



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 1, 2017 – 05:34 PM EDT

PDB ID : 5T62  
EMDB ID: : EMD-8362  
Title : Nmd3 is a structural mimic of eIF5A, and activates the cpGTPase Lsg1 during  
60S ribosome biogenesis: 60S-Nmd3-Tif6-Lsg1 Complex  
Authors : Malyutin, A.G.; Musalgaonkar, S.; Patchett, S.; Frank, J.; Johnson, A.W.  
Deposited on : unknown  
Resolution : 3.30 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

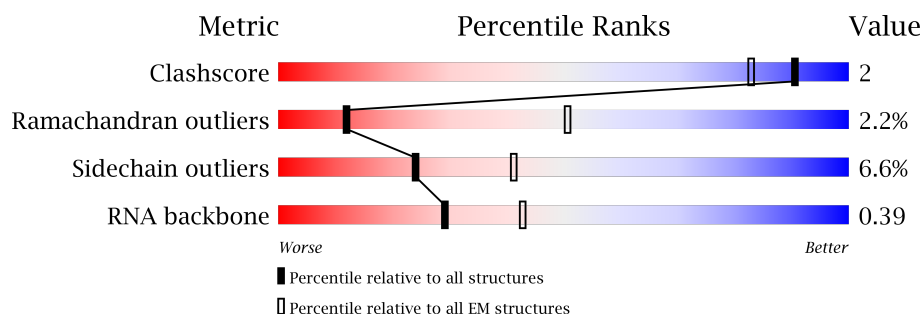
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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.











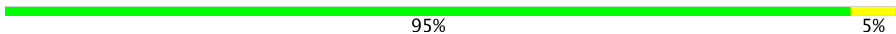
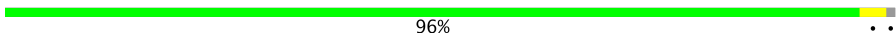
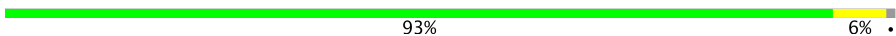
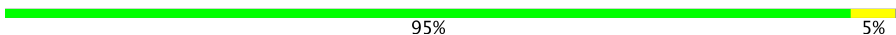




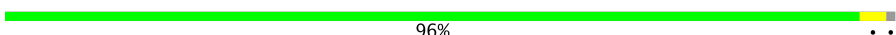



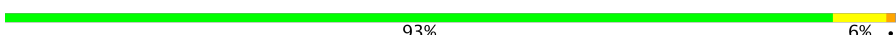




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	X	264	81% 15% .
2	A	3396	66% 26% 6% .
3	B	121	72% 26% .
4	C	158	73% 27% .
5	D	254	91% 8% .
6	E	387	90% 10%
7	F	362	89% 10% .
8	G	297	92% 7% .

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Mol	Chain	Length	Quality of chain
9	H	176	
10	I	244	
11	J	256	
12	K	191	
13	L	221	
14	M	174	
15	N	199	
16	O	138	
17	a	204	
18	b	199	
19	c	184	
20	d	186	
21	e	189	
22	f	172	
23	g	160	
24	h	121	
25	i	137	
26	j	155	
27	k	142	
28	l	127	
29	m	136	
30	n	149	
31	o	59	
32	p	105	
33	q	113	

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Mol	Chain	Length	Quality of chain
34	r	130	 91% 7% .
35	s	107	 91% 8% .
36	t	121	 86% 7% 7%
37	u	120	 90% 8% ..
38	v	100	 94% 5% .
39	w	88	 88% 11% .
40	x	78	 91% 8% .
41	y	51	 94% . .
42	z	128	 38% . 59%
43	Q	106	 86% 11% ..
44	R	92	 90% 9% .
45	S	217	 96% . .
46	V	524	 48% 13% 5% 33%
47	W	651	 34% 10% . 53%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PSU	A	2264	-	-	X	-
2	PSU	A	2266	-	-	X	-
50	GNP	W	701	-	-	X	-

## 2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 131766 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 Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	224	Total	C	N	O	S	0	0
			1633	1019	279	328	7		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-18	MET	-	initiating methionine	UNP Q12522
X	-17	GLY	-	expression tag	UNP Q12522
X	-16	SER	-	expression tag	UNP Q12522
X	-15	SER	-	expression tag	UNP Q12522
X	-14	HIS	-	expression tag	UNP Q12522
X	-13	HIS	-	expression tag	UNP Q12522
X	-12	HIS	-	expression tag	UNP Q12522
X	-11	HIS	-	expression tag	UNP Q12522
X	-10	HIS	-	expression tag	UNP Q12522
X	-9	HIS	-	expression tag	UNP Q12522
X	-8	SER	-	expression tag	UNP Q12522
X	-7	LEU	-	expression tag	UNP Q12522
X	-6	ARG	-	expression tag	UNP Q12522
X	-5	ARG	-	expression tag	UNP Q12522
X	-4	ALA	-	expression tag	UNP Q12522
X	-3	SER	-	expression tag	UNP Q12522
X	-2	LEU	-	expression tag	UNP Q12522
X	-1	GLY	-	expression tag	UNP Q12522
X	0	SER	-	expression tag	UNP Q12522

- Molecule 2 is a RNA chain called *Saccharomyces cerevisiae* S288c 35S pre-ribosomal RNA miscRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	3204	Total	C	N	O	P	0	0
			68535	30613	12358	22360	3204		

- Molecule 3 is a RNA chain called *Saccharomyces cerevisiae* strain HB\_C\_OMARUNUI\_6

chromosome XII sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 4 is a RNA chain called *Saccharomyces cerevisiae* culture-collection CBS:2888 large subunit ribosomal RNA gene, partial sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 5 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	252	Total	C	N	O	S	0	0
			1914	1191	388	334	1		

- Molecule 6 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 7 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 8 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 9 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 10 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 11 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 12 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 13 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	211	Total	C	N	O	S	0	0
			1705	1083	322	294	6		

- Molecule 14 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 15 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	N	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 16 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 17 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 18 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 19 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	c	183	Total	C	N	O	S	0	0
			1420	882	281	257			

- Molecule 20 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	d	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 21 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	e	188	Total	C	N	O	S	0	0
			1521	935	326	260			

- Molecule 22 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	f	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 23 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	g	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 24 is a protein called 60S ribosomal protein L22-A.



