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Title	:	State A of the human mitoribosomal large subunit assembly intermediate
Authors	:	Lenarcic, T.; Jaskolowski, M.; Leibundgut, M.; Scaiola, A.; Schoenhut, T.;
		Saurer, M.; Lee, R.G.; Rackham, O.; Filipovska, A.; Ban, N.
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This is	a I	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.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 Å.

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

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



2 Entry composition (i)

There are 63 unique types of molecules in this entry. The entry contains 107464 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 Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues		\mathbf{A}	AltConf	Trace			
1	u	110	Total 919	C 591	N 154	0 164	S 10	0	0

• Molecule 2 is a protein called MIEF1 upstream open reading frame protein.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
2	V	60	Total	С	N	Ō	0	0
	v	03	588	372	116	100	0	0

• Molecule 3 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues		Ate	\mathbf{oms}	AltConf	Trace		
3	W	79	Total 638	C 410	N 95	0 128	${f S}{5}$	0	0

• Molecule 4 is a protein called 5-methylcytosine rRNA methyltransferase NSUN4.

Mol	Chain	Residues		At	AltConf	Trace			
4	x	336	Total 2660	C 1694	N 465	0 484	S 17	0	0

• Molecule 5 is a protein called Transcription termination factor 4, mitochondrial.

Mol	Chain	Residues		At	AltConf	Trace			
5	У	244	Total 1980	C 1264	N 342	O 362	S 12	0	0

• Molecule 6 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
6	0	110	Total 898	C 554	N 176	0 162	S 6	0	0



• Molecule 7 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
7	1	55	Total 455	C 290	N 87	O 76	${ m S} { m 2}$	0	0

• Molecule 8 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
8	2	46	Total	С	Ν	Ο	S	0	0
0		40	377	233	83	60	1		0

• Molecule 9 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
9	3	95	Total 832	C 539	N 162	0 128	${ m S} { m 3}$	0	0

• Molecule 10 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
10	4	38	Total 342	C 217	N 72	O 49	${S \atop 4}$	0	0

• Molecule 11 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	5	394	Total 3210	C 2073	N 560	O 566	S 11	0	0

• Molecule 12 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	6	354	Total 2948	C 1881	N 525	0 533	S 9	0	0

• Molecule 13 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues		At	AltConf	Trace			
13	7	294	Total 2390	C 1529	N 405	O 438	S 18	0	0

• Molecule 14 is a protein called 39S ribosomal protein L40, mitochondrial.



Mol	Chain	Residues		At	oms	AltConf	Trace		
14	8	102	Total 860	C 543	N 152	O 163	${ m S} { m 2}$	0	0

• Molecule 15 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
15	9	124	Total 997	С 644	N 170	0 181	${S \over 2}$	0	0

• Molecule 16 is a RNA chain called 16S mitochondrial rRNA, DNA (31-MER),16S mitochondrial rRNA.

Mol	Chain	Residues		A	Atoms					
16	А	1448	Total 30460	C 13658	N 5442	O 9912	Р 1448	0	0	

• Molecule 17 is a RNA chain called mitochondrial tRNAVal.

Mol	Chain	Residues		A	toms			AltConf	Trace
17	В	72	Total 1522	C 683	N 269	0 498	Р 72	0	0

• Molecule 18 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues		At	AltConf	Trace			
18	D	240	Total 1872	C 1165	N 378	O 320	S 9	0	0

• Molecule 19 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues		At	AltConf	Trace			
19	Е	305	Total 2406	C 1545	N 418	0 432	S 11	0	0

• Molecule 20 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues		Ate	AltConf	Trace			
20	F	252	Total 2031	C 1305	N 370	O 350	S 6	0	0

• Molecule 21 is a protein called 39S ribosomal protein L9, mitochondrial.



Mol	Chain	Residues		Ato	ms		AltConf	Trace
21	Н	97	Total 802	C 508	N 155	O 139	0	0

• Molecule 22 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues		A	toms	AltConf	Trace		
22	Ι	163	Total 1324	C 854	N 240	O 220	S 10	0	0

• Molecule 23 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	J	175	Total 1330	C 847	N 237	0 244	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 24 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
24	K	177	Total 1455	C 936	N 259	O 253	S 7	0	0

• Molecule 25 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues		At	oms		AltConf	Trace	
25	L	115	Total 890	$\begin{array}{c} \mathrm{C} \\ 559 \end{array}$	N 171	O 155	${ m S}{ m 5}$	0	0

• Molecule 26 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues		At		AltConf	Trace		
26	М	291	Total 2327	C 1483	N 430	O 408	S 6	0	0

• Molecule 27 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Ν	212	Total 1723	C 1107	N 310	O 297	S 9	0	0

• Molecule 28 is a protein called 39S ribosomal protein L17, mitochondrial.



