2 CL2 CL2 CL2		
• Molecule 19: NADE	I dehydrogenase [ubiquino	ne] 1 alpha subcomplex subunit 2	
Chain S:	77%	8% 15%	
MET ALA ALA ALA ALA ALA ALA ALA CI CI CI CI CI CI CI CI CI CI CI CI CI	K38 K38 K45 K74 M92 S96 LYS ALA		
• Molecule 20: Acyl o	arrier protein, mitochondr	rial	







Chain Z:	83%	14% •
MET ALA ALA SER KS KS C14 C14 C14 C14	E66 A67 E89 E89 E89 E92 E93 E92 E92 E92 E102 M120 M120 M120 M120 M120 E123 E123 E123 E123 E123 T137 T137	
• Molecule 26:	NADH dehydrogenase [ubiquinone] 1 alpha	subcomplex subunit 1
Chain a:	99%	
D70		
• Molecule 27:	NADH dehydrogenase [ubiquinone] 1 alpha	subcomplex subunit 3
Chain b:	95%	•••
MET ALA E2 R3 V4 T33 N61	◆ 881 1	
• Molecule 28:	NADH dehydrogenase [ubiquinone] 1 subun	it C1, mitochondrial
Chain c:	58% 5%	37%
MET ALA PRO SER SER ALA LEU LEU LEU PRO PHE TRP	LYS LEU ALA ALA ALA ALA ALA ARG SER SER SER SER SER SER SER SER SER SER	
• Molecule 29:	NADH dehydrogenase [ubiquinone] 1 subun	it C2
Chain d:	03%	. 6%
AME MET ARG GLN GLN AS AS AS AS	K1005 K1	
• Molecule 30:	NADH dehydrogenase [ubiquinone] iron-sult	fur protein 5
Chain e:	89%	• 8%
MET P1 T15 T18 K87	P83 H97 SER GLU PRO PRO ARG SER	
• Molecule 31:	NADH dehydrogenase [ubiquinone] 1 beta s	subcomplex subunit 1
Chain f:	88%	• 9%





 \bullet Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:	59%	5%	36%	I	
				**	
MET ALA ALA ALA ARG ARG CVS CVS CVS CVS CVS CVS ARG ARG	LEU LALA ALAA ALAA ALAA ALAA ALAA ALAA A	SER SER SER SER ALA ALA TLE ALA ALA PRLA SER THR	LEU ALA ALA ALA ALA ALA ALA PRO GLU FRO CLU LEU LEU LEU VZG	E33 D34 N57	
886 E109 C112 S116 E122 ASP GLU	ASP				
• Molecule 33: drial	NADH dehydrogenase [ubiquinone] 1	beta subcomplex	subunit 5,	mitochon-
Chain h:	72%		27%		
MET ALA ALA ALA MET SER SER LEU HIS ALA SER SER VAL	SER ALA VAL ALA ALA ALA ALA ALA CLA CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	PHE LEU LEU ARG ARG PHE PRO LYS THR VAL ALA	PRO VAL ARG HITS SER GLY GLY KC3 KC3 KC3	N143	
• Molecule 34: N	NADH dehydrogenase [ub	iquinone] 1 beta	a subcomplex sub	unit 6	
Chain i:	78%		• 20%		
S1 Q12 GLN GLN ARG VAL PRO VAL VAL CLU	ASC PHE TRP ASP CLVS PHE LVS CLV CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	К62 Н66 К120 D124 0125 H125	STH		
• Molecule 35: drial	NADH dehydrogenase [ubiquinone] 1	beta subcomplex	subunit 2,	mitochon-
Chain j:	58%	•	38%		
MET ALA GLY GLY MET AEA LEU LEU ARG LEU ALA PRO	PHE ALLA HIS VAL GLY GLY GLY GLY ARG ARG ARG ALA ALA ALA ALA ALA	ARG GLY VAL ARG ARG ARG CLY GLY GLY GLY	He F40 B70 E71 ASP		

• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



 \bullet Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



Chain l:	82%	• 17%
MET ALA ALA ALA ALA ARG GLY VAL VAL	CLT CLT CLT CLT CLT CLT CLT CLT CLT CLT	E18 K25 E32 E32 E149 F150 E151 E151
• Molecule	38: NADH dehydrogenase [ubiquinone]	1 beta subcomplex subunit 4
Chain m:	7%	
MET SER F2 F2 Y22 D23	226 826 827 829 128 187 128 128 128 128	
• Molecule	39: NADH dehydrogenase [ubiquinone]	1 beta subcomplex subunit 9
Chain n:	95%	
MET ALLA PHE LEU SER SER GLY A7	X8 W159 M178 M178	
• Molecule	40: NADH dehydrogenase [ubiquinone]	1 beta subcomplex subunit 7
Chain o:	84%	• 12%
MET G1 M21 K69 K80	q109 R110 R117 E118 A119 A119 A119 A114 A14 A14 CLV CLV CLV CLV CLV CLV CLV CLV CLV CLV	
• Molecule	41: NADH dehydrogenase [ubiquinone]	1 beta subcomplex subunit 10
Chain p:	96%	
MET PRO D2 R42 K126	A172 ALA ALA ALA	
• Molecule	42: NADH dehydrogenase [ubiquinone]	1 alpha subcomplex subunit 12
Chain q:	99%	·
M1 E2 V26 V144 K145		
• Molecule	43: NADH dehydrogenase [ubiquinone]	1 alpha subcomplex subunit 7
Chain r:	81%	• 17%

