



wwPDB EM Validation Summary Report ⓘ

Nov 5, 2024 – 06:21 PM EST

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 : 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	: 4.02b-467
buster-report	: 1.1.7 (2018)
Percentile statistics	: 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	: FAILED
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.39

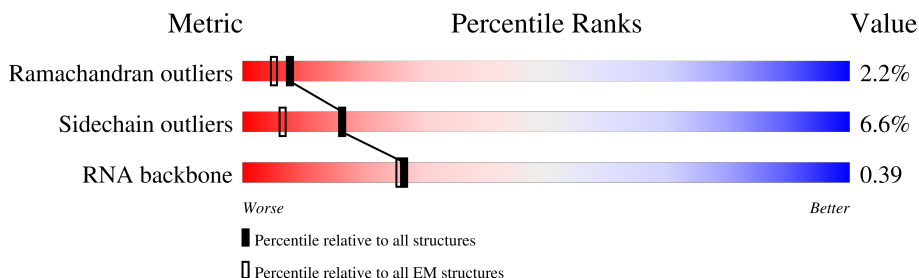
1 Overall quality at a glance

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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	
2	A	3396	
3	B	121	
4	C	158	
5	D	254	
6	E	387	
7	F	362	
8	G	297	
9	H	176	

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Mol	Chain	Length	Quality of chain
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	
34	r	130	

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Mol	Chain	Length	Quality of chain
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	 90% 9% .
44	R	92	 95% . .
45	S	217	 97% .
46	V	524	 57% 9% . 33%
47	W	651	 40% 7% 53%

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

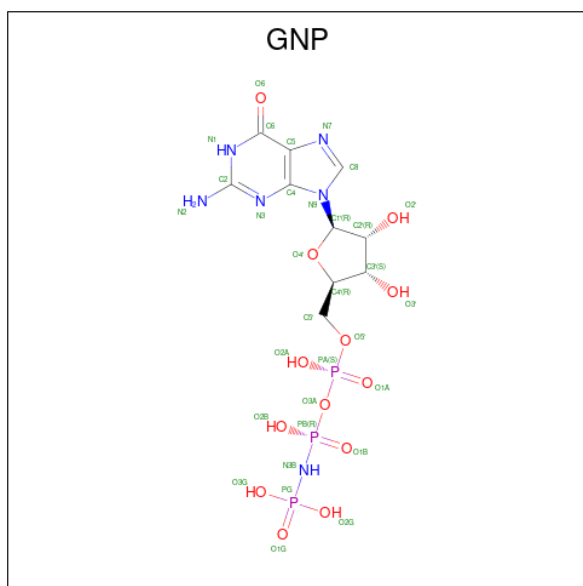
- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 (three-letter code: K) (formula: K).

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

- 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	0
			5	5	
51	e	1	Total	O	0
			1	1	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

