



wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 02:47 PM UTC

PDB ID : 5T62 / pdb_00005t62
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 : 2016-09-01
Resolution : 3.10 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis	: FAILED
Mogul	: 2022.3.0, CSD as543be (2022)
MolProbity	: 4-5-2 with Phenix2.0
Buster-report	: wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	: NOT EXECUTED
MapQ	: FAILED
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.49

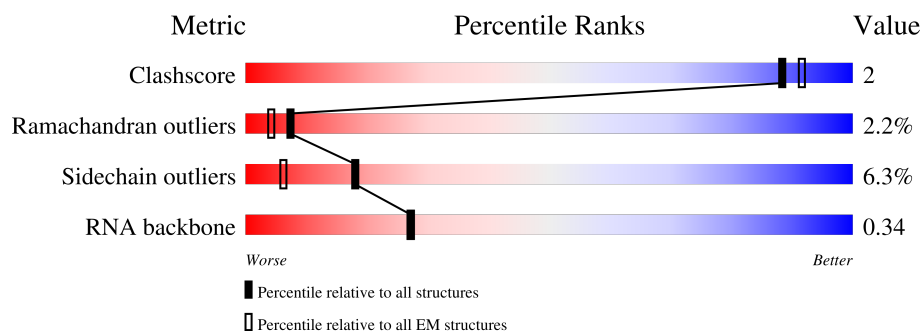
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.



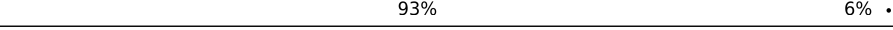
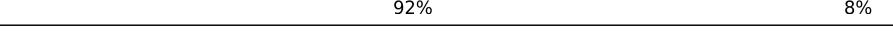
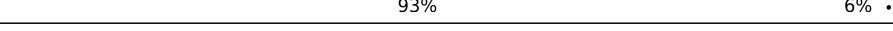
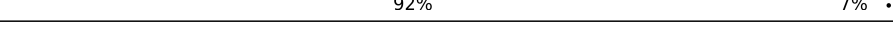
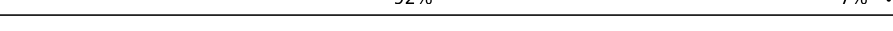
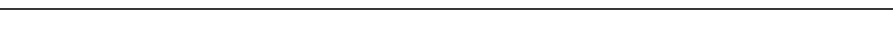
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	X	264	81% 15% . .
2	A	3396	65% 26% . 6%
3	B	121	71% 27% .
4	C	158	73% 25% .
5	D	254	92% 7% .
6	E	387	88% 11%
7	F	362	90% 10% .

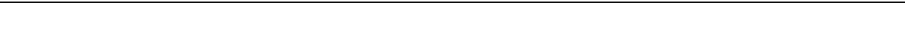
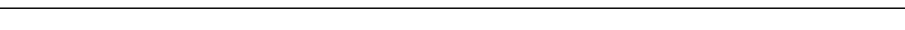
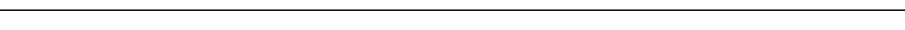
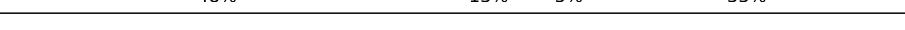
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Mol	Chain	Length	Quality of chain
8	G	297	 92% 8%
9	H	176	 83% 5% 11%
10	I	244	 82% 7% 9%
11	J	256	 80% 10% 9%
12	K	191	 89% 9% ..
13	L	221	 85% 10% 5%
14	M	174	 90% 7% ..
15	N	199	 84% 12% ..
16	O	138	 89% 8% ..
17	a	204	 91% 7% .
18	b	199	 93% 6% .
19	c	184	 92% 8% .
20	d	186	 93% 6% ..
21	e	189	 92% 7% ..
22	f	172	 88% 12%
23	g	160	 89% 10% ..
24	h	121	 80% . 17%
25	i	137	 92% 7% .
26	j	155	 61% .. 37%
27	k	142	 75% 10% . 15%
28	l	127	 92% 5% ..
29	m	136	 90% 8% ..
30	n	149	 83% 15% ..
31	o	59	 85% 10% ..
32	p	105	 88% 5% 8%

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Mol	Chain	Length	Quality of chain
33	q	113	 86% 10% . .
34	r	130	 89% 7% . .
35	s	107	 89% 7% . .
36	t	121	 83% 9% 7%
37	u	120	 88% 10% . .
38	v	100	 91% 8% .
39	w	88	 81% 17% . .
40	x	78	 94% 5% .
41	y	51	 90% 8% .
42	z	128	 37% . 59%
43	Q	106	 87% 11% . .
44	R	92	 88% 11% .
45	S	217	 96% . .
46	V	524	 48% 13% 5% . 33%
47	W	651	 33% 11% . 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 TPA_inf: Saccharomyces cerevisiae S288C chromosome XII, complete sequence.

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 5S Ribosomal RNA.

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 5.8S Ribosomal RNA.

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	conflict	UNP P53145
W	136	UNK	PRO	conflict	UNP P53145
W	137	UNK	GLU	conflict	UNP P53145
W	138	UNK	TRP	conflict	UNP P53145
W	139	UNK	ASN	conflict	UNP P53145
W	140	UNK	GLU	conflict	UNP P53145
W	141	UNK	GLY	conflict	UNP P53145
W	142	UNK	MET	conflict	UNP P53145
W	143	UNK	SER	conflict	UNP P53145
W	144	UNK	LYS	conflict	UNP P53145
W	145	UNK	PHE	conflict	UNP P53145
W	146	UNK	GLN	conflict	UNP P53145
W	147	UNK	LEU	conflict	UNP P53145
W	148	UNK	ASP	conflict	UNP P53145
W	149	UNK	ARG	conflict	UNP P53145