L112

ATA BANK

E10

MET

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

Chain s:

40%

60%





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48367	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	34.153	Depositor
Minimum map value	-13.918	Depositor
Average map value	0.004	Depositor
Map value standard deviation	1.021	Depositor
Recommended contour level	5.0	Depositor
Map size (Å)	482.46, 482.46, 482.46	wwPDB
Map dimensions	660, 660, 660	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	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: FME, LMT, SAC, FES, NDP, MG, PC1, FMN, AYA, EHZ, 2MR, SF4, CDL, K, I49, ZN, 3PE, GTP, MYR

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

Mol Chain		Bond lengths		Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.32	0/936	0.42	0/1281	
2	В	0.42	0/1272	0.46	0/1720	
3	С	0.37	0/1772	0.46	0/2413	
4	D	0.37	0/3537	0.45	0/4794	
5	Е	0.34	0/1695	0.46	0/2307	
6	F	0.35	0/3384	0.45	0/4572	
7	G	0.34	0/5367	0.46	0/7274	
8	Н	0.35	0/2571	0.44	0/3513	
9	Ι	0.38	0/1445	0.48	0/1956	
10	J	0.34	0/1362	0.43	0/1848	
11	Κ	0.29	0/745	0.43	0/1008	
12	L	0.33	0/4908	0.42	0/6679	
13	М	0.34	0/3738	0.43	0/5097	
14	Ν	0.32	0/2792	0.44	0/3800	
15	0	0.35	0/2651	0.42	0/3587	
16	Р	0.34	0/2824	0.45	0/3831	
17	Q	0.33	0/1039	0.46	0/1404	
18	R	0.38	0/742	0.46	0/999	
19	S	0.31	0/688	0.46	0/927	
20	Т	0.30	0/621	0.41	0/837	
20	U	0.37	0/705	0.43	0/952	
21	V	0.31	0/931	0.38	0/1261	
22	W	0.32	0/995	0.42	0/1337	
23	Х	0.32	0/1439	0.42	0/1942	
$2\overline{4}$	Y	0.28	$0/1\overline{042}$	0.44	$0/1\overline{414}$	
25	Ζ	0.34	0/1175	0.45	0/1584	
$\overline{26}$	a	0.35	$0/\overline{584}$	0.44	0/786	
27	b	0.31	0/667	0.43	0/916	
28	с	0.33	0/418	0.37	0/567	
29	d	0.38	0/975	0.40	0/1319	
30	е	0.32	0/840	0.42	0/1123	



Mal	Chain	Bond lengths		Bond	angles
10101	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
31	f	0.32	0/464	0.43	0/626
32	g	0.35	0/850	0.39	0/1154
33	h	0.35	0/1188	0.41	0/1607
34	i	0.34	0/900	0.44	0/1224
35	j	0.34	0/607	0.39	0/833
36	k	0.34	0/657	0.42	0/887
37	1	0.35	0/1358	0.42	0/1858
38	m	0.34	0/1088	0.42	0/1472
39	n	0.37	0/1545	0.40	0/2092
40	0	0.36	0/1060	0.42	0/1420
41	р	0.36	0/1476	0.41	0/1990
42	q	0.35	0/1250	0.45	0/1698
43	r	0.35	0/780	0.45	0/1056
44	s	0.31	0/383	0.41	0/518
All	All	0.34	0/67466	0.44	0/91483