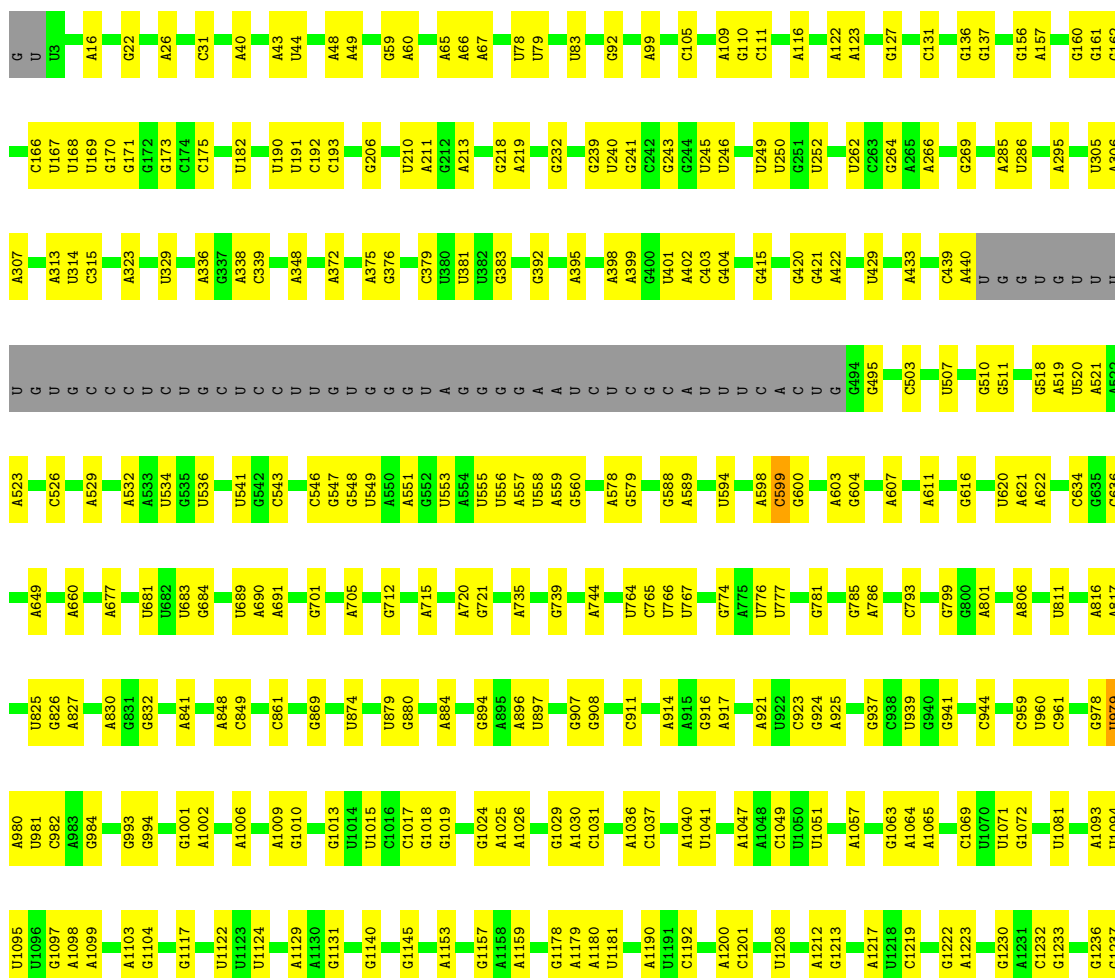
- Molecule 1: Eukaryotic translation initiation factor 6

Chain X: 

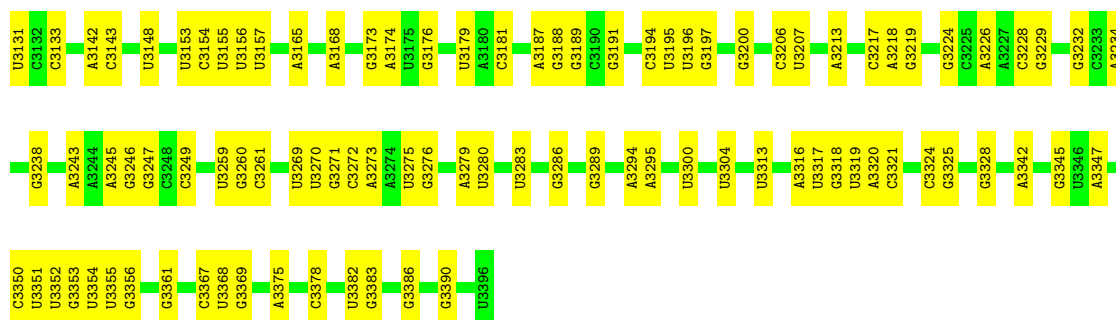


- Molecule 2: TPA_inf: *Saccharomyces cerevisiae* S288C chromosome XII, complete sequence

Chain A: 