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

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Chain	Residue	Modelled	Actual	Comment	Reference
W	292	UNK	PRO	conflict	UNP P53145
W	293	UNK	LEU	conflict	UNP P53145
W	294	UNK	PRO	conflict	UNP P53145
W	295	UNK	GLY	conflict	UNP P53145
W	296	UNK	GLN	conflict	UNP P53145
W	297	UNK	PRO	conflict	UNP P53145
W	298	UNK	PRO	conflict	UNP P53145
W	299	UNK	LEU	conflict	UNP P53145
W	504	UNK	HIS	conflict	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

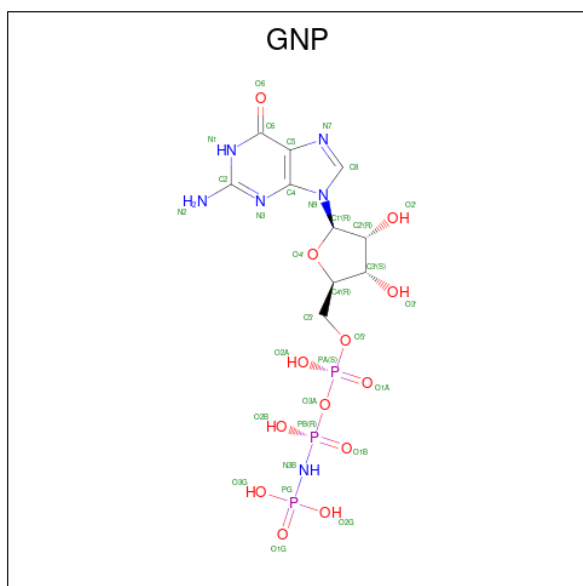
- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 49 is POTASSIUM ION (CCD ID: K) (formula: K).

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

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

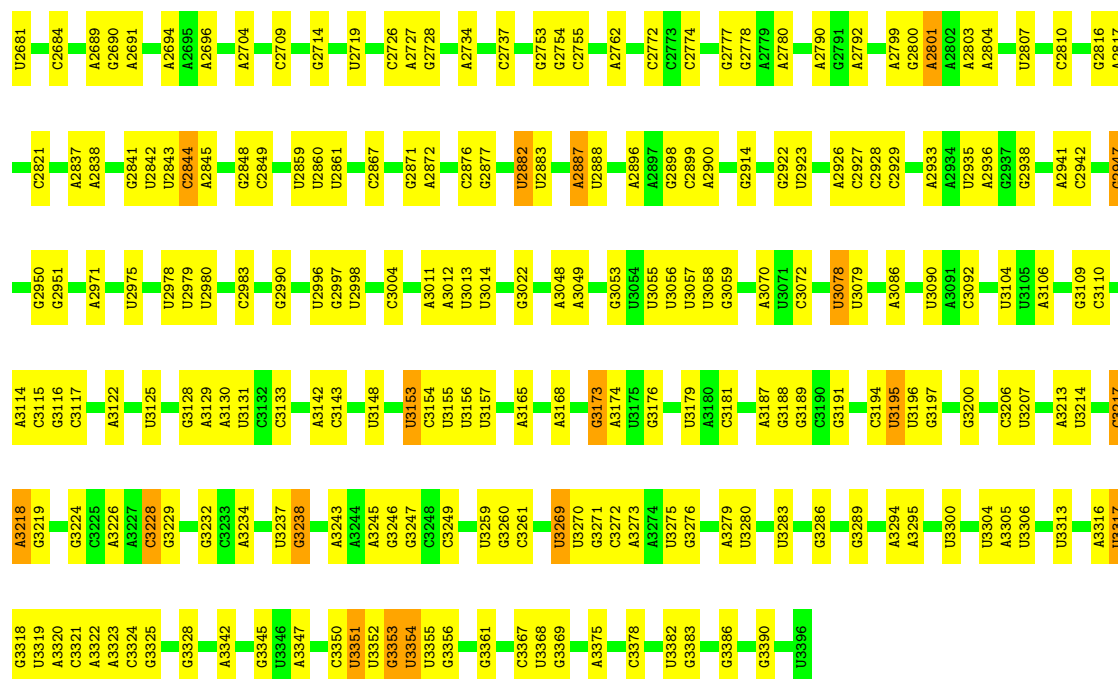


Mol	Chain	Residues	Atoms					AltConf
50	W	1	Total	C	N	O	P	0
			32	10	6	13	3	

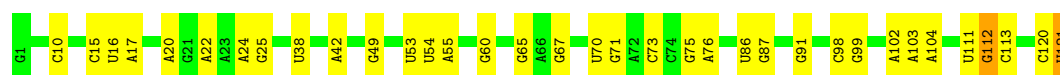
- Molecule 51 is water.