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	85	2MR	Mainchain

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	921	0	952	4	0
2	В	1241	0	1251	9	0
3	С	1721	0	1675	7	0
4	D	3459	0	3404	25	0
5	Е	1655	0	1661	13	0
6	F	3310	0	3266	16	0
7	G	5279	0	5301	26	0
8	Н	2509	0	2621	20	0
9	Ι	1414	0	1370	5	0
10	J	1337	0	1346	15	0
11	Κ	745	0	785	5	0
12	L	4791	0	4942	43	0
13	М	3654	0	3852	21	0
14	Ν	2733	0	2912	17	0
15	0	2589	0	2566	19	0
16	Р	2747	0	2766	16	0
17	Q	1016	0	1014	4	0
18	R	730	0	707	1	0
19	S	677	0	688	3	0
20	Т	612	0	604	10	0
20	U	693	0	688	3	0
21	V	911	0	950	7	0
22	W	971	0	989	4	0
23	Х	1402	0	1383	8	0
24	Y	1030	0	1039	7	0
25	Ζ	1146	0	1146	14	0
26	a	569	0	568	0	0
27	b	646	0	654	0	0
28	с	405	0	409	0	0
29	d	945	0	932	0	0
30	е	819	0	821	0	0
31	f	451	0	453	0	0
32	g	824	0	772	0	0
33	h	1154	0	1168	0	0
34	i	879	0	892	0	0
35	j	580	0	519	0	0
36	k	638	0	621	0	0
37	1	1304	0	1203	0	0
38	m	1061	0	1059	0	0
39	n	1492	0	1438	0	0
40	0	1035	0	1003	0	0
41	р	1443	0	1415	0	0
42	q	1209	0	1182	0	0



Continuea from previous page							
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes	
43	r	767	0	776	0	0	
44	s	371	0	344	0	0	
45	А	70	0	92	1	0	
45	J	35	0	46	1	0	
45	L	105	0	138	1	0	
45	М	105	0	138	4	0	
45	N	35	0	46	0	0	
45	Y	105	0	138	4	0	
45	h	35	0	46	0	0	
45	j	35	0	46	0	0	
45	1	35	0	46	0	0	
46	А	21	0	18	1	0	
46	В	89	0	132	2	0	
46	L	49	0	75	0	0	
47	В	8	0	0	1	0	
47	F	8	0	0	1	0	
47	G	16	0	0	0	0	
47	Ι	16	0	0	0	0	
48	Е	4	0	0	0	0	
48	G	4	0	0	0	0	
49	F	31	0	19	2	0	
50	G	1	0	0	0	0	
51	Н	78	0	112	1	0	
51	Ι	51	0	82	0	0	
51	L	94	0	142	0	0	
51	М	97	0	151	4	0	
51	N	121	0	170	2	0	
51	Р	37	0	48	0	0	
51	Х	51	0	82	4	0	
51	Y	35	0	44	0	0	
51	d	51	0	82	0	0	
52	J	62	0	68	1	0	
52	K	71	0	86	0	0	
52	L	69	0	82	0	0	
52	h	67	0	81	0	0	
52	q	76	0	96	0	0	
53	Ν	17	0	0	1	0	
54	0	32	0	12	3	0	
55	0	1	0	0	0	0	
56	P	48	0	26	1	0	
57	R	1	0	0	0	0	
58	Т	37	0	0	0	0	

Continued from previous page...


		i previous		TT (111)		0 01 1
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	U	37	0	0	0	0
59	0	6	0	6	0	0
60	A	21	0	0	0	0
60	B	62	0	0	2	0
60	C	83	0	0	3	0
60	D	155	0	0	9	0
60	E	13	0	0	1	0
60	F	59	0	0	3	0
60	G	183	0	0	7	0
60	Н	61	0	0	2	0
60	I	91	0	0	3	0
60	J	21	0	0	1	0
60	K	15	0	0	0	0
60	L	31	0	0	2	0
60	М	49	0	0	3	0
60	Ν	49	0	0	3	0
60	Ο	21	0	0	2	0
60	Р	58	0	0	1	0
60	Q	59	0	0	1	0
60	R	39	0	0	0	0
60	S	2	0	0	0	0
60	V	15	0	0	2	0
60	W	10	0	0	1	0
60	Х	23	0	0	3	0
60	Y	3	0	0	0	0
60	Ζ	24	0	0	2	0
60	a	11	0	0	0	0
60	b	7	0	0	0	0
60	d	9	0	0	0	0
60	е	15	0	0	0	0
60	f	1	0	0	0	0
60	g	4	0	0	0	0
60	h	15	0	0	0	0
60	i	2	0	0	0	0
60	j	1	0	0	0	0
60	k	2	0	0	0	0
60	1	3	0	0	0	0
60	m	7	0	0	0	0
60	n	9	0	0	0	0
60	р	10	0	0	0	0
60	q	35	0	0	0	0
60	r	25	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	s	4	0	0	0	0
All	All	69138	0	68457	313	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 313 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:479:GLN:NE2	12:L:481:THR:O	2.08	0.87
16:P:51:CYS:O	60:P:601:HOH:O	1.96	0.83
21:V:105:GLU:O	60:V:201:HOH:O	1.94	0.83
4:D:72:MET:SD	60:D:653:HOH:O	2.35	0.82
2:B:44:SER:OG	8:H:51:ASP:OD1	1.97	0.82