U2976	G2816	A2674	A2547	A2452	A2372	U2209	A	C	G1953	C1788	G1623	U1501	U1334	A1240
U2979	A2817	A2677	C2548	G2463	A2373	G2210	C	U	G1954	G1789	U1627	C1502	U1348	U1241
U2980	C2821	G2677	U2550	U2464	C2374	G2211	G	U	U1955	G1790	C1628	A1503	U1349	G1242
C2983	A2837	U2681	U2551	A2468	G2375	G2221	C	U	A	U1795	U1630	C1508	A1350	G1243
G2990	A2838	C2684	U2553	G2469	U2379	A2228	C	U	G	A1797	C1631	G1521	U1351	A1244
U2996	U2842	A2689	A2554	C2470	U2379	G2239	G	U	A	A1798	A1632	C1527	A1352	A1245
G2997	U2843	A2690	G2555	C2471	G2385	G2240	C	U	G	C1803	A1642	C1531	G1354	A1246
U2998	C2844	A2691	A2561	G2474	U2388	A2244	U	U	G	A1643	A1643	C1531	G1355	C1248
C3004	A2845	A2694	A2562	G2475	G2393	G2245	C	U	C	G1808	C1644	C1532	U1356	G1249
A3011	G2848	A2694	G2563	C2476	G2393	G2246	U	U	C	G1812	U1645	U1533	G1357	U1253
A3012	C2849	A2695	G2564	G2477	A2397	G2249	A	A	G	A1813	C1657	G1536	C1364	C1257
U3013	U2859	A2696	U2565	C2478	A2397	G2250	C	U	U	A1814	G1658	A1537	U1258	U1258
U3014	U2860	A2704	A2566	A2480	A2401	G2253	A	A	U	U1815	G1664	G1547	G1383	G1262
U3014	U2861	C2709	U2570	U2482	C2403	U2254	U	U	C	A1816	C1665	U1553	A1386	A1263
G3022	C2867	C2709	U2571	G2483	A2404	A2255	U	U	C	G1817	G1666	U1553	C1391	G1264
A3048	G2871	G2714	C2572	A2484	C2405	A2257	A	G	G	U1820	C1674	U1554	G1392	U1265
A3049	A2872	G2573	G2573	A2485	C2406	C2257	C	A	C	U1821	G1678	U1555	A1393	G1267
U3055	U2882	U2719	G2574	A2488	C2407	U2258	G	U	G	A1839	U1678	A1557	A1394	U1267
U3056	A2726	C2726	G2576	A2491	U2411	U2260	G	C	C	U1840	U1682	G1560	A1399	A1270
U3057	A2727	A2727	C2577	A2491	G2412	G2261	C	A	A	A1841	U1683	G1561	G1400	A1271
U3058	A2887	G2728	U2581	A2494	G2418	A2262	U	C	U	A1842	U1703	C1562	A1286	A1274
G3059	U2888	A2734	G2585	C2495	A2419	C2263	C	C	C	G1845	U1564	C1563	G1409	C1275
A3070	A2896	C2737	G2586	U2497	G2425	C2265	G	G	G	C1849	U1716	U1564	U1414	U1276
U3071	G2897	C2737	A2593	U2498	U2428	U2266	U	U	C	A1850	U1717	A1566	U1415	C1277
C3072	G2898	G2753	C2594	U2501	G2429	C2267	G	U	G	U1867	U1574	U1567	U1416	A1278
U3078	C2899	G2754	G2602	A2502	U2434	U2268	A	U	U	U1871	C1725	U1568	A1419	C1279
U3079	A2914	C2755	G2606	U2506	G2437	A2270	G	C	C	U1880	G1733	U1570	G1285	G1285
A3086	U2923	A2762	G2607	U2508	G2437	U2274	A	U	U	U1886	G1734	A1571	A1287	A1286
U3090	C2928	C2772	G2614	C2507	G2440	A2281	C	U	G	A1886	G1735	U1572	U1288	U1288
A3091	A2933	C2773	G2614	U2513	A2441	U2282	G	U	U	A1893	A1741	G1576	G1434	A1290
C3092	U2935	G2774	G2621	U2514	G2442	U2283	C	G	C	A1894	C1437	C1577	C1437	A1291
U3104	U2935	G2777	A2626	A2515	C2443	G2288	U	A	A	A1895	G1446	C1579	A1446	A1303
G3109	A2936	G2778	C2627	G2522	A2445	U2288	U	C	U	G1906	G1450	C1582	G1450	U1305
C3110	G2937	A2780	A2628	G2531	G2450	G2307	G	G	C	A1907	A1750	A1583	U1455	U1306
A3114	U2938	A2790	A2635	U2532	G2451	C2308	A	U	U	A1908	G1751	A1587	U1455	G1307
C3115	G2941	G2791	C2644	G2533	G2452	U2309	G	U	G	A1909	A1760	A1588	A1460	A1308
C3117	C2942	A2792	C2644	U2537	G2453	U2310	U	G	C	G1917	C1761	A1589	A1460	U1309
U3122	G2947	A2799	G2648	U2538	U2453	A2313	U	C	U	U1765	U1765	G1599	G1466	G1313
A3122	G2950	A2801	U2652	U2539	G2454	U2314	C	U	G	C1926	G1766	A1605	G1480	C1314
U3125	G2951	A2803	U2652	U2540	A2456	G2315	U	G	U	A1930	G1770	C1615	A1481	U1315
A3129	A2971	C2810	U2655	U2542	A2458	A2330	G	C	C	A1936	G1775	A1619	A1482	G1319
A3130	U2975	A2975	A2657	U2544	A2459	G2336	U	U	U	C1951	U1780	A1620	G1489	U1329
			G2658	U2544	A2461	C2337	A	G	G	U1952			C1496	A1330