Mol	Chain	Residues	Atoms				AltConf	Trace
24	h	100	Total	C	N	O	0	0
			796	516	131	149		

- Molecule 25 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	i	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 26 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	j	98	Total	C	N	O	S	0	0
			699	443	137	118	1		

- Molecule 27 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	k	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 28 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	l	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 29 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	m	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 30 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	n	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 31 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	o	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 32 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	p	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 33 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	q	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 34 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	r	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 35 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	s	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 36 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	t	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 37 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	u	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 38 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	v	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 39 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	w	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 40 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	x	77	Total	C	N	O	S	0	0
			612	391	115	106			

- Molecule 41 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	y	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 42 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	z	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 43 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Q	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	R	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 45 is a protein called Ribosomal Protein uL1.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	S	210	Total	C	N	O	0	0
			1050	630	210	210		

- Molecule 46 is a protein called 60S ribosomal export protein NMD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	V	350	Total	C	N	O	S	0	0
			2713	1729	468	504	12		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	-5	HIS	-	expression tag	UNP P38861
V	-4	HIS	-	expression tag	UNP P38861
V	-3	HIS	-	expression tag	UNP P38861
V	-2	HIS	-	expression tag	UNP P38861
V	-1	HIS	-	expression tag	UNP P38861
V	0	HIS	-	expression tag	UNP P38861

- Molecule 47 is a protein called Large subunit GTPase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	W	306	Total	C	N	O	S	0	0
			2236	1432	390	409	5		

There are 77 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	135	UNK	ARG	see remark 999	UNP P53145
W	136	UNK	PRO	see remark 999	UNP P53145
W	137	UNK	GLU	see remark 999	UNP P53145
W	138	UNK	TRP	see remark 999	UNP P53145
W	139	UNK	ASN	see remark 999	UNP P53145
W	140	UNK	GLU	see remark 999	UNP P53145
W	141	UNK	GLY	see remark 999	UNP P53145
W	142	UNK	MET	see remark 999	UNP P53145
W	143	UNK	SER	see remark 999	UNP P53145
W	144	UNK	LYS	see remark 999	UNP P53145
W	145	UNK	PHE	see remark 999	UNP P53145
W	146	UNK	GLN	see remark 999	UNP P53145
W	147	UNK	LEU	see remark 999	UNP P53145
W	148	UNK	ASP	see remark 999	UNP P53145
W	149	UNK	ARG	see remark 999	UNP P53145

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Chain	Residue	Modelled	Actual	Comment	Reference
W	150	UNK	GLN	see remark 999	UNP P53145
W	151	UNK	GLU	see remark 999	UNP P53145
W	152	UNK	LYS	see remark 999	UNP P53145
W	153	UNK	GLU	see remark 999	UNP P53145
W	154	UNK	ALA	see remark 999	UNP P53145
W	155	UNK	PHE	see remark 999	UNP P53145
W	156	UNK	LEU	see remark 999	UNP P53145
W	157	UNK	GLU	see remark 999	UNP P53145
W	158	UNK	TRP	see remark 999	UNP P53145
W	159	UNK	ARG	see remark 999	UNP P53145
W	160	UNK	ARG	see remark 999	UNP P53145
W	161	UNK	LYS	see remark 999	UNP P53145
W	162	UNK	LEU	see remark 999	UNP P53145
W	163	UNK	ALA	see remark 999	UNP P53145
W	164	UNK	HIS	see remark 999	UNP P53145
W	165	UNK	LEU	see remark 999	UNP P53145
W	166	UNK	GLN	see remark 999	UNP P53145
W	167	UNK	GLU	see remark 999	UNP P53145
W	168	UNK	SER	see remark 999	UNP P53145
W	169	UNK	ASN	see remark 999	UNP P53145
W	170	UNK	GLU	see remark 999	UNP P53145
W	171	UNK	ASP	see remark 999	UNP P53145
W	172	UNK	LEU	see remark 999	UNP P53145
W	173	UNK	LEU	see remark 999	UNP P53145
W	174	UNK	LEU	see remark 999	UNP P53145
W	175	UNK	THR	see remark 999	UNP P53145
W	276	UNK	LEU	see remark 999	UNP P53145
W	277	UNK	GLU	see remark 999	UNP P53145
W	278	UNK	GLU	see remark 999	UNP P53145
W	279	UNK	LEU	see remark 999	UNP P53145
W	280	UNK	PHE	see remark 999	UNP P53145
W	281	UNK	LEU	see remark 999	UNP P53145
W	282	UNK	SER	see remark 999	UNP P53145
W	283	UNK	LYS	see remark 999	UNP P53145
W	284	UNK	ALA	see remark 999	UNP P53145
W	285	UNK	PRO	see remark 999	UNP P53145
W	286	UNK	ASN	see remark 999	UNP P53145
W	287	UNK	GLU	see remark 999	UNP P53145
W	288	UNK	PRO	see remark 999	UNP P53145
W	289	UNK	LEU	see remark 999	UNP P53145
W	290	UNK	LEU	see remark 999	UNP P53145
W	291	UNK	PRO	see remark 999	UNP P53145

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Chain	Residue	Modelled	Actual	Comment	Reference
W	292	UNK	PRO	see remark 999	UNP P53145
W	293	UNK	LEU	see remark 999	UNP P53145
W	294	UNK	PRO	see remark 999	UNP P53145
W	295	UNK	GLY	see remark 999	UNP P53145
W	296	UNK	GLN	see remark 999	UNP P53145
W	297	UNK	PRO	see remark 999	UNP P53145
W	298	UNK	PRO	see remark 999	UNP P53145
W	299	UNK	LEU	see remark 999	UNP P53145
W	504	UNK	HIS	see remark 999	UNP P53145
W	641	ALA	-	expression tag	UNP P53145
W	642	ALA	-	expression tag	UNP P53145
W	643	ALA	-	expression tag	UNP P53145
W	644	LEU	-	expression tag	UNP P53145
W	645	GLU	-	expression tag	UNP P53145
W	646	HIS	-	expression tag	UNP P53145
W	647	HIS	-	expression tag	UNP P53145
W	648	HIS	-	expression tag	UNP P53145
W	649	HIS	-	expression tag	UNP P53145
W	650	HIS	-	expression tag	UNP P53145
W	651	HIS	-	expression tag	UNP P53145