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

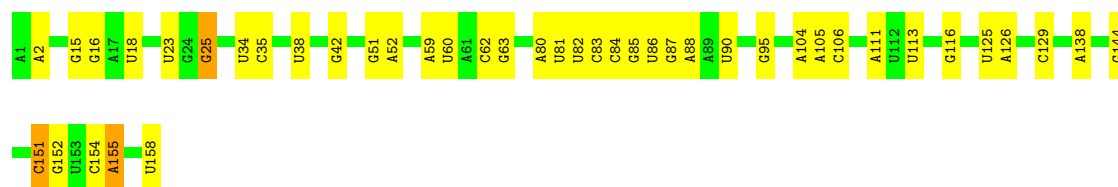
A2561	C2476	G2401	G2261	C2118	A1867	G1747	A1605	A1482	U1329	G1236	U1122	A1009
A2562	C2477	A2402	A2262	G2121	U1871	G1748	A1606	G1483	A1330	G1237	U1123	G1010
G2563	C2478	G2403	U2264	A	U	A1749	C1615	A1489	U1334	U1240	U1124	G1013
G2564	C2479	A2404	C2265	U	U1880	A1750	C1616	A1490	U1348	U1241	A1129	U1014
U2565	A2405	C2406	U2266	G	U	G1751	A1619	G1496	U1352	U1242	A1130	U1015
C2566	C2407	C2407	C2267	U	U1886	A1760	U1620	U1501	U1353	U1243	A1131	G1016
U2569	G2484	U2410	U2268	C	U	C1761	G1623	C1502	U1354	U1244	G1140	C1017
U2571	A2485	A2270	A2270	U	A1893	U1765	U1627	A1503	A1350	U1245	A1141	G1018
C2572	U2411	A2271	A2143	C	U1894	G1766	C1628	A1503	A1352	U1246	G1142	G1019
G2573	G2412	G2272	A2144	U	A1895	U1770	U1629	G1508	U1353	U1247	G1145	G1024
G2574	U2487	G2273	A2145	G	G1906	G1770	U1630	G1521	G1352	U1248	A1025	A1026
G2575	G2418	U2274	U	C	C1907	U1775	U1631	G1522	A1355	U1249	A1153	
G2576	A2419	G2281	A2157	U	A1908	U1776	A1632	C1527	U1356	U1253	G1157	G1029
C2577	G2425	U2282	A2158	U	A1909	G1780	U1633	C1527	G1357	U1258	A1030	C1031
U2581	U2428	G2283	U2159	G	C1917	U1785	C1639	G1531	C1364	C1257	A1159	G1035
G2585	G2429	U2288	C2163	U	U	U1786	A1642	C1532	U1383	A1262	A1169	A1036
G2586	U2434	C2290	G2169	G	C1926	C1788	A1643	U1533	A1386	A1263	C1175	C1037
A2593	G2435	C2293	G2185	U	A1930	G1789	U1645	G1536	C1391	U1265	G1176	U1040
C2594	U2436	U2294	U2186	G	U	G1790	U1645	A1537	G1392	G1266	G1177	U1041
G2602	G2437	A2295	G2187	U	A1936	U1795	C1657	G1547	A1393	U1267	G1178	A1047
U2505	G2440	U2298	U2191	U	C1951	G1796	G1658	U1553	G1409	C1275	A1189	U1051
U2506	A2441	C2307	C2192	C	G1952	A1797	U1659	U1554	G1414	U1276	U1191	A1057
C2507	G2442	C2308	G2196	A	U1953	G1798	C1660	A1555	G1415	C1277	A1192	G1063
U2508	A2443	C2310	C2197	C	G1954	U1803	G1661	C1556	C1416	C1278	A1193	A1064
U2513	U2444	U2311	C2198	U	U1955	A1804	C1662	A1557	U1427	C1279	A1195	A1065
U2514	U2446	A2312	A2198	G	A	C1805	G1664	U1563	U1430	A1285	C1196	U1069
A2515	G2447	G2313	U2205	U	U	C1806	C1665	U1564	C1420	A1286	U1200	U1070
G2522	A2448	A2314	U2209	G	U	G1808	G1666	U1567	U1427	U1287	C1201	G1072
C2531	G2450	G2315	G2210	U	U	U1812	G1674	U1568	U1430	A1288	U1208	U1081
U2532	G2451	U2316	G2221	C	U	A1813	G1678	G1565	G1434	A1289	A1212	A1083
G2533	U2452	C2332	A2228	G	U	A1814	U1682	U1566	C1437	A1286	G1213	U1094
U2537	U2453	U2336	G2229	U	C	U1815	A1683	U1567	U1446	U1287	A1217	U1095
C2538	G2454	C2337	G2239	C	U	A1816	U1683	U1568	A1446	G1306	U1218	U1096
U2539	A2456	G2355	A2244	U	U	G1817	A1696	U1569	G1450	G1307	C1219	G1097
C2541	U2457	C2355	C2245	G	U	U1820	A1697	A1570	G1450	A1308	A1098	A1098
U2542	A2458	A2372	G2246	C	U	U1821	U1703	U1572	G1434	U1309	G1222	A1099
U2543	U2460	A2374	G2246	A	U	A1839	G1576	G1573	C1437	A1303	A1223	U1100
U2544	A2461	C2374	G2246	G	U	U1840	U1716	U1573	U1455	A1304	G1224	G1101
U2544	G2462	G2375	G2249	C	U	A1841	U1717	C1577	U1455	G1306	A1225	A1102
A2547	G2463	U2379	G2251	G	C	A1842	G1718	C1578	G1450	G1307	A1231	A1103
C2548	U2464	U2379	G2252	U	U	G1845	U1724	C1579	G1450	A1308	G1230	G1104
G2549	A2468	C2253	A2252	G	C	U1845	C1725	C1582	U1455	U1309	A1232	G1117
U2550	G2469	U2254	G2253	C	A	C1849	G1733	A1582	U1455	G1313	G1232	
U2551	C2470	A2255	U2102	U	U	A1850	G1733	A1583	A1460	G1314	A1233	
U2552	U2471	A2256	G2111	U	C	A1858	G1735	A1587	A1460	U1315	A1233	
U2553	U2472	C2257	U2112	G	G	A1864	A1741	A1588	G1466	G1319	G1233	
G2554	G2473	U2258	A2113	U	U	U1864		A1589	G1480	G1319	G1233	
G2555	G2474	C2259	C2114	U	C			A1599	A1481	U1325	G1233	
	G2475	U2260		G	G			U1599				



• Molecule 3: 5S Ribosomal RNA



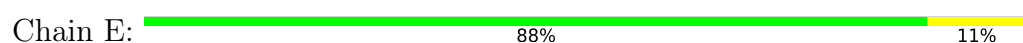
• Molecule 4: 5.8S Ribosomal RNA



• Molecule 5: 60S ribosomal protein L2-A



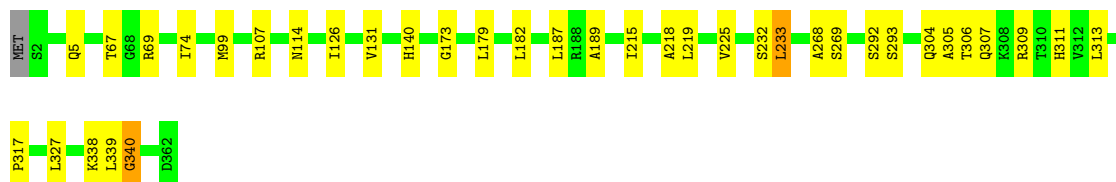
• Molecule 6: 60S ribosomal protein L3





- Molecule 7: 60S ribosomal protein L4-A

Chain F: 90% 10%



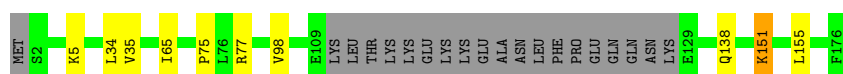
- Molecule 8: 60S ribosomal protein L5

Chain G: 92% 8%



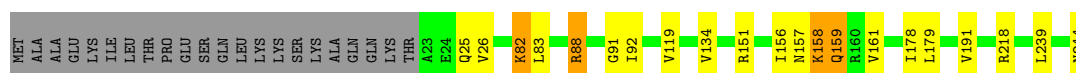
- Molecule 9: 60S ribosomal protein L6-A