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	Outliers	Perce	entiles
1	А	113/115~(98%)	111 (98%)	2 (2%)	0	100	100
2	В	153/216~(71%)	146 (95%)	7 (5%)	0	100	100
3	С	205/266~(77%)	200 (98%)	5 (2%)	0	100	100
4	D	427/463~(92%)	415 (97%)	12 (3%)	0	100	100
5	Е	211/249~(85%)	206 (98%)	5 (2%)	0	100	100
6	F	428/464 (92%)	420 (98%)	8 (2%)	0	100	100
7	G	686/727~(94%)	668 (97%)	18 (3%)	0	100	100
8	Н	316/318~(99%)	303 (96%)	13 (4%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
9	Ι	174/212~(82%)	169~(97%)	5 (3%)	0	100	100
10	J	172/175~(98%)	161 (94%)	11~(6%)	0	100	100
11	Κ	96/98~(98%)	95~(99%)	1 (1%)	0	100	100
12	L	604/606~(100%)	580 (96%)	23~(4%)	1 (0%)	47	58
13	М	457/459~(100%)	451 (99%)	6 (1%)	0	100	100
14	Ν	345/347~(99%)	339~(98%)	6(2%)	0	100	100
15	О	318/343~(93%)	313 (98%)	5(2%)	0	100	100
16	Р	339/380~(89%)	332 (98%)	7(2%)	0	100	100
17	Q	123/175~(70%)	123 (100%)	0	0	100	100
18	R	93/124~(75%)	90~(97%)	3(3%)	0	100	100
19	S	82/99~(83%)	80 (98%)	2(2%)	0	100	100
20	Т	74/156~(47%)	73~(99%)	1 (1%)	0	100	100
20	U	84/156~(54%)	83~(99%)	1 (1%)	0	100	100
21	V	110/116~(95%)	109 (99%)	1 (1%)	0	100	100
22	W	112/128 (88%)	109 (97%)	3(3%)	0	100	100
23	Х	169/172~(98%)	168 (99%)	1 (1%)	0	100	100
24	Y	138/141 (98%)	134 (97%)	4 (3%)	0	100	100
25	Ζ	138/144 (96%)	135 (98%)	2(1%)	1 (1%)	22	26
26	a	68/70~(97%)	66~(97%)	2(3%)	0	100	100
27	b	80/84~(95%)	76~(95%)	4 (5%)	0	100	100
28	с	46/76~(60%)	46 (100%)	0	0	100	100
29	d	111/120 (92%)	110 (99%)	1 (1%)	0	100	100
30	е	95/106~(90%)	93~(98%)	2(2%)	0	100	100
31	f	50/57~(88%)	49 (98%)	1 (2%)	0	100	100
32	g	96/154~(62%)	91 (95%)	5(5%)	0	100	100
33	h	136/189~(72%)	135 (99%)	1 (1%)	0	100	100
34	i	98/127~(77%)	95~(97%)	3(3%)	0	100	100
35	j	65/108~(60%)	65 (100%)	0	0	100	100
36	k	77/98~(79%)	76~(99%)	1 (1%)	0	100	100
37	1	153/186~(82%)	149 (97%)	4 (3%)	0	100	100
38	m	125/129~(97%)	121 (97%)	4 (3%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
39	n	170/179~(95%)	165~(97%)	5(3%)	0	100	100
40	О	118/137~(86%)	113 (96%)	5 (4%)	0	100	100
41	р	169/176~(96%)	167~(99%)	2(1%)	0	100	100
42	q	143/145~(99%)	142 (99%)	1 (1%)	0	100	100
43	r	90/113~(80%)	86 (96%)	4 (4%)	0	100	100
44	s	42/109~(38%)	41 (98%)	1 (2%)	0	100	100
All	All	8099/9212 (88%)	7899 (98%)	198 (2%)	2(0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	562	LEU
25	Ζ	102	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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	100/100~(100%)	100 (100%)	0	100	100
2	В	131/175~(75%)	127 (97%)	4 (3%)	40	55
3	С	188/228~(82%)	188 (100%)	0	100	100
4	D	370/392~(94%)	367~(99%)	3 (1%)	81	91
5	Е	183/205~(89%)	182 (100%)	1 (0%)	88	95
6	F	344/368~(94%)	335~(97%)	9~(3%)	46	63
7	G	578/608~(95%)	570 (99%)	8 (1%)	67	81
8	Н	274/274~(100%)	268~(98%)	6(2%)	52	69
9	Ι	151/175~(86%)	150 (99%)	1 (1%)	84	92
10	J	140/141~(99%)	138 (99%)	2(1%)	67	81
11	Κ	85/85~(100%)	82 (96%)	3 (4%)	36	50
12	L	531/533~(100%)	523 (98%)	8 (2%)	65	79