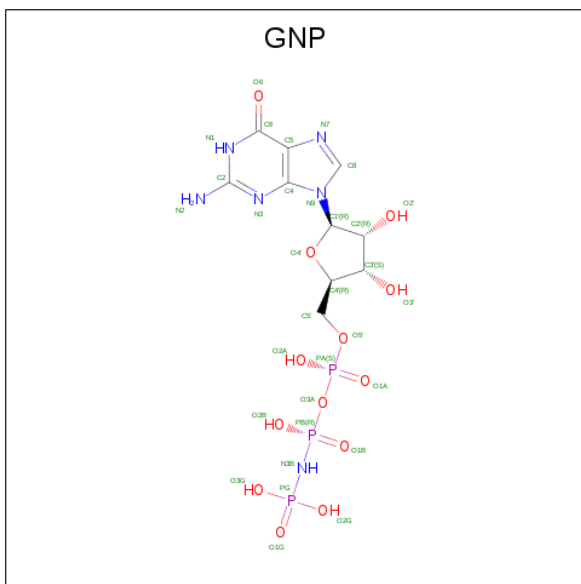
- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
48	D	1	Total Mg 1 1	0
48	B	5	Total Mg 5 5	0
48	i	1	Total Mg 1 1	0
48	C	2	Total Mg 2 2	0
48	a	1	Total Mg 1 1	0
48	c	1	Total Mg 1 1	0
48	W	1	Total Mg 1 1	0
48	A	148	Total Mg 148 148	0

- Molecule 49 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
49	A	2	Total K 2 2	0

- Molecule 50 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula:  $C_{10}H_{17}N_6O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
50	W	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 51 is water.

Mol	Chain	Residues	Atoms	AltConf
51	A	5	Total O 5 5	0
51	e	1	Total O 1 1	0



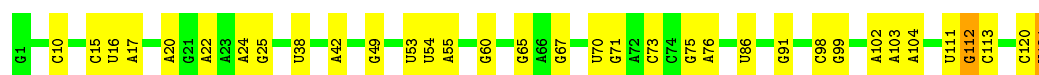


G2898	A2762	G2621	U2514	U2446	A2309	C2197	G1954	A1798	G1661	U1553	G1392	U1267	C1175
G2899	C2772	G2624	A2515	A2447	U2310	A2198	U1955	C1803	G1662	U1554	A1393	A1270	C1176
A2900	C2773	G2625	G2522	G2448	A2311	U2205	A	A1804	G1663	U1555	A1394	A1271	G1177
G2914	C2774	A2626	G2522	A2449	A2312	U2205	G	C1805	G1664	U1556	A1399	A1274	G1178
G2922	G2777	A2627	C2531	G2450	A2313	U2209	U	G1808	G1665	A1557	G1400	C1275	A1179
U2923	G2778	A2628	U2532	G2452	U2314	G2210	G	A	G1666	G1560	G1409	U1276	A1180
A2926	G2779	A2635	G2533	U2453	G2315	G2211	A	G1808	G1674	G1561	G1409	U1277	U1181
C2927	A2780	A2636	U2537	G2454	A2332	G2221	G	G1812	G1678	G1562	G1414	C1276	C1189
C2928	A2790	U2641	U2538	A2455	G2335	A2228	G	A1813	G1678	U1563	U1278	C1279	A1190
C2929	A2792	C2644	C2539	G2457	U2336	G2239	C	U1815	U1682	U1564	U1415	C1279	U1191
A2933	A2793	C2644	A2540	A2458	C2337	G2239	U	A1816	U1683	U1565	C1416	G1285	C1192
U2934	A2799	C2648	U2541	A2459	A2372	A2244	U	G1817	A1696	U1567	A1419	A1286	A1200
A2935	G2800	A2657	U2542	U2460	A2373	C2245	G	U1820	A1697	U1568	C1420	A1287	A1201
A2936	A2801	U2652	U2544	A2463	C2374	G2246	U	U1821	U1703	U1569	U1430	G1289	U1208
U2937	A2802	U2652	U2544	A2463	C2375	G2246	C	A1839	U1703	A1571	G1434	A1291	U1208
G2938	A2803	U2655	A2547	U2464	U2379	G2249	A	U1840	U1716	U1572	G1434	A1291	A1212
C2941	C2810	A2656	C2548	A2468	G2385	G2250	G	A1841	U1717	G1573	C1437	A1303	G1213
C2942	G2816	G2658	U2550	G2469	G2385	G2251	C	A1842	G1718	G1576	A1446	A1304	A1217
G2947	A2817	C2674	C2552	U2471	U2388	G2252	U	G1845	U1724	G1577	A1446	G1306	U1218
G2950	C2821	C2677	U2553	U2472	G2393	A2255	C	C1849	C1725	C1578	G1450	G1307	C1219
G2951	A2837	U2681	A2554	C2473	G2393	A2256	G	A1850	G1733	U1582	U1455	A1308	G1222
A2971	A2838	C2684	G2555	G2475	A2397	C2257	U	U1858	G1734	A1583	U1460	G1313	A1223
U2975	G2841	A2689	A2561	G2476	A2401	A2258	C	A1864	G1741	A1587	G1466	U1315	A1225
U2978	U2842	G2690	A2562	C2477	A2402	U2260	G	A1867	G1747	A1588	G1480	G1319	G1230
U2979	C2843	A2691	U2566	U2480	G2403	G2261	U	U1871	G1748	A1589	A1481	U1325	A1231
U2980	A2845	C2694	A2569	U2482	C2406	C2262	C	U1880	A1750	A1605	A1482	U1325	G1233
C2983	G2848	A2696	A2570	G2483	C2407	U2266	U	U1886	G1751	C1615	A1489	U1329	G1236
G2990	U2859	U2696	U2571	A2485	U2410	U2267	G	A1886	A1760	A1619	C1496	A1330	G1237
U2996	U2860	C2704	C2572	G2486	U2411	U2268	U	A1893	C1761	U1620	U1334	U1241	A1240
G2997	U2861	C2709	G2573	U2487	G2412	A2271	C	U1894	U1765	U1501	U1348	G1242	G1242
U2998	C2867	G2714	C2577	A2490	G2418	G2272	U	A1895	G1766	C1502	G1349	G1243	G1243
C3004	G2871	U2719	U2581	A2494	G2425	U2274	G	G1906	G1770	A1503	A1350	A1244	A1244
A3011	A2872	C2726	G2585	C2495	U2428	A2281	U	C1907	G1775	C1508	U1351	A1245	A1245
U3013	C2876	A2727	G2586	U2496	G2429	U2282	A	A1908	G1775	U1629	A1352	U1247	U1247
U3014	G2877	G2728	A2593	U2498	U2434	G2288	G	U1909	G1780	G1521	G1354	C1248	C1248
G3022	U2882	A2734	C2594	U2501	G2435	U2289	U	C1917	G1784	C1527	U1355	G1249	G1249
A3048	U2883	C2737	G2602	A2502	U2436	G2290	C	G1926	U1785	C1531	U1356	U1253	U1253
A3049	A2887	G2753	G2606	U2505	G2437	C2293	U	A1930	C1788	C1532	C1364	U1258	U1258
G3053	U2888	G2754	G2607	U2506	G2441	U2294	G	A1936	G1789	U1645	G1383	G1262	G1262
U3054	A2896	C2755	G2614	C2507	G2442	A2295	U	C1951	G1790	A1657	U1382	A1263	A1263
U3055	C2897	C2755	G2614	U2508	A2443	U2298	A	G1952	U1796	G1658	A1386	G1264	G1264
				U2513	A2445	C2307	G	G1963	A1797	C1660	G1547	U1265	U1265
						C2308	C						G1266