Chain H: 83% 5% 11%



- Molecule 10: 60S ribosomal protein L7-A

Chain I: 82% 7% 9%



- Molecule 11: 60S ribosomal protein L8-A

Chain J: 80% 10% 9%



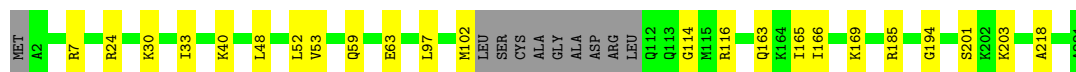
- Molecule 12: 60S ribosomal protein L9-A

Chain K: 89% 9%



- 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: 84% 12% ..



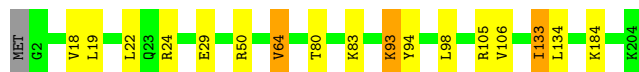
- Molecule 16: 60S ribosomal protein L14-A

Chain O: 89% 8% ..



- Molecule 17: 60S ribosomal protein L15-A

Chain a: 91% 7% .



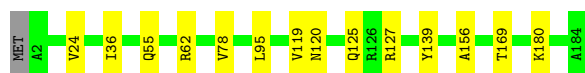
- Molecule 18: 60S ribosomal protein L16-A

Chain b: 93% 6% .



- Molecule 19: 60S ribosomal protein L17-A

Chain c: 92% 8% .



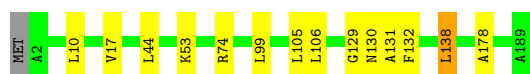
- Molecule 20: 60S ribosomal protein L18-A

Chain d: 93% 6% ..



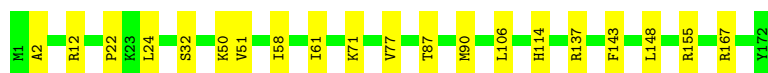
- Molecule 21: 60S ribosomal protein L19-A

Chain e: 92% 7% ..



- Molecule 22: 60S ribosomal protein L20-A

Chain f: 88% 12%



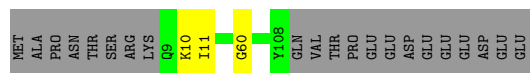
- Molecule 23: 60S ribosomal protein L21-A

Chain g: 89% 10% ..



- Molecule 24: 60S ribosomal protein L22-A

Chain h: 80% 17%



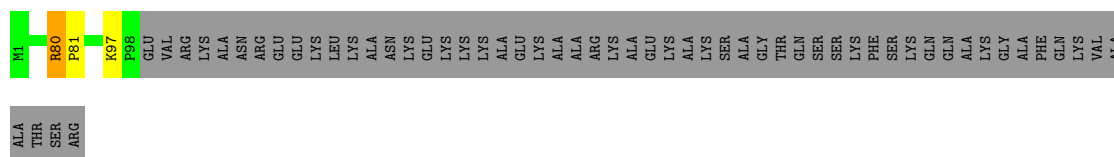
- Molecule 25: 60S ribosomal protein L23-A

Chain i: 92% 7% .



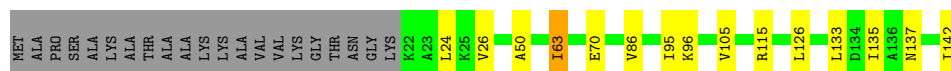
- Molecule 26: 60S ribosomal protein L24-A

Chain j: 61% .. 37%



- Molecule 27: 60S ribosomal protein L25

Chain k: 75% 10% 15%



- Molecule 28: 60S ribosomal protein L26-A

Chain l: 92% 5% ..



- Molecule 29: 60S ribosomal protein L27-A

Chain m: 90% 8% ..



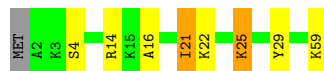
- Molecule 30: 60S ribosomal protein L28

Chain n: 83% 15% ..



- Molecule 31: 60S ribosomal protein L29

Chain o: 85% 10% ..



- Molecule 32: 60S ribosomal protein L30

Chain p: 88% 5% 8%



- Molecule 33: 60S ribosomal protein L31-A

Chain q:  86% 10% ..



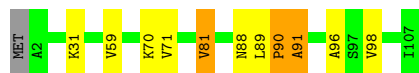
- Molecule 34: 60S ribosomal protein L32

Chain r:  89% 7% ..



- Molecule 35: 60S ribosomal protein L33-A

Chain s:  89% 7% ..



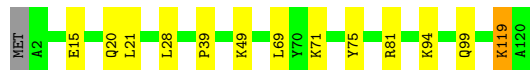
- Molecule 36: 60S ribosomal protein L34-A

Chain t:  83% 9% 7%



- Molecule 37: 60S ribosomal protein L35-A

Chain u:  88% 10% ..



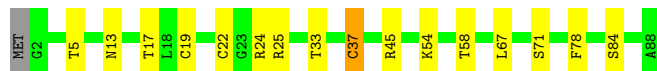
- Molecule 38: 60S ribosomal protein L36-A

Chain v:  91% 8% .

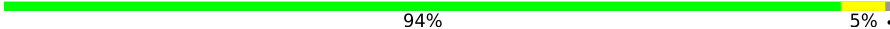


- Molecule 39: 60S ribosomal protein L37-A

Chain w:  81% 17% ..