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Mol	Chain	Analysed	Rotameric	Outliers Percent		ntiles
13	М	412/412~(100%)	404~(98%)	8 (2%)	57	73
14	Ν	315/315~(100%)	312~(99%)	3~(1%)	76	87
15	Ο	283/303~(93%)	274~(97%)	9~(3%)	39	54
16	Р	295/327~(90%)	292~(99%)	3~(1%)	76	87
17	Q	112/153~(73%)	112 (100%)	0	100	100
18	R	78/97~(80%)	76~(97%)	2(3%)	46	63
19	S	75/82~(92%)	72 (96%)	3(4%)	31	44
20	Т	70/135~(52%)	67~(96%)	3 (4%)	29	40
20	U	79/135~(58%)	79 (100%)	0	100	100
21	V	100/102~(98%)	100 (100%)	0	100	100
22	W	107/114 (94%)	106 (99%)	1 (1%)	78	89
23	Х	154/155~(99%)	151 (98%)	3~(2%)	57	73
24	Y	101/102~(99%)	98~(97%)	3~(3%)	41	57
25	Ζ	119/121~(98%)	117 (98%)	2(2%)	60	76
26	a	59/59~(100%)	58~(98%)	1 (2%)	60	76
27	b	71/72~(99%)	69~(97%)	2(3%)	43	60
28	с	44/68~(65%)	40 (91%)	4 (9%)	9	11
29	d	101/105~(96%)	100 (99%)	1 (1%)	76	87
30	е	88/96~(92%)	85~(97%)	3~(3%)	37	51
31	f	49/54~(91%)	47 (96%)	2~(4%)	30	43
32	g	89/131~(68%)	82 (92%)	7 (8%)	12	15
33	h	121/158~(77%)	120 (99%)	1 (1%)	81	91
34	i	97/120~(81%)	95~(98%)	2(2%)	53	70
35	j	61/84~(73%)	57~(93%)	4 (7%)	16	22
36	k	61/76~(80%)	60~(98%)	1 (2%)	62	78
37	1	139/159~(87%)	137~(99%)	2(1%)	67	81
38	m	113/115~(98%)	110 (97%)	3(3%)	44	61
39	n	156/161~(97%)	154 (99%)	2(1%)	69	82
40	0	109/120~(91%)	104 (95%)	5 (5%)	27	38
41	р	155/157~(99%)	153~(99%)	2(1%)	69	82
42	q	131/131 (100%)	129 (98%)	2(2%)	65	79



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles	
43	r	84/97~(87%)	82~(98%)	2(2%)	49	66	
44	s	43/92~(47%)	43 (100%)	0	100	100	
All	All	7146/7892~(90%)	7015 (98%)	131 (2%)	61	75	

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
38	m	26	SER
39	n	84	SER
43	r	104	GLU
13	М	114	GLU
13	М	80	SER

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such side chains are listed below:

Mol	Chain	Res	Type
16	Р	87	HIS
35	j	6	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).

Mol T	True	Chain	Chain Res	Tinle	Bo	ond leng	$_{\rm sths}$	E	Bond ang	gles
NIOI	туре	Chain		LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	SAC	i	1	34	7,8,9	0.97	0	8,9,11	1.29	2 (25%)
1	FME	А	1	1	8,9,10	0.92	0	7,9,11	1.13	1 (14%)
10	FME	J	1	10	8,9,10	0.96	0	7,9,11	0.99	0



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	ths	E	ond ang	gles
INIOI	туре	Unain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
8	FME	Н	1	8	8,9,10	0.96	0	7,9,11	0.78	0
14	FME	N	1	14	8,9,10	0.93	0	7,9,11	1.05	0
4	2MR	D	85	4	10,12,13	2.62	4 (40%)	5,13,15	1.15	1 (20%)
43	AYA	r	1	43	6,7,8	1.80	2 (33%)	5,8,10	1.28	1 (20%)
11	FME	K	1	11	8,9,10	0.93	0	7,9,11	0.86	0
12	FME	L	1	12	8,9,10	0.99	1 (12%)	7,9,11	0.75	0
13	FME	М	1	13	8,9,10	0.99	1 (12%)	7,9,11	1.01	1 (14%)
24	AYA	Y	1	24	6,7,8	1.79	2 (33%)	5,8,10	1.38	1 (20%)

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
34	SAC	i	1	34	-	2/7/8/10	-
1	FME	А	1	1	-	0/7/9/11	-
10	FME	J	1	10	-	3/7/9/11	-
8	FME	Н	1	8	-	4/7/9/11	-
14	FME	Ν	1	14	-	3/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
43	AYA	r	1	43	-	0/4/6/8	-
11	FME	Κ	1	11	-	1/7/9/11	-
12	FME	L	1	12	-	2/7/9/11	-
13	FME	М	1	13	-	0/7/9/11	-
24	AYA	Y	1	24	-	0/4/6/8	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	4.86	1.44	1.33
4	D	85	2MR	CZ-NE	4.54	1.44	1.34
4	D	85	2MR	O-C	3.94	1.35	1.19
24	Y	1	AYA	CT-N	3.26	1.45	1.34
43	r	1	AYA	CT-N	3.13	1.45	1.34