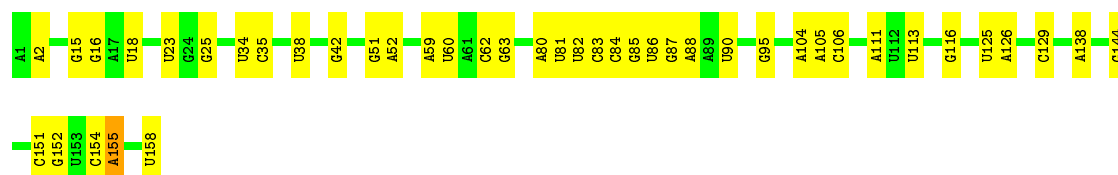
- Molecule 3: *Saccharomyces cerevisiae* strain HB\_C\_OMARUNUI\_6 chromosome XII sequence

Chain B: 72% 26%



- Molecule 4: *Saccharomyces cerevisiae* culture-collection CBS:2888 large subunit ribosomal RNA gene, partial sequence

Chain C: 73% 27%



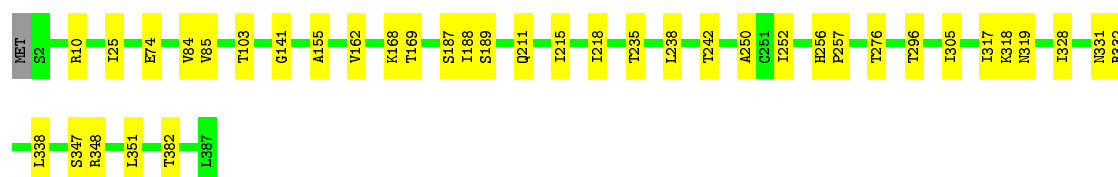
- Molecule 5: 60S ribosomal protein L2-A

Chain D: 91% 8%



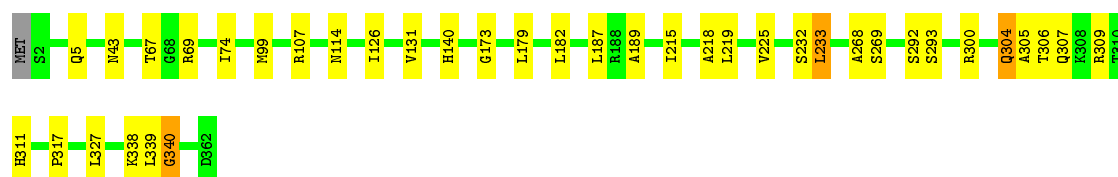
- Molecule 6: 60S ribosomal protein L3

Chain E: 90% 10%



- Molecule 7: 60S ribosomal protein L4-A

Chain F: 89% 10%



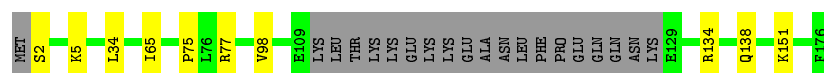
- Molecule 8: 60S ribosomal protein L5

Chain G: 92% 7%



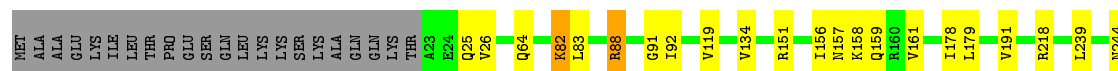
- Molecule 9: 60S ribosomal protein L6-A

Chain H: 83% 6% 11%



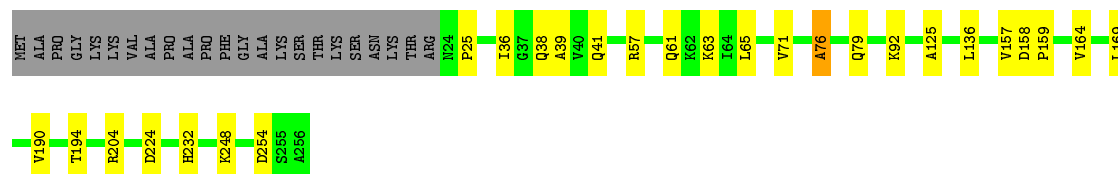
- Molecule 10: 60S ribosomal protein L7-A

Chain I: 82% 8% 9%



- Molecule 11: 60S ribosomal protein L8-A

Chain J: 80% 10% 9%



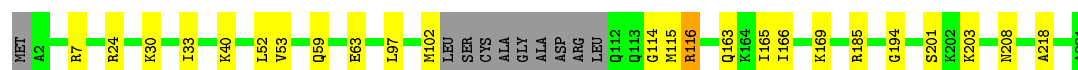
- Molecule 12: 60S ribosomal protein L9-A

Chain K: 88% 10% 2%




- Molecule 13: 60S ribosomal protein L10

Chain L: 85% 10% 5%




- Molecule 14: 60S ribosomal protein L11-A

Chain M:  90% 7% ..