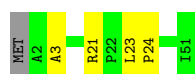
- Molecule 40: 60S ribosomal protein L38

Chain x:  94% 5%



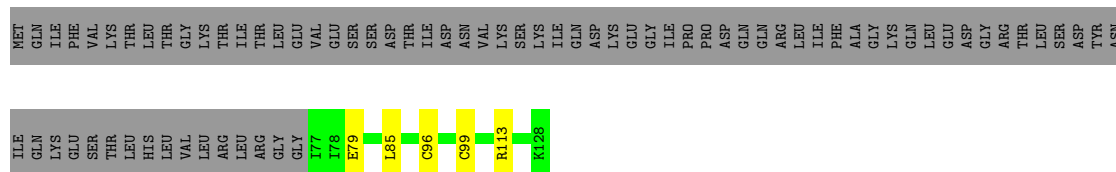
- Molecule 41: 60S ribosomal protein L39

Chain y:  90% 8%



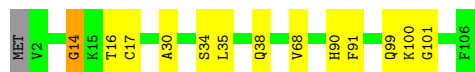
- Molecule 42: Ubiquitin-60S ribosomal protein L40

Chain z:  37% 59%



- Molecule 43: 60S ribosomal protein L42-A

Chain Q:  87% 11%

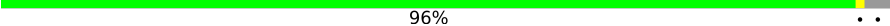


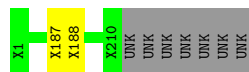
- Molecule 44: 60S ribosomal protein L43-A

Chain R:  88% 11%



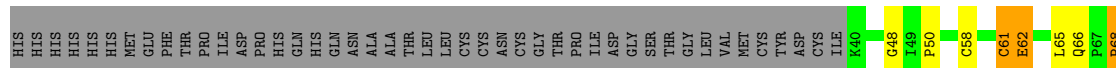
- Molecule 45: Ribosomal Protein uL1

Chain S:  96%

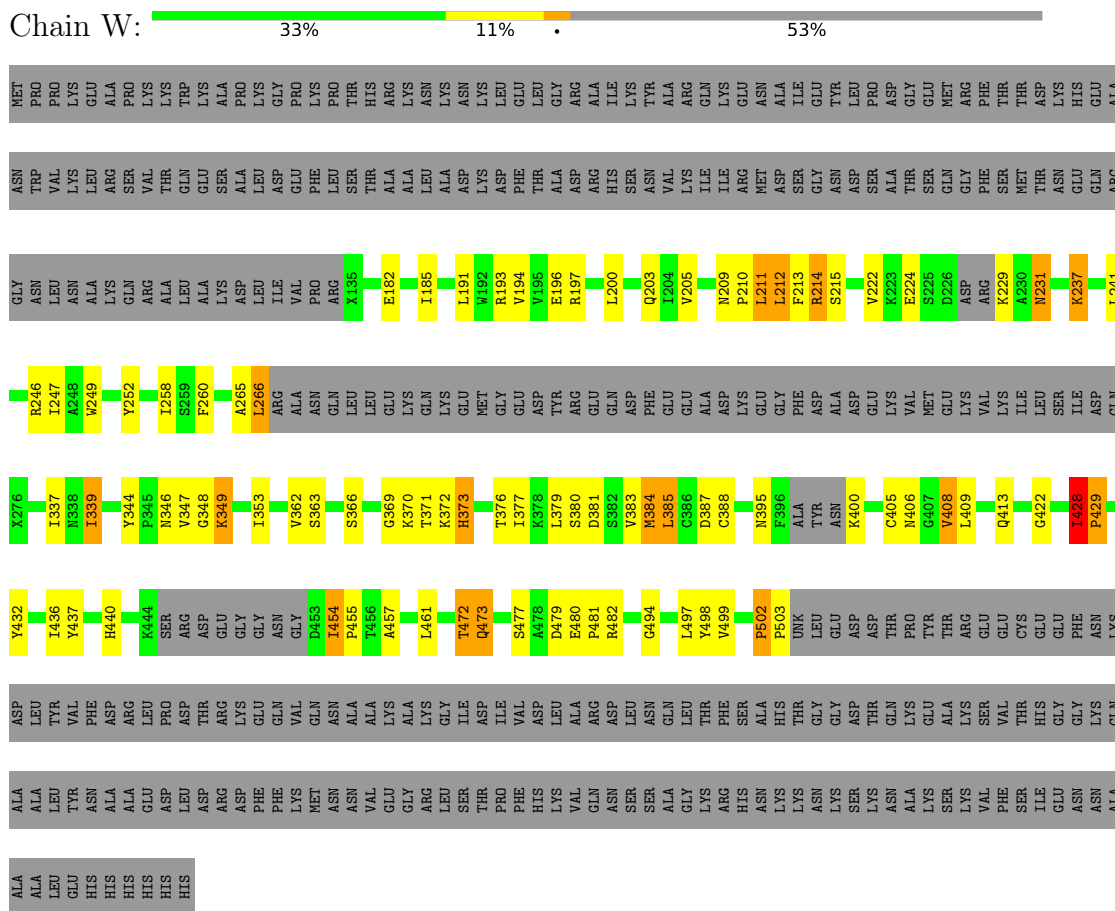


- Molecule 46: 60S ribosomal export protein NMD3

Chain V:  48% 13% 5% 33%



- Molecule 47: Large subunit GTPase 1



4 Experimental information

Property	Value	Source
EM 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: GNP, MG, PSU, K

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	X	0.64	0/1653	0.86	2/2255 (0.1%)
2	A	0.40	0/76629	0.73	47/119475 (0.0%)
3	B	0.40	0/2883	0.71	0/4491
4	C	0.40	0/3746	0.71	0/5832
5	D	0.62	0/1948	0.83	0/2617
6	E	0.59	0/3146	0.80	0/4228
7	F	0.59	0/2800	0.86	0/3790
8	G	0.59	0/2425	0.80	0/3271
9	H	0.57	0/1260	0.78	0/1694
10	I	0.62	0/1821	0.88	0/2451
11	J	0.63	0/1836	0.85	0/2481
12	K	0.59	0/1539	0.78	1/2073 (0.0%)
13	L	0.60	0/1741	0.72	0/2335
14	M	0.60	0/1374	0.81	0/1842
15	N	0.64	0/1568	0.87	0/2106
16	O	0.57	0/1068	0.84	0/1438
17	a	0.60	0/1757	0.85	2/2354 (0.1%)
18	b	0.60	0/1585	0.92	3/2128 (0.1%)
19	c	0.60	0/1443	0.87	0/1944
20	d	0.59	0/1465	0.85	0/1965
21	e	0.60	0/1538	0.85	0/2050
22	f	0.60	0/1481	0.82	1/1990 (0.1%)
23	g	0.59	0/1300	0.79	0/1743
24	h	0.61	0/812	0.71	0/1099
25	i	0.61	0/1018	0.81	0/1369
26	j	0.61	0/712	0.89	2/958 (0.2%)
27	k	0.59	0/979	0.77	0/1321
28	l	0.57	0/1004	0.78	0/1341
29	m	0.58	0/1118	0.78	0/1497
30	n	0.57	0/1204	0.83	0/1612
31	o	0.57	0/473	0.86	0/629
32	p	0.62	0/751	0.80	0/1008