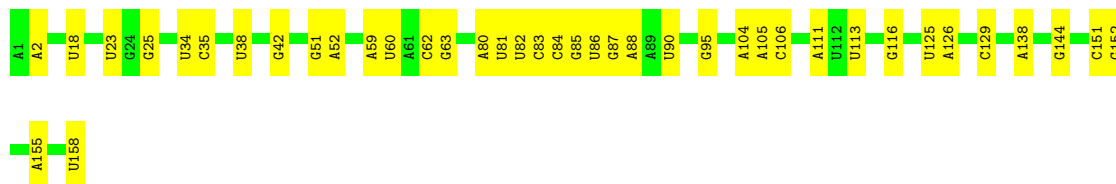
- Molecule 3: 5S Ribosomal RNA

Chain B: 77% 23%



- Molecule 4: 5.8S Ribosomal RNA

Chain C: 75% 25%



- Molecule 5: 60S ribosomal protein L2-A

Chain D: 94% 6%



- Molecule 6: 60S ribosomal protein L3

Chain E: 93% 7%



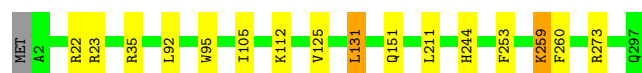
- Molecule 7: 60S ribosomal protein L4-A

Chain F: 92% 8%




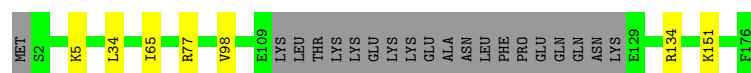
- Molecule 8: 60S ribosomal protein L5

Chain G:  94% 5%




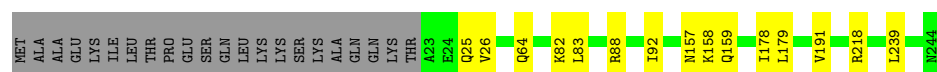
- Molecule 9: 60S ribosomal protein L6-A

Chain H:  85% 11%




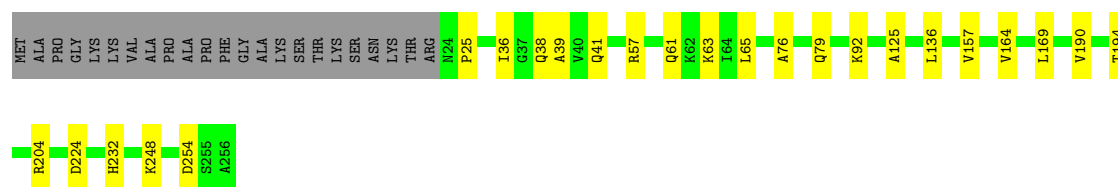
- Molecule 10: 60S ribosomal protein L7-A

Chain I:  85% 6% 9%



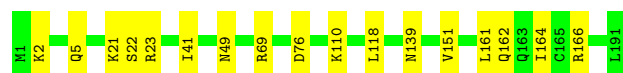
- Molecule 11: 60S ribosomal protein L8-A

Chain J:  82% 9% 9%




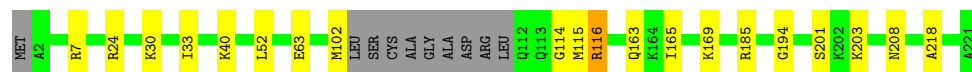
- Molecule 12: 60S ribosomal protein L9-A

Chain K:  91% 9%



- Molecule 13: 60S ribosomal protein L10

Chain L:  86% 9% 5%




- Molecule 14: 60S ribosomal protein L11-A

Chain M:  90% 6%




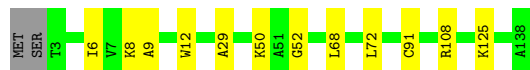
- Molecule 15: 60S ribosomal protein L13-A

Chain N:  88% 8% ..



- Molecule 16: 60S ribosomal protein L14-A

Chain O:  90% 9% .



- Molecule 17: 60S ribosomal protein L15-A

Chain a:  95% 5%



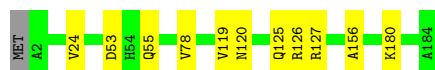
- Molecule 18: 60S ribosomal protein L16-A

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

Chain e:  94% 6% .