- Molecule 15: 60S ribosomal protein L13-A

Chain N:  85% 11% ..



- Molecule 16: 60S ribosomal protein L14-A

Chain O:  88% 10% ..



- Molecule 17: 60S ribosomal protein L15-A

Chain a:  95% 5%



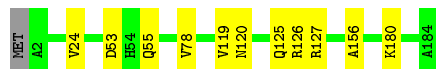
- Molecule 18: 60S ribosomal protein L16-A

Chain b:  96% ..



- Molecule 19: 60S ribosomal protein L17-A

Chain c:  93% 6% .



- Molecule 20: 60S ribosomal protein L18-A

Chain d:  95% 5%



- Molecule 21: 60S ribosomal protein L19-A

- Molecule 22: 60S ribosomal protein L20-A

- Molecule 23: 60S ribosomal protein L21-A


- Molecule 24: 60S ribosomal protein L22-A

- Molecule 25: 60S ribosomal protein L23-A

- Molecule 26: 60S ribosomal protein L24-A

- Molecule 27: 60S ribosomal protein L25

- Molecule 28: 60S ribosomal protein L26-A

Chain l:  93% 6% ..




- Molecule 29: 60S ribosomal protein L27-A

Chain m:  93% 6% ..




- Molecule 30: 60S ribosomal protein L28

Chain n:  88% 11% ..




- Molecule 31: 60S ribosomal protein L29

Chain o:  88% 8% ..




- Molecule 32: 60S ribosomal protein L30

Chain p:  90% 8% .



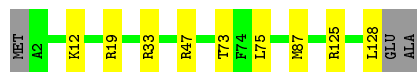
- Molecule 33: 60S ribosomal protein L31-A

Chain q:  89% 7% .



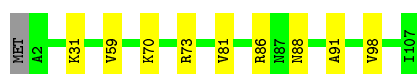
- Molecule 34: 60S ribosomal protein L32

Chain r:  91% 7% .



- Molecule 35: 60S ribosomal protein L33-A

Chain s:  91% 8% .



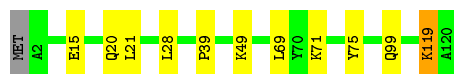
- Molecule 36: 60S ribosomal protein L34-A

Chain t: 86% 7% 7%



- Molecule 37: 60S ribosomal protein L35-A

Chain u: 90% 8% ..



- Molecule 38: 60S ribosomal protein L36-A

Chain v: 94% 5% .



- Molecule 39: 60S ribosomal protein L37-A

Chain w: 88% 11% .



- Molecule 40: 60S ribosomal protein L38

Chain x: 91% 8% .



- Molecule 41: 60S ribosomal protein L39

Chain y: 94% . .



- Molecule 42: Ubiquitin-60S ribosomal protein L40

Chain z: 38% . 59%







HIS	ASN	PHE	H440	T339	R246	GLY	ASN	ASN	TRP	ASN
HIS	ALA	ASP	K444	Y344	W249	ASN	LEU	LEU	VAL	TRP
HIS	GLU	ARG	P345	N346	Y252	ALA	LEU	LEU	VAL	LEU
HIS	ASP	PRO	N347	G348	I258	LYS	ARG	ARG	ARG	ARG
	ASP	THR	G349	S259	F260	GLN	THR	VAL	VAL	SER
	ARG	LYS	T353			ALA	GLN	THR	THR	THR
	ARG	GLU				LEU	LEU	GLN	GLN	GLU
	PHE	GLN	ASN			ALA	SER	SER	GLU	SER
	LYS	VAL	GLY			LYS	ALA	ALA	ALA	ALA
	GLN	GLN	D453	V362	L265	ASP	ASP	ASP	ASP	ASP
	ASN	ASN	I454	S363	ARG	LEU	LEU	LEU	LEU	LEU
	ALA	ALA	P455			ILE	ILE	ASP	ASP	ASP
	VAL	ALA	T456	S366		VAL	VAL	GLU	GLU	GLU
	GLU	LYS	A457			PRO	PRO	PHE	PHE	PHE
	GLY	ALA		G369		GLN	LEU	LEU	LEU	LEU
	ARG	LYS	L461	K370		LEU	LEU	LEU	SER	SER
	LEU	GLY		T371		GLU	GLU	THR	THR	THR
	SER	ILE	T472	K372		LYS	LYS	ALA	ALA	ALA
	THR	ASP	Q473	H373		GLN	GLN	GLN	GLN	GLN
	PRO	ILE				LYS	LYS	LYS	LYS	LYS
	PHE	VAL	S477	T376		GLU	GLU	GLU	GLU	GLU
	HIS	ASP	A478	I377		MET	MET	ASP	ASP	ASP
	LYS	LEU	D479	K378		GLY	GLY	LYS	LYS	LYS
	VAL	ALA	E480	L379		GLU	GLU	ASP	ASP	ASP
	GLN	ARG	P481	S380		ASP	ASP	PHE	PHE	PHE
	ASN	ASP	R482	D381		TYR	TYR	ALA	ALA	ALA
	SER	LEU				ARG	ARG	ASP	ASP	ASP
	SER	ASN	R485	N384		GLU	GLU	GLN	GLN	GLN
	ALA	GLN		L385		ASP	ASP	ASP	HIS	HIS
	GLY	LEU	L497	C386		PHE	PHE	LYS	LYS	LYS
	LYS	THR	Y498	D387		GLU	GLU	VAL	VAL	VAL
	ARG	PHE	V499	C388		GLU	GLU	VAL	VAL	VAL
	HIS	SER				ALA	ALA	ASP	ASP	ASP
	ASN	ALA	P502	F396		ASP	ASP	ILE	ILE	ILE
	LYS	HIS	P503	ALA		ASP	ASP	ILE	ILE	ILE
	LYS	THR	UNK	TYR		LYS	LYS	ARG	ARG	ARG
	ASN	GLY	LEU	ASN		GLU	GLU	GLY	GLY	GLY
	LYS	GLY		K400		GLY	GLY	GLY	MET	MET
	LYS	ASP	ASP			PHE	PHE	ASP	ASP	ASP
	LYS	THR	THR			ASP	ASP	GLY	GLY	GLY
	ASN	GLN	THR	C405		ALA	ALA	ASN	ASN	ASN
	ALA	LYS	PRO	M406		ASP	ASP	ASP	ASP	ASP
	LYS	GLU	TYR	G407		GLU	GLU	ASP	ASP	ASP
	SER	ALA	THR	V408		LYS	LYS	ASP	ASP	ASP
	LYS	LYS	ARG	L409		VAL	VAL	SER	SER	SER
	VAL	SER	GLU	Q413		MET	MET	ALA	ALA	ALA
	PHE	VAL	GLU			GLU	GLU	THR	THR	THR
	SER	THR	CYS	G422		LYS	LYS	SER	SER	SER
	ILE	HIS	GLU			VAL	VAL	GLN	GLN	GLN
	GLU	GLY	GLU	I428		ASP	ASP	GLY	GLY	GLY
	ASN	GLY	P429	K229		ARG	ARG	PHE	PHE	PHE
	ASN	LYS	K430	A230		LEU	LEU	SER	SER	SER
	ALA	GLN	Y431	M231		THR	THR	MET	MET	MET
	ALA	ALA	LYS			THR	THR	THR	THR	THR
	ALA	ALA	ASP	Y432		ILE	ILE	ASN	ASN	ASN
	ALA	ALA	LEU			ASP	ASP	GLN	GLN	GLN
	LEU	LEU	TYR	I436		GLN	GLN	GLU	GLU	GLU
	GLU	TYR	VAL	Y437		ARG	ARG	ARG	ARG	ARG