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	q	0.58	0/890	0.76	0/1196
34	r	0.58	0/1041	0.81	1/1394 (0.1%)
35	s	0.56	0/868	0.81	3/1168 (0.3%)
36	t	0.62	0/890	0.85	0/1189
37	u	0.63	0/978	0.88	0/1301
38	v	0.65	0/778	0.87	0/1034
39	w	0.71	0/696	0.93	1/923 (0.1%)
40	x	0.61	0/618	0.72	0/826
41	y	0.57	0/443	0.81	0/588
42	z	0.60	0/423	0.79	0/562
43	Q	0.61	0/860	0.74	0/1136
44	R	0.67	0/701	0.87	0/934
46	V	0.63	0/2766	0.94	5/3759 (0.1%)
47	W	0.70	0/1950	0.98	2/2640 (0.1%)
All	All	0.49	0/139979	0.77	70/206037 (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 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	j	80	ARG	CA-C-N	9.53	131.76	119.84
26	j	80	ARG	C-N-CA	9.53	131.76	119.84
2	A	3078	U	C4'-C3'-O3'	9.18	123.17	109.40
18	b	109	PRO	CA-C-N	8.93	129.58	120.38
18	b	109	PRO	C-N-CA	8.93	129.58	120.38

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	11	0
2	A	68535	0	34438	193	0
3	B	2579	0	1304	5	0
4	C	3353	0	1695	4	0
5	D	1914	0	1981	6	0
6	E	3075	0	3142	7	0
7	F	2748	0	2859	8	0
8	G	2375	0	2325	4	0
9	H	1239	0	1326	1	0
10	I	1784	0	1862	6	0
11	J	1804	0	1877	2	0
12	K	1518	0	1587	7	0
13	L	1705	0	1736	2	0
14	M	1353	0	1383	2	0
15	N	1543	0	1608	6	0
16	O	1053	0	1149	4	0
17	a	1720	0	1779	4	0
18	b	1555	0	1659	2	0
19	c	1420	0	1437	4	0
20	d	1441	0	1543	3	0
21	e	1521	0	1617	3	0
22	f	1445	0	1487	5	0
23	g	1276	0	1323	7	0
24	h	796	0	812	0	0
25	i	1003	0	1048	7	0
26	j	699	0	640	0	0
27	k	964	0	1025	5	0
28	l	993	0	1081	3	0
29	m	1092	0	1155	4	0
30	n	1173	0	1215	10	0
31	o	462	0	491	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	p	743	0	797	2	0
33	q	876	0	912	2	0
34	r	1020	0	1090	2	0
35	s	850	0	880	3	0
36	t	880	0	945	3	0
37	u	969	0	1078	1	0
38	v	771	0	849	1	0
39	w	681	0	685	5	0
40	x	612	0	682	0	0
41	y	436	0	475	1	0
42	z	417	0	459	1	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	71	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	436	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 436 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 [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	Percentiles	
1	X	222/264 (84%)	202 (91%)	20 (9%)	0	100	100
5	D	250/254 (98%)	226 (90%)	22 (9%)	2 (1%)	16	47
6	E	384/387 (99%)	346 (90%)	31 (8%)	7 (2%)	6	28
7	F	359/362 (99%)	311 (87%)	32 (9%)	16 (4%)	2	12
8	G	294/297 (99%)	265 (90%)	25 (8%)	4 (1%)	9	34
9	H	152/176 (86%)	133 (88%)	16 (10%)	3 (2%)	6	25
10	I	220/244 (90%)	200 (91%)	14 (6%)	6 (3%)	4	20
11	J	231/256 (90%)	207 (90%)	17 (7%)	7 (3%)	3	19
12	K	189/191 (99%)	169 (89%)	17 (9%)	3 (2%)	7	30
13	L	207/221 (94%)	186 (90%)	16 (8%)	5 (2%)	4	22
14	M	167/174 (96%)	143 (86%)	19 (11%)	5 (3%)	3	19
15	N	191/199 (96%)	168 (88%)	18 (9%)	5 (3%)	4	21
16	O	134/138 (97%)	119 (89%)	10 (8%)	5 (4%)	2	15
17	a	201/204 (98%)	188 (94%)	11 (6%)	2 (1%)	12	41
18	b	195/199 (98%)	184 (94%)	11 (6%)	0	100	100
19	c	181/184 (98%)	163 (90%)	17 (9%)	1 (1%)	21	52
20	d	183/186 (98%)	162 (88%)	18 (10%)	3 (2%)	7	30
21	e	186/189 (98%)	173 (93%)	9 (5%)	4 (2%)	5	24
22	f	170/172 (99%)	156 (92%)	11 (6%)	3 (2%)	6	28
23	g	157/160 (98%)	141 (90%)	13 (8%)	3 (2%)	6	27
24	h	98/121 (81%)	79 (81%)	17 (17%)	2 (2%)	6	25
25	i	134/137 (98%)	124 (92%)	9 (7%)	1 (1%)	18	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	j	96/155 (62%)	81 (84%)	12 (12%)	3 (3%)	3	18
27	k	119/142 (84%)	107 (90%)	11 (9%)	1 (1%)	16	47
28	l	124/127 (98%)	115 (93%)	7 (6%)	2 (2%)	7	30
29	m	133/136 (98%)	111 (84%)	18 (14%)	4 (3%)	3	19
30	n	146/149 (98%)	126 (86%)	13 (9%)	7 (5%)	2	11
31	o	56/59 (95%)	48 (86%)	5 (9%)	3 (5%)	1	9
32	p	95/105 (90%)	88 (93%)	7 (7%)	0	100	100
33	q	107/113 (95%)	98 (92%)	6 (6%)	3 (3%)	4	20
34	r	125/130 (96%)	121 (97%)	3 (2%)	1 (1%)	16	47
35	s	104/107 (97%)	95 (91%)	7 (7%)	2 (2%)	6	27
36	t	110/121 (91%)	102 (93%)	6 (6%)	2 (2%)	6	28
37	u	117/120 (98%)	109 (93%)	4 (3%)	4 (3%)	3	16
38	v	97/100 (97%)	88 (91%)	8 (8%)	1 (1%)	12	41
39	w	85/88 (97%)	77 (91%)	6 (7%)	2 (2%)	4	22
40	x	75/78 (96%)	67 (89%)	5 (7%)	3 (4%)	2	13
41	y	48/51 (94%)	44 (92%)	3 (6%)	1 (2%)	5	25
42	z	50/128 (39%)	47 (94%)	2 (4%)	1 (2%)	6	25
43	Q	103/106 (97%)	88 (85%)	10 (10%)	5 (5%)	1	11
44	R	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
46	V	344/524 (66%)	302 (88%)	27 (8%)	15 (4%)	2	12
47	W	231/651 (36%)	198 (86%)	25 (11%)	8 (4%)	3	16
All	All	6959/7997 (87%)	6240 (90%)	564 (8%)	155 (2%)	7	24