Mol	Chain	Residues		At	oms			AltConf	Trace
28	О	154	Total 1259	C 792	N 241	O 219	${ m S} 7$	0	0

• Molecule 29 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Р	144	Total 1173	C 733	N 224	0 211	${f S}{5}$	0	0

• Molecule 30 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Q	221	Total 1843	C 1179	N 327	0 328	S 9	0	0

• Molecule 31 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
31	R	140	Total 1154	C 732	N 231	0 187	${S \atop 4}$	0	0

• Molecule 32 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues		Atoms					Trace
32	S	161	Total 1293	C 835	N 227	0 227	$\begin{array}{c} \mathrm{S} \\ \mathrm{4} \end{array}$	0	0

• Molecule 33 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
33	Т	166	Total 1369	C 875	N 254	0 233	${ m S} 7$	0	0

• Molecule 34 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
34	U	152	Total 1251	C 788	N 234	O 226	${ m S} { m 3}$	0	0

• Molecule 35 is a protein called 39S ribosomal protein L24, mitochondrial.



Mol	Chain	Residues		At	AltConf	Trace			
35	V	205	Total 1676	C 1068	N 298	O 302	S 8	0	0

• Molecule 36 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
36	W	106	Total 835	C 536	N 157	O 139	${ m S} { m 3}$	0	0

• Molecule 37 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues		Ate	AltConf	Trace			
37	Х	244	Total 2044	C 1322	N 352	O 365	$\frac{S}{5}$	0	0

• Molecule 38 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Y	181	Total 1556	C 995	N 298	O 259	${S \atop 4}$	0	0

• Molecule 39 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
39	Z	122	Total 996	C 636	N 186	0 171	${ m S} { m 3}$	0	0

• Molecule 40 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
40	a	100	Total 840	C 529	N 152	0 154	${f S}{5}$	0	0

• Molecule 41 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
41	b	149	Total 1189	C 739	N 230	0 217	${ m S} { m 3}$	0	0

• Molecule 42 is a protein called 39S ribosomal protein L44, mitochondrial.



Mol	Chain	Residues		At	AltConf	Trace			
42	с	286	Total 2299	C 1470	N 397	O 423	S 9	0	0

• Molecule 43 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues		At	AltConf	Trace			
43	d	259	Total 2124	C 1357	N 369	0 384	S 14	0	0

• Molecule 44 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	е	228	Total 1848	C 1174	N 326	0 342	S 6	0	0

• Molecule 45 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	f	150	Total 1196	C 764	N 197	0 231	${f S}$ 4	0	0

• Molecule 46 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
46	g	134	Total 1113	C 719	N 193	0 199	${S \over 2}$	0	0

• Molecule 47 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
47	h	110	Total 895	C 568	N 156	0 168	${ m S} { m 3}$	0	0

• Molecule 48 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues		At	oms		AltConf	Trace	
48	i	97	Total 828	C 532	N 165	0 127	${S \atop 4}$	0	0

• Molecule 49 is a protein called 39S ribosomal protein L52, mitochondrial.



Mol	Chain	Residues		At	oms			AltConf	Trace
49	j	94	Total 745	C 463	N 144	0 136	${ m S} { m 2}$	0	0

• Molecule 50 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
50	k	101	Total 774	C 479	N 148	0 142	${ m S}{ m 5}$	0	0

• Molecule 51 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
51	1	82	Total 688	C 437	N 120	0 128	${ m S} { m 3}$	0	0

• Molecule 52 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues		Ato	\mathbf{ms}			AltConf	Trace
52	m	51	Total	С	N	0	S	0	0
			419	262	82	73	2		, in the second s

• Molecule 53 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
53	О	94	Total 798	C 501	N 165	0 129	${ m S} { m 3}$	0	0

• Molecule 54 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
54	р	147	Total 1205	C 748	N 228	0 225	$\frac{S}{4}$	0	0

• Molecule 55 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues		At	oms			AltConf	Trace
55	q	141	Total 1177	C 732	N 229	0 211	${ m S}{ m 5}$	0	0

• Molecule 56 is a protein called 39S ribosomal protein S18a, mitochondrial.



Mol	Chain	Residues		At	oms	AltConf	Trace		
56	r	162	Total 1322	C 839	N 252	O 223	S 8	0	0

• Molecule 57 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues		At		AltConf	Trace		
57	S	386	Total 3155	C 2023	N 559	O 559	S 14	0	0

• Molecule 58 is S-(2-{[N-(2-HYDROXY-4-{[HYDROXY(OXIDO)PHOSPHINO]OXY}-3,3-DIMETHYLBUTANOYL)-BETA-ALANYL]AMINO}ETHYL) DECANETHIOATE (three-letter code: PM8) (formula: $C_{21}H_{41}N_2O_7PS$).



Mol	Chain	Residues		Α	tom	IS			AltConf
59		1	Total	С	Ν	Ο	Р	S	0
00	W	1	32	21	2	7	1	1	0

• Molecule 59 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).