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT	Depositor
Number of particles used	226516, 19411	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30, FEI TITAN KRIOS	Depositor
Voltage (kV)	300, 300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40, 59.5	Depositor
Minimum defocus (nm)	1500, Not provided	Depositor
Maximum defocus (nm)	4000, Not provided	Depositor
Magnification	31000, Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, MG, GNP, PSU

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	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	X	0.40	0/1653	0.55	0/2255
10	I	0.43	0/1821	0.63	0/2451
11	J	0.41	0/1836	0.58	0/2481
12	K	0.40	0/1539	0.60	0/2073
13	L	0.41	0/1741	0.61	0/2335
14	M	0.41	0/1374	0.65	0/1842
15	N	0.44	0/1568	0.69	0/2106
16	O	0.38	0/1068	0.61	0/1438
17	a	0.43	0/1757	0.74	0/2354
18	b	0.42	0/1585	0.61	0/2128
19	c	0.40	0/1443	0.66	0/1944
2	A	0.28	0/76629	0.70	3/119475 (0.0%)
20	d	0.40	0/1465	0.72	0/1965
21	e	0.40	0/1538	0.67	0/2050
22	f	0.41	0/1481	0.64	0/1990
23	g	0.40	0/1300	0.62	0/1743
24	h	0.41	0/812	0.52	0/1099
25	i	0.40	0/1018	0.64	0/1369
26	j	0.41	0/712	0.59	0/958
27	k	0.39	0/979	0.59	0/1321
28	l	0.38	0/1004	0.64	0/1341
29	m	0.39	0/1118	0.56	0/1497
3	B	0.26	0/2883	0.68	0/4491
30	n	0.40	0/1204	0.67	0/1612
31	o	0.39	0/473	0.67	0/629
32	p	0.40	0/751	0.55	0/1008
33	q	0.39	0/890	0.64	0/1196
34	r	0.39	0/1041	0.67	0/1394
35	s	0.39	0/868	0.69	0/1168
36	t	0.40	0/890	0.71	0/1189
37	u	0.41	0/978	0.65	0/1301
38	v	0.42	0/778	0.62	0/1034

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	w	0.49	0/696	0.81	1/923 (0.1%)
4	C	0.29	0/3746	0.71	0/5832
40	x	0.40	0/618	0.57	0/826
41	y	0.41	0/443	0.73	0/588
42	z	0.39	0/423	0.64	0/562
43	Q	0.42	0/860	0.64	0/1136
44	R	0.45	0/701	0.71	0/934
46	V	0.41	0/2766	0.67	2/3759 (0.1%)
47	W	0.46	0/1950	0.68	1/2640 (0.0%)
5	D	0.41	0/1948	0.68	0/2617
6	E	0.42	0/3146	0.66	0/4228
7	F	0.39	0/2800	0.65	0/3790
8	G	0.41	0/2425	0.62	1/3271 (0.0%)
9	H	0.39	0/1260	0.59	0/1694
All	All	0.34	0/139979	0.68	8/206037 (0.0%)

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
11	J	0	1
30	n	0	1
31	o	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	V	143	CYS	C-N-CD	-10.95	96.51	120.60
47	W	369	GLY	N-CA-C	6.68	129.79	113.10
46	V	50	PRO	N-CA-CB	5.54	109.94	103.30
2	A	599	C	C2'-C3'-O3'	5.33	122.23	113.70
2	A	979	U	C2'-C3'-O3'	5.25	122.10	113.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	J	76	ALA	Peptide
30	n	46	ASP	Peptide
31	o	4	SER	Peptide