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%)	65	78
5	D	193/196 (98%)	184 (95%)	9 (5%)	23	55
6	E	320/323 (99%)	293 (92%)	27 (8%)	10	35
7	F	288/289 (100%)	278 (96%)	10 (4%)	32	62
8	G	244/245 (100%)	230 (94%)	14 (6%)	18	49
9	H	134/153 (88%)	128 (96%)	6 (4%)	24	56
10	I	186/205 (91%)	178 (96%)	8 (4%)	26	57
11	J	187/208 (90%)	171 (91%)	16 (9%)	10	34
12	K	171/171 (100%)	159 (93%)	12 (7%)	14	41
13	L	177/187 (95%)	163 (92%)	14 (8%)	11	37
14	M	147/150 (98%)	141 (96%)	6 (4%)	27	59
15	N	154/159 (97%)	140 (91%)	14 (9%)	9	32
16	O	107/109 (98%)	103 (96%)	4 (4%)	30	61
17	a	175/176 (99%)	164 (94%)	11 (6%)	16	45
18	b	160/162 (99%)	154 (96%)	6 (4%)	29	60
19	c	140/146 (96%)	132 (94%)	8 (6%)	18	49
20	d	150/151 (99%)	144 (96%)	6 (4%)	28	60
21	e	153/154 (99%)	147 (96%)	6 (4%)	28	60
22	f	156/156 (100%)	148 (95%)	8 (5%)	21	52
23	g	136/137 (99%)	129 (95%)	7 (5%)	21	52
24	h	87/107 (81%)	86 (99%)	1 (1%)	65	78
25	i	104/105 (99%)	99 (95%)	5 (5%)	23	54
26	j	57/129 (44%)	57 (100%)	0	100	100
27	k	104/118 (88%)	95 (91%)	9 (9%)	9	34
28	l	109/110 (99%)	103 (94%)	6 (6%)	19	50
29	m	115/116 (99%)	109 (95%)	6 (5%)	21	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	n	118/119 (99%)	111 (94%)	7 (6%)	18	48
31	o	46/47 (98%)	42 (91%)	4 (9%)	9	34
32	p	81/88 (92%)	79 (98%)	2 (2%)	42	69
33	q	92/97 (95%)	86 (94%)	6 (6%)	15	44
34	r	109/111 (98%)	100 (92%)	9 (8%)	10	35
35	s	90/91 (99%)	85 (94%)	5 (6%)	19	49
36	t	95/103 (92%)	90 (95%)	5 (5%)	20	51
37	u	104/105 (99%)	95 (91%)	9 (9%)	9	34
38	v	81/82 (99%)	75 (93%)	6 (7%)	13	40
39	w	70/71 (99%)	63 (90%)	7 (10%)	7	29
40	x	68/69 (99%)	67 (98%)	1 (2%)	57	75
41	y	45/46 (98%)	44 (98%)	1 (2%)	45	71
42	z	47/116 (40%)	45 (96%)	2 (4%)	26	57
43	Q	90/91 (99%)	87 (97%)	3 (3%)	33	63
44	R	71/72 (99%)	65 (92%)	6 (8%)	10	35
46	V	291/473 (62%)	257 (88%)	34 (12%)	5	22
47	W	209/502 (42%)	168 (80%)	41 (20%)	1	6
All	All	5838/6672 (88%)	5469 (94%)	369 (6%)	18	45

5 of 369 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	o	59	LYS
43	Q	99	GLN
33	q	82	GLU
37	u	20	GLN
46	V	145	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
21	e	68	GLN
28	l	42	GLN
47	W	209	ASN
22	f	63	GLN

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Mol	Chain	Res	Type
24	h	87	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	3201/3396 (94%)	852 (26%)	100 (3%)
3	B	120/121 (99%)	27 (22%)	3 (2%)
4	C	157/158 (99%)	39 (24%)	3 (1%)
All	All	3478/3675 (94%)	918 (26%)	106 (3%)

5 of 918 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	2404	A
2	A	2644	C
2	A	3353	G
2	A	2434	U
2	A	2513	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	2260	2	18,21,22	1.36	2 (11%)	21,30,33	2.08	4 (19%)
2	PSU	A	2264	2	18,21,22	1.34	2 (11%)	21,30,33	2.14	6 (28%)
2	PSU	A	2258	2	18,21,22	1.40	2 (11%)	21,30,33	2.10	5 (23%)
2	PSU	A	2266	2	18,21,22	1.38	2 (11%)	21,30,33	2.13	5 (23%)