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
34	i	1	SAC	C-CA-N	2.55	114.33	109.73



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	1	FME	C-CA-N	2.47	114.18	109.73
24	Y	1	AYA	CM-CT-N	2.37	120.11	116.10
4	D	85	2MR	NE-CZ-NH2	-2.31	117.36	119.48
43	r	1	AYA	CM-CT-N	2.27	119.94	116.10

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
8	Н	1	FME	C-CA-CB-CG
8	Н	1	FME	CA-CB-CG-SD
10	J	1	FME	O1-CN-N-CA
12	L	1	FME	O1-CN-N-CA
14	Ν	1	FME	O1-CN-N-CA

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 57 ligands modelled in this entry, 3 are monoatomic - leaving 54 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	Mol Type	Chain	Dec	Link	B	ond leng	gths	B	ond ang	$\begin{array}{c c} \mathbf{ngles} \\ Z & \# Z > 2 \end{array}$		
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2		
52	CDL	K	401	-	70,70,99	1.03	8 (11%)	76,82,111	1.04	4 (5%)		
45	LMT	М	602	-	36,36,36	1.13	2 (5%)	47,47,47	0.93	1 (2%)		
51	3PE	Ν	1301	-	50,50,50	0.87	3 (6%)	53,55,55	1.07	2 (3%)		
51	3PE	Ν	1303	-	40,40,50	0.96	4 (10%)	43,45,55	1.08	2 (4%)		



N <i>T</i> - 1	—		D	T 1.	Bond lengths		B	ond ang	les	
NIOI	Type	Chain	Res	LINK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
51	3PE	Y	802	-	34,34,50	1.04	3 (8%)	37,39,55	1.20	2 (5%)
47	SF4	F	502	6	0,12,12	-	-	-		
58	EHZ	Т	101	20	29,36,37	1.68	6 (20%)	35,44,47	1.88	6 (17%)
59	MYR	0	201	40	5,5,15	0.85	0	4,4,15	1.01	0
45	LMT	М	603	-	36,36,36	1.16	2(5%)	47,47,47	0.89	1 (2%)
45	LMT	L	702	-	36,36,36	1.18	2(5%)	47,47,47	0.94	1 (2%)
45	LMT	J	702	-	36,36,36	1.22	3 (8%)	47,47,47	1.12	2 (4%)
49	FMN	F	501	-	33,33,33	1.11	2 (6%)	48,50,50	1.24	6 (12%)
53	I49	N	1305	-	15,17,17	1.46	2 (13%)	21,22,22	2.11	4 (19%)
52	CDL	J	701	-	61,61,99	1.08	8 (13%)	67,73,111	1.28	4 (5%)
47	SF4	G	802	7	0,12,12	-	-	-		
51	3PE	L	701	-	48,48,50	0.90	4 (8%)	51,53,55	1.13	2 (3%)
51	3PE	М	601	-	45,45,50	0.91	3 (6%)	48,50,55	1.04	2 (4%)
51	3PE	М	605	-	50,50,50	0.85	3 (6%)	53,55,55	1.06	2 (3%)
51	3PE	L	705	-	44,44,50	0.91	3 (6%)	47,49,55	1.24	3 (6%)
46	PC1	А	303	-	20,20,53	1.86	3 (15%)	24,27,61	1.14	1 (4%)
45	LMT	j	101	_	36,36,36	1.22	4 (11%)	47,47,47	0.88	1 (2%)
45	LMT	Y	803	_	36,36,36	1.19	3 (8%)	47,47,47	1.00	1 (2%)
56	NDP	Р	501	_	45,52,52	2.15	4 (8%)	53,80,80	1.69	12 (22%)
47	SF4	Ι	203	9	0,12,12	-		-		
45	LMT	А	301	-	36,36,36	1.15	2 (5%)	47,47,47	1.01	2 (4%)
52	CDL	L	703	-	68,68,99	1.04	5 (7%)	74,80,111	1.09	4 (5%)
46	PC1	L	707	_	48,48,53	0.98	4 (8%)	54,56,61	1.07	2 (3%)
48	FES	G	803	7	0,4,4	-	-	-		
45	LMT	М	604	-	36,36,36	1.21	3 (8%)	47,47,47	0.90	0
51	3PE	N	1304	-	28,28,50	1.14	4 (14%)	31,33,55	1.13	2 (6%)
45	LMT	L	706	-	36,36,36	1.17	2 (5%)	47,47,47	1.04	2 (4%)
45	LMT	N	1302	-	36,36,36	1.18	3 (8%)	47,47,47	0.93	0
45	LMT	L	704	_	36,36,36	1.25	4 (11%)	47,47,47	1.01	2 (4%)
47	SF4	В	201	2	0,12,12	_		-		
46	PC1	В	203	-	34,34,53	1.16	4 (11%)	40,42,61	1.12	2 (5%)
51	3PE	X	401	-	50,50,50	0.86	4 (8%)	53,55,55	1.11	2 (3%)
54	GTP	0	401	55	26,34,34	2.90	11 (42%)	32,54,54	1.64	9 (28%)
51	3PE	Ι	201	_	50,50,50	0.87	4 (8%)	53,55,55	1.09	2 (3%)
45	LMT	Y	801	-	36,36,36	1.19	3 (8%)	47,47,47	0.99	0
58	EHZ	U	101	20	29,36,37	1.65	6 (20%)	35,44,47	1.42	3 (8%)