Mol	Chain	Residues	Atoms				AltConf	
59	х	1	Total 27	C 15	N 6	O 5	S 1	0

• Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
60	0	1	Total Zn 1 1	0
60	4	1	Total Zn 1 1	0

• Molecule 61 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
61	9	1	Total Mg 1 1	0
61	А	92	TotalMg9292	0
61	D	1	Total Mg 1 1	0
61	М	1	Total Mg 1 1	0
61	О	1	Total Mg 1 1	0
61	g	1	Total Mg 1 1	0



• Molecule 62 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
62	А	2	Total K 2 2	0

• Molecule 63 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	AltConf
63	r	1	TotalFeS422	0

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



3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123267	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor



4 Model quality (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

4.3.2 Protein sidechains (i)

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

4.3.3 RNA (i)

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

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

4 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 Type	Turne	Chain	Dec	Link	B	ond leng	\mathbf{gths}	Bond angles			
MOI	туре	Unain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
50	AYA	k	2	50	6,7,8	1.24	1 (16%)	5,8,10	1.32	1 (20%)	
24	SAC	K	2	24	7,8,9	1.02	0	8,9,11	0.81	0	
34	AYA	U	2	34	6,7,8	1.30	1 (16%)	5,8,10	1.22	1 (20%)	
41	THC	b	2	41	8,9,10	1.06	1 (12%)	9,11,13	0.71	0	



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	AYA	k	2	50	-	0/4/6/8	-
24	SAC	К	2	24	-	2/7/8/10	-
34	AYA	U	2	34	-	0/4/6/8	-
41	THC	b	2	41	-	0/8/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
34	U	2	AYA	CA-N	-2.57	1.43	1.46
50	k	2	AYA	CA-N	-2.27	1.44	1.46
41	b	2	THC	CA-N1	-2.15	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
50	k	2	AYA	CB-CA-N	2.71	112.63	109.61
34	U	2	AYA	CB-CA-N	2.58	112.48	109.61

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	Κ	2	SAC	N-CA-CB-OG
24	Κ	2	SAC	C-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 104 ligands modelled in this entry, 101 are monoatomic - leaving 3 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).

	Turne	Type Chain	Res	Jan Link	Bond lengths			Bond angles		
	туре	Unann			Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
59	SAM	х	401	-	24,29,29	1.21	3 (12%)	23,42,42	1.59	4 (17%)
58	PM8	W	200	3	25,31,31	0.22	0	30,38,38	0.43	0
63	FES	r	201	22,56	0,4,4	-	-	-		

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
59	SAM	х	401	-	-	5/12/33/33	0/3/3/3
58	PM8	W	200	3	-	14/36/38/38	-
63	FES	r	201	22,56	-	-	0/1/1/1

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
59	Х	401	SAM	C2-N3	4.01	1.38	1.32
59	Х	401	SAM	C2-N1	2.46	1.38	1.33
59	Х	401	SAM	OXT-C	-2.17	1.23	1.30

All (3) bond length outliers are listed below:

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
59	Х	401	SAM	N3-C2-N1	-5.45	120.16	128.68
59	Х	401	SAM	OXT-C-O	-2.84	117.63	124.09
59	Х	401	SAM	C3'-C2'-C1'	2.79	105.18	100.98
59	Х	401	SAM	OXT-C-CA	2.21	120.91	113.38

There are no chirality outliers.

All (19) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
58	W	200	PM8	O27-C28-C29-C32
58	W	200	PM8	C32-C34-N36-C37
58	W	200	PM8	O1-C1-S1-C43
58	W	200	PM8	C2-C1-S1-C43
59	Х	401	SAM	N-CA-CB-CG
59	Х	401	SAM	C-CA-CB-CG
59	Х	401	SAM	CB-CG-SD-C5'
58	W	200	PM8	C38-C39-N41-C42
58	W	200	PM8	O35-C34-N36-C37
58	W	200	PM8	O40-C39-N41-C42
58	W	200	PM8	O27-C28-C29-C30
58	W	200	PM8	O27-C28-C29-C31
58	W	200	PM8	O33-C32-C34-O35
59	Х	401	SAM	CB-CG-SD-CE
58	W	200	PM8	O33-C32-C34-N36
58	W	200	PM8	C42-C43-S1-C1
58	W	200	PM8	C31-C29-C32-C34
59	Х	401	SAM	OXT-C-CA-N
58	W	200	PM8	C28-C29-C32-C34

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
16	А	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3251:N	O3'	3252:N	Р	17.10
1	A	3236:N	O3'	3237:N	Р	13.81



5 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12845. 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.

5.1 Orthogonal projections (i)

This section was not generated.

5.2 Central slices (i)

This section was not generated.

5.3 Largest variance slices (i)

This section was not generated.

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

This section was not generated.

5.5 Orthogonal surface views (i)

This section was not generated.

5.6 Mask visualisation (i)

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



6 Map analysis (i)

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

6.1 Map-value distribution (i)

This section was not generated.

6.2 Volume estimate versus contour level (i)

This section was not generated.

6.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



7 Fourier-Shell correlation (i)

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



8 Map-model fit (i)

This section was not generated.