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	2260	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2264	2	-	1/7/25/26	0/2/2/2
2	PSU	A	2258	2	-	2/7/25/26	0/2/2/2
2	PSU	A	2266	2	-	1/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2264	PSU	C6-C5	3.26	1.38	1.35
2	A	2260	PSU	C6-C5	3.25	1.38	1.35
2	A	2258	PSU	C6-C5	3.25	1.38	1.35
2	A	2266	PSU	C6-C5	3.10	1.38	1.35
2	A	2260	PSU	C4-N3	-2.74	1.33	1.38

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2260	PSU	N1-C2-N3	6.47	121.99	115.17
2	A	2258	PSU	N1-C2-N3	6.46	121.98	115.17
2	A	2266	PSU	N1-C2-N3	6.39	121.91	115.17
2	A	2264	PSU	N1-C2-N3	6.38	121.90	115.17
2	A	2258	PSU	C4-N3-C2	-4.27	120.48	126.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2258	PSU	C3'-C4'-C5'-O5'
2	A	2258	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	A	2264	PSU	C2'-C1'-C5-C4
2	A	2266	PSU	O4'-C1'-C5-C4

There are no ring outliers.

3 monomers are involved in 32 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	34,34,34	1.62	5 (14%)	47,54,54	1.82	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
50	GNP	W	701	48	-	6/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	W	701	GNP	PG-N3B	4.46	1.75	1.63
50	W	701	GNP	PB-N3B	4.45	1.75	1.63
50	W	701	GNP	C5-C4	3.13	1.47	1.38
50	W	701	GNP	C6-N1	-2.49	1.34	1.38
50	W	701	GNP	C5-N7	-2.12	1.34	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	W	701	GNP	C5-C4-N3	-6.39	118.22	128.39
50	W	701	GNP	C2-N3-C4	5.13	121.14	112.30
50	W	701	GNP	N9-C4-N3	4.81	135.57	125.95
50	W	701	GNP	C6-C5-N7	3.05	135.85	130.29
50	W	701	GNP	C4-C5-N7	-2.53	106.67	110.67

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

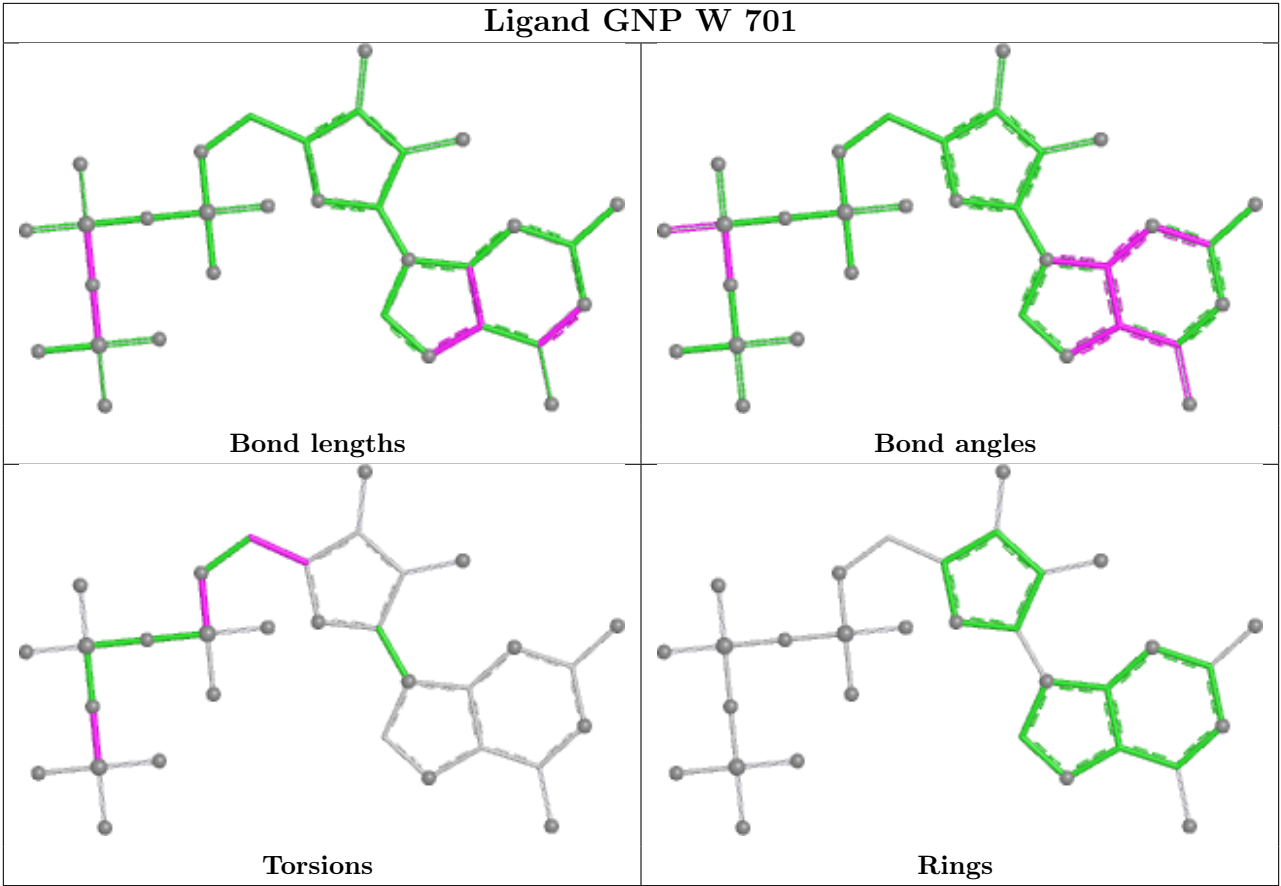
Mol	Chain	Res	Type	Atoms
50	W	701	GNP	PB-N3B-PG-O1G
50	W	701	GNP	C5'-O5'-PA-O3A
50	W	701	GNP	C5'-O5'-PA-O1A
50	W	701	GNP	C5'-O5'-PA-O2A
50	W	701	GNP	O4'-C4'-C5'-O5'

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

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 than 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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