Mol	Tuno	Chain	Dog	Link	B	ond leng	gths	B	ond ang	les
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
46	PC1	В	202	-	$53,\!53,\!53$	0.93	3 (5%)	59,61,61	1.01	2 (3%)
51	3PE	Р	502	-	36,36,50	1.03	4 (11%)	39,41,55	1.10	2(5%)
47	SF4	G	801	7	0,12,12	-	-	-		
51	3PE	d	301	-	$50,\!50,\!50$	0.83	3 (6%)	53,55,55	1.18	4 (7%)
45	LMT	h	1002	-	36,36,36	1.13	2 (5%)	47,47,47	1.04	1 (2%)
52	CDL	h	1001	-	66,66,99	1.05	7 (10%)	72,78,111	1.20	4 (5%)
45	LMT	1	201	-	36,36,36	1.20	3 (8%)	47,47,47	1.00	2 (4%)
48	FES	Е	301	5	0,4,4	-	-	-		
51	3PE	Н	402	-	33,33,50	1.35	3 (9%)	34,37,55	1.15	2(5%)
47	SF4	Ι	202	9	0,12,12	-	-	-		
52	CDL	q	201	-	75,75,99	0.99	6 (8%)	81,87,111	1.11	4 (4%)
45	LMT	Y	804	-	36,36,36	1.20	3 (8%)	47,47,47	1.11	3 (6%)
51	3PE	Н	401	-	43,43,50	0.93	3 (6%)	46,48,55	1.08	2 (4%)
45	LMT	А	302	-	36,36,36	1.14	2 (5%)	47,47,47	1.64	7 (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
52	CDL	К	401	-	-	29/81/81/110	-
45	LMT	М	602	-	-	8/21/61/61	0/2/2/2
51	3PE	Ν	1301	-	-	20/54/54/54	-
51	3PE	Ν	1303	-	-	22/44/44/54	-
51	3PE	Y	802	-	-	17/38/38/54	-
58	EHZ	Т	101	20	-	11/42/44/45	-
47	SF4	F	502	6	-	-	0/6/5/5
59	MYR	0	201	40	-	2/2/3/13	-
45	LMT	М	603	-	-	13/21/61/61	0/2/2/2
45	LMT	L	702	-	-	10/21/61/61	0/2/2/2
45	LMT	J	702	-	-	10/21/61/61	0/2/2/2
49	FMN	F	501	-	-	1/18/18/18	0/3/3/3
53	I49	Ν	1305	-	-	5/10/10/10	0/1/1/1
52	CDL	J	701	-	-	37/71/71/110	-
51	3PE	L	701	-	-	28/52/52/54	-
47	SF4	G	802	7	-	-	0/6/5/5



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	3PE	М	601	-	-	19/49/49/54	-
51	3PE	М	605	-	-	24/54/54/54	-
51	3PE	L	705	-	-	20/48/48/54	-
46	PC1	А	303	-	-	4/22/22/57	-
45	LMT	j	101	-	-	4/21/61/61	0/2/2/2
45	LMT	Y	803	-	-	8/21/61/61	0/2/2/2
56	NDP	Р	501	-	_	7/30/77/77	0/5/5/5
47	SF4	Ι	203	9	-	-	0/6/5/5
45	LMT	А	301	-	-	5/21/61/61	0/2/2/2
52	CDL	L	703	-	-	34/79/79/110	-
46	PC1	L	707	-	-	25/52/52/57	-
48	FES	G	803	7	-	-	0/1/1/1
45	LMT	М	604	-	-	8/21/61/61	0/2/2/2
51	3PE	N	1304	-	-	17/32/32/54	-
45	LMT	L	706	-	-	8/21/61/61	0/2/2/2
45	LMT	N	1302	-	-	9/21/61/61	0/2/2/2
45	LMT	L	704	-	-	10/21/61/61	0/2/2/2
51	3PE	X	401	-	-	25/54/54/54	-
46	PC1	В	203	-	-	17/38/38/57	-
47	SF4	В	201	2	-	-	0/6/5/5
54	GTP	0	401	55	-	4/18/38/38	0/3/3/3
51	3PE	Ι	201	-	-	16/54/54/54	-
45	LMT	Y	801	-	-	8/21/61/61	0/2/2/2
58	EHZ	U	101	20	-	7/42/44/45	-
46	PC1	В	202	-	-	20/57/57/57	-
51	3PE	Р	502	-	-	21/40/40/54	-
47	SF4	G	801	7	-	-	0/6/5/5
51	3PE	d	301	-	-	23/54/54/54	-
45	LMT	h	1002	-	-	8/21/61/61	0/2/2/2
52	CDL	h	1001	-	-	39/77/77/110	-
45	LMT	1	201	-	-	9/21/61/61	0/2/2/2
51	3PE	Н	402	-	-	19/36/36/54	-
48	FES	E	301	5	-	-	0/1/1/1
47	SF4	Ι	202	9	-	-	0/6/5/5
52	CDL	q	201	-	-	36/86/86/110	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	LMT	Y	804	-	-	6/21/61/61	0/2/2/2
51	3PE	Н	401	-	-	18/47/47/54	-
45	LMT	А	302	-	-	11/21/61/61	0/2/2/2