## 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	X	1633	0	1596	5	0
2	A	68535	0	34438	174	0
3	B	2579	0	1304	5	0
4	C	3353	0	1695	2	0
5	D	1914	0	1981	5	0
6	E	3075	0	3142	7	0
7	F	2748	0	2859	8	0
8	G	2375	0	2325	3	0
9	H	1239	0	1326	2	0
10	I	1784	0	1862	5	0
11	J	1804	0	1877	2	0
12	K	1518	0	1587	6	0
13	L	1705	0	1736	2	0
14	M	1353	0	1383	1	0
15	N	1543	0	1608	5	0
16	O	1053	0	1149	2	0
17	a	1720	0	1779	0	0
18	b	1555	0	1659	0	0
19	c	1420	0	1437	0	0
20	d	1441	0	1543	0	0
21	e	1521	0	1617	0	0
22	f	1445	0	1487	0	0
23	g	1276	0	1323	0	0
24	h	796	0	812	0	0
25	i	1003	0	1048	0	0
26	j	699	0	640	0	0
27	k	964	0	1025	0	0
28	l	993	0	1081	0	0
29	m	1092	0	1155	0	0
30	n	1173	0	1215	0	0
31	o	462	0	491	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	p	743	0	797	0	0
33	q	876	0	912	0	0
34	r	1020	0	1090	0	0
35	s	850	0	880	0	0
36	t	880	0	945	0	0
37	u	969	0	1078	0	0
38	v	771	0	849	0	0
39	w	681	0	685	0	0
40	x	612	0	682	0	0
41	y	436	0	475	0	0
42	z	417	0	459	0	0
43	Q	847	0	918	4	0
44	R	694	0	738	2	0
45	S	1050	0	246	1	0
46	V	2713	0	2644	70	0
47	W	2236	0	2029	67	0
48	A	148	0	0	0	0
48	B	5	0	0	0	0
48	C	2	0	0	0	0
48	D	1	0	0	0	0
48	W	1	0	0	0	0
48	a	1	0	0	0	0
48	c	1	0	0	0	0
48	i	1	0	0	0	0
49	A	2	0	0	0	0
50	W	32	0	13	12	0
51	A	5	0	0	0	0
51	e	1	0	0	0	0
All	All	131766	0	95620	356	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 2.

The worst 5 of 356 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)
2:A:2410:U:O4	2:A:2801:A:N1	1.61	1.33
47:W:349:LYS:HG2	50:W:701:GNP:O2B	1.32	1.30
2:A:2264:PSU:O2'	2:A:2265:C:H6	0.96	1.28
2:A:2252:A:N6	2:A:2264:PSU:O2	1.69	1.24
46:V:388:ASN:O	46:V:390:ASP:N	1.73	1.20

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	Percentiles	
1	X	222/264 (84%)	202 (91%)	20 (9%)	0	100	100
5	D	250/254 (98%)	226 (90%)	22 (9%)	2 (1%)	22	57
6	E	384/387 (99%)	346 (90%)	31 (8%)	7 (2%)	10	42
7	F	359/362 (99%)	311 (87%)	32 (9%)	16 (4%)	3	20
8	G	294/297 (99%)	265 (90%)	25 (8%)	4 (1%)	13	46
9	H	152/176 (86%)	133 (88%)	16 (10%)	3 (2%)	9	39
10	I	220/244 (90%)	200 (91%)	14 (6%)	6 (3%)	6	32
11	J	231/256 (90%)	207 (90%)	17 (7%)	7 (3%)	5	30
12	K	189/191 (99%)	169 (89%)	17 (9%)	3 (2%)	11	43
13	L	207/221 (94%)	186 (90%)	16 (8%)	5 (2%)	7	35
14	M	167/174 (96%)	143 (86%)	19 (11%)	5 (3%)	5	30
15	N	191/199 (96%)	168 (88%)	18 (9%)	5 (3%)	6	33
16	O	134/138 (97%)	119 (89%)	10 (8%)	5 (4%)	4	25
17	a	201/204 (98%)	188 (94%)	11 (6%)	2 (1%)	18	53
18	b	195/199 (98%)	184 (94%)	11 (6%)	0	100	100
19	c	181/184 (98%)	163 (90%)	17 (9%)	1 (1%)	28	63
20	d	183/186 (98%)	162 (88%)	18 (10%)	3 (2%)	11	43
21	e	186/189 (98%)	173 (93%)	9 (5%)	4 (2%)	8	37
22	f	170/172 (99%)	156 (92%)	11 (6%)	3 (2%)	10	42
23	g	157/160 (98%)	141 (90%)	13 (8%)	3 (2%)	9	41
24	h	98/121 (81%)	79 (81%)	17 (17%)	2 (2%)	9	39
25	i	134/137 (98%)	124 (92%)	9 (7%)	1 (1%)	25	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	j	96/155 (62%)	81 (84%)	12 (12%)	3 (3%)	5	30
27	k	119/142 (84%)	107 (90%)	11 (9%)	1 (1%)	22	57
28	l	124/127 (98%)	115 (93%)	7 (6%)	2 (2%)	11	43
29	m	133/136 (98%)	111 (84%)	18 (14%)	4 (3%)	5	30
30	n	146/149 (98%)	126 (86%)	13 (9%)	7 (5%)	2	18
31	o	56/59 (95%)	48 (86%)	5 (9%)	3 (5%)	2	15
32	p	95/105 (90%)	88 (93%)	7 (7%)	0	100	100
33	q	107/113 (95%)	98 (92%)	6 (6%)	3 (3%)	6	32
34	r	125/130 (96%)	121 (97%)	3 (2%)	1 (1%)	22	57
35	s	104/107 (97%)	95 (91%)	7 (7%)	2 (2%)	9	41
36	t	110/121 (91%)	102 (93%)	6 (6%)	2 (2%)	10	42
37	u	117/120 (98%)	109 (93%)	4 (3%)	4 (3%)	4	27
38	v	97/100 (97%)	88 (91%)	8 (8%)	1 (1%)	18	53
39	w	85/88 (97%)	77 (91%)	6 (7%)	2 (2%)	7	35
40	x	75/78 (96%)	67 (89%)	5 (7%)	3 (4%)	3	23
41	y	48/51 (94%)	44 (92%)	3 (6%)	1 (2%)	8	38
42	z	50/128 (39%)	47 (94%)	2 (4%)	1 (2%)	9	39
43	Q	103/106 (97%)	88 (85%)	10 (10%)	5 (5%)	2	18
44	R	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
46	V	344/524 (66%)	302 (88%)	27 (8%)	15 (4%)	3	20
47	W	231/651 (36%)	198 (86%)	25 (11%)	8 (4%)	4	26
All	All	6959/7997 (87%)	6240 (90%)	564 (8%)	155 (2%)	12	37

5 of 155 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	E	351	LEU
10	I	159	GLN
11	J	157	VAL
15	N	47	ALA
17	a	184	LYS



### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain 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	Percentiles	
1	X	177/227 (78%)	175 (99%)	2 (1%)	78	88
5	D	193/196 (98%)	181 (94%)	12 (6%)	21	56
6	E	320/323 (99%)	300 (94%)	20 (6%)	21	56
7	F	288/289 (100%)	276 (96%)	12 (4%)	34	69
8	G	244/245 (100%)	231 (95%)	13 (5%)	26	62
9	H	134/153 (88%)	130 (97%)	4 (3%)	46	75
10	I	186/205 (91%)	177 (95%)	9 (5%)	30	65
11	J	187/208 (90%)	171 (91%)	16 (9%)	12	42
12	K	171/171 (100%)	157 (92%)	14 (8%)	13	44
13	L	177/187 (95%)	161 (91%)	16 (9%)	11	39
14	M	147/150 (98%)	139 (95%)	8 (5%)	26	62
15	N	154/159 (97%)	141 (92%)	13 (8%)	13	43
16	O	107/109 (98%)	100 (94%)	7 (6%)	20	55
17	a	175/176 (99%)	167 (95%)	8 (5%)	31	67
18	b	160/162 (99%)	154 (96%)	6 (4%)	38	70
19	c	140/146 (96%)	130 (93%)	10 (7%)	17	51
20	d	150/151 (99%)	144 (96%)	6 (4%)	36	70
21	e	153/154 (99%)	146 (95%)	7 (5%)	31	67
22	f	156/156 (100%)	145 (93%)	11 (7%)	17	51
23	g	136/137 (99%)	125 (92%)	11 (8%)	14	44
24	h	87/107 (81%)	85 (98%)	2 (2%)	56	79
25	i	104/105 (99%)	101 (97%)	3 (3%)	48	75
26	j	57/129 (44%)	57 (100%)	0	100	100
27	k	104/118 (88%)	96 (92%)	8 (8%)	15	47
28	l	109/110 (99%)	102 (94%)	7 (6%)	20	55
29	m	115/116 (99%)	109 (95%)	6 (5%)	27	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	n	118/119 (99%)	108 (92%)	10 (8%)	12	42
31	o	46/47 (98%)	43 (94%)	3 (6%)	20	55
32	p	81/88 (92%)	78 (96%)	3 (4%)	39	71
33	q	92/97 (95%)	87 (95%)	5 (5%)	26	62
34	r	109/111 (98%)	101 (93%)	8 (7%)	16	49
35	s	90/91 (99%)	83 (92%)	7 (8%)	15	46
36	t	95/103 (92%)	89 (94%)	6 (6%)	21	56
37	u	104/105 (99%)	96 (92%)	8 (8%)	15	47
38	v	81/82 (99%)	77 (95%)	4 (5%)	29	65
39	w	70/71 (99%)	63 (90%)	7 (10%)	9	33
40	x	68/69 (99%)	65 (96%)	3 (4%)	33	67
41	y	45/46 (98%)	44 (98%)	1 (2%)	57	80
42	z	47/116 (40%)	44 (94%)	3 (6%)	20	55
43	Q	90/91 (99%)	85 (94%)	5 (6%)	25	60
44	R	71/72 (99%)	67 (94%)	4 (6%)	25	60
46	V	291/473 (62%)	254 (87%)	37 (13%)	5	23
47	W	209/502 (42%)	171 (82%)	38 (18%)	2	9
All	All	5838/6672 (88%)	5455 (93%)	383 (7%)	24	54

5 of 383 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	d	135	GLN
27	k	133	LEU
47	W	214	ARG
21	e	36	ASN
23	g	12	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
15	N	137	GLN
20	d	9	GLN
47	W	442	GLN
19	c	120	ASN

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Mol	Chain	Res	Type
20	d	73	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	3201/3396 (94%)	839 (26%)	100 (3%)
3	B	120/121 (99%)	25 (20%)	3 (2%)
4	C	157/158 (99%)	39 (24%)	3 (1%)
All	All	3478/3675 (94%)	903 (25%)	106 (3%)

5 of 903 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	16	A
2	A	22	G
2	A	26	A
2	A	31	C
2	A	40	A

5 of 106 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	2157	G
2	A	2434	U
2	A	3350	C
2	A	2209	U
2	A	2269	U

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

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	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PSU	A	2258	2	16,21,22	1.58	2 (12%)	20,30,33	3.76	7 (35%)
2	PSU	A	2260	2	16,21,22	1.43	1 (6%)	20,30,33	3.43	6 (30%)
2	PSU	A	2264	2	16,21,22	1.47	1 (6%)	20,30,33	3.58	8 (40%)
2	PSU	A	2266	2	16,21,22	1.56	2 (12%)	20,30,33	3.85	8 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	A	2258	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2260	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2264	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2266	2	-	0/7/25/26	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2258	PSU	C5-C1'	-4.96	1.47	1.52
2	A	2266	PSU	C5-C1'	-4.96	1.47	1.52
2	A	2264	PSU	C5-C1'	-4.73	1.48	1.52
2	A	2260	PSU	C5-C1'	-4.42	1.48	1.52
2	A	2258	PSU	C2'-C1'	-2.48	1.51	1.53

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2264	PSU	N1-C2-N3	-9.04	121.90	128.40
2	A	2266	PSU	N1-C2-N3	-9.03	121.91	128.40
2	A	2258	PSU	N1-C2-N3	-8.92	121.98	128.40
2	A	2260	PSU	N1-C2-N3	-8.91	121.99	128.40
2	A	2266	PSU	C5-C4-N3	-8.68	118.31	125.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2258	PSU	6	0
2	A	2264	PSU	18	0
2	A	2266	PSU	8	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 163 ligands modelled in this entry, 162 are monoatomic - leaving 1 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
50	GNP	W	701	48	27,34,34	2.65	6 (22%)	26,54,54	1.26	2 (7%)

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	GNP	W	701	48	-	0/16/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	W	701	GNP	C4-N9	-10.21	1.34	1.47
50	W	701	GNP	C8-N9	-3.92	1.34	1.46
50	W	701	GNP	C5-C6	-2.39	1.48	1.53
50	W	701	GNP	C2-N1	-2.26	1.34	1.44
50	W	701	GNP	PB-N3B	4.40	1.75	1.63

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	W	701	GNP	PA-O3A-PB	-3.57	119.78	132.38
50	W	701	GNP	O1B-PB-N3B	-2.19	108.52	111.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	W	701	GNP	12	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
47	W	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	175:UNK	C	180:PRO	N	16.95
1	W	299:UNK	C	337:ILE	N	5.51