The worst 5 of 170 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Р	501	NDP	P2B-O2B	11.88	1.81	1.59
54	0	401	GTP	O6-C6	8.07	1.39	1.23
46	А	303	PC1	O21-C2	-5.79	1.40	1.46
54	0	401	GTP	O4'-C1'	5.41	1.48	1.41
58	Т	101	EHZ	C12-N1	5.12	1.45	1.33

The worst 5 of 124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
58	Т	101	EHZ	C8-C9-S1	7.27	122.62	113.63
56	Р	501	NDP	PN-O3-PA	-6.84	109.37	132.83
58	U	101	EHZ	C8-C9-S1	5.82	120.83	113.63
53	Ν	1305	I49	C14-N02-C15	-5.66	115.78	125.21
45	А	302	LMT	C1-O1'-C1'	5.27	122.58	113.84

There are no chirality outliers.

5 of 702 torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
45	А	302	LMT	C2'-C1'-O1'-C1
45	L	702	LMT	C2-C1-O1'-C1'
45	L	704	LMT	C2'-C1'-O1'-C1
45	L	706	LMT	C2'-C1'-O1'-C1
45	L	706	LMT	O5'-C1'-O1'-C1

There are no ring outliers.

21 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	М	602	LMT	4	0
51	Ν	1301	3PE	2	0
47	F	502	SF4	1	0
45	J	702	LMT	1	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	F	501	FMN	2	0
53	N	1305	I49	1	0
52	J	701	CDL	1	0
51	М	601	3PE	3	0
51	М	605	3PE	1	0
46	А	303	PC1	1	0
56	Р	501	NDP	1	0
45	L	706	LMT	1	0
47	В	201	SF4	1	0
46	В	203	PC1	1	0
51	Х	401	3PE	4	0
54	0	401	GTP	3	0
45	Y	801	LMT	2	0
46	В	202	PC1	1	0
45	Y	804	LMT	2	0
51	Н	401	3PE	1	0
45	А	302	LMT	1	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-14251. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map



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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 330

Y Index: 330





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: 353

Y Index: 333

Z Index: 423

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


6.5 Mask visualisation (i)

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



7 Map analysis (i)

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

7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)



The volume at the recommended contour level is 299 $\rm nm^3;$ this corresponds to an approximate mass of 270 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 0.435 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-14251 and PDB model 7R41. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 5.0 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 (5.0).



9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (5.0) and Q-score for the entire model and for each chain.

\mathbf{Chain}	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.8992	0.6860
А	0.8863	0.6930
В	0.9519	0.7230
С	0.9636	0.7270
D	0.9526	0.7240
Е	0.8923	0.6780
F	0.9478	0.6960
G	0.9283	0.7030
Н	0.9635	0.7150
Ι	0.9708	0.7290
J	0.8836	0.6840
Κ	0.9198	0.7050
L	0.8983	0.6670
М	0.9519	0.6950
Ν	0.9472	0.7040
О	0.8972	0.6720
Р	0.8970	0.6960
Q	0.9315	0.7130
R	0.9046	0.7040
S	0.8647	0.6730
Т	0.6273	0.5950
U	0.9116	0.6660
V	0.8884	0.6930
W	0.8917	0.6960
Х	0.8834	0.6700
Y	0.6975	0.6350
Z	0.8827	0.6780
a	0.9435	0.6960
b	0.8623	0.6590
С	0.7551	0.6470
d	0.8810	0.6790
е	0.8379	0.6660
f	0.8014	0.6470
g	0.8940	0.6700
h	0.9053	0.6820

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Chain	Atom inclusion	Q-score
i	0.8232	0.6480
j	0.8083	0.6350
k	0.8682	0.6390
1	0.8058	0.6420
m	0.7777	0.6540
n	0.8839	0.6670
0	0.8730	0.6420
р	0.8890	0.6650
q	0.8873	0.6950
r	0.9245	0.7040
S	0.8702	0.6780