- Molecule 22: 60S ribosomal protein L20-A

Item	Category
M1	Yellow
P22	Green
R23	Green
L24	Green
V51	Green
I58	Green
I61	Green
K71	Green
D82	Green
T87	Green
E93	Green
D134	Green
R137	Green
R155	Green
R167	Green
Y172	Green

- | |
|------|
| MET |
| G2 |
| R12 |
| K32 |
| L75 |
| M79 |
| R88 |
| I96 |
| R102 |
| V124 |
| A125 |
| V126 |
| Q127 |
| L128 |
| R139 |
| F159 |
| T160 |

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|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ALA | PRO | ASN | THR | SER | ARG | LYS | Q9 | K10 | I11 | G60 | K70 | I108 | GLN | VAL | THR | PRO | GLU | GLU | ASP | GLU | GLU | GLU | ASP | GLU | GLU |
|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ALA | THR | SER | ARG | MT | R80 | P81 | K97 | P98 | GLU | VAL | ARG | LYS | ALA | ASN | ARG | GLU | GLU | LYS | LEU | LYS | ALA | ALA | ASN | LYS | GLU | LYS | LYS | LYS | ALA | ALA | ARG | LYS | ALA | GLU | LYS | LYS | GLY | THR | GLN | SER | SER | LYS | PHE | SER | LYS | GLN | GLN | ALA | ALA | LYS | GLY | ALA | PHE | GLN | LYS | VAL |
|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|
| MET | ALA | PRO | SER | LYS | THR | ALA | ALA | LYS | VAL | VAL | LYS | GLY | THR | ASN | GLY | LYS | K22 | A50 | K61 | V62 | I63 | E70 | R115 | L133 | D134 | I135 | A136 | N137 | I142 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|


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- Diagram illustrating the protein structure of the E127 mutant, showing residues MET, A2, K3, Q4, R13, K37, I50, D53, Y74, K84, L126, and E127.

- 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% .




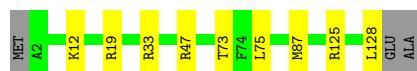
- Molecule 33: 60S ribosomal protein L31-A

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% .



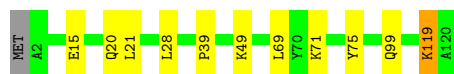
- Molecule 36: 60S ribosomal protein L34-A

Chain t:  86% 7% 7%



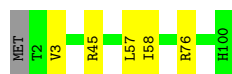
- Molecule 37: 60S ribosomal protein L35-A

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% .



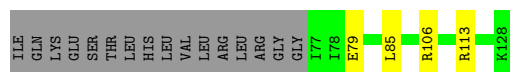
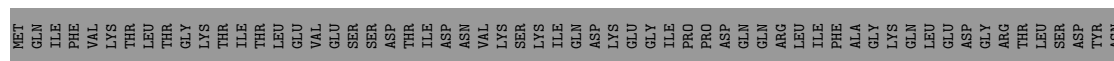
- Molecule 41: 60S ribosomal protein L39

Chain y:  94% . .



- Molecule 42: Ubiquitin-60S ribosomal protein L40

Chain z:  38% . 59%



GLU	ASN	ASN	ALA	ALA	ALA	GLU	HIS	HIS	HIS	HIS	HIS	GLY	ASN	PHE	GLY	GLN	VAL	GLN	ASN	GLY	ILE	ASP	ILE	VAL	GLY	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GL
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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: PSU, GNP, K, MG

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	0.40	0/1653	0.55	0/2255
2	A	0.28	0/76629	0.70	3/119475 (0.0%)
3	B	0.26	0/2883	0.68	0/4491
4	C	0.29	0/3746	0.71	0/5832
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
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
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
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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
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
39	w	0.49	0/696	0.81	1/923 (0.1%)
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%)
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](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	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	48
6	E	384/387 (99%)	346 (90%)	31 (8%)	7 (2%)	7	29
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	26
10	I	220/244 (90%)	200 (91%)	14 (6%)	6 (3%)	4	21
11	J	231/256 (90%)	207 (90%)	17 (7%)	7 (3%)	3	19
12	K	189/191 (99%)	169 (89%)	17 (9%)	3 (2%)	8	31
13	L	207/221 (94%)	186 (90%)	16 (8%)	5 (2%)	5	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	16
17	a	201/204 (98%)	188 (94%)	11 (6%)	2 (1%)	13	42
18	b	195/199 (98%)	184 (94%)	11 (6%)	0	100	100
19	c	181/184 (98%)	163 (90%)	17 (9%)	1 (1%)	22	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	d	183/186 (98%)	162 (88%)	18 (10%)	3 (2%)	8	31
21	e	186/189 (98%)	173 (93%)	9 (5%)	4 (2%)	5	24
22	f	170/172 (99%)	156 (92%)	11 (6%)	3 (2%)	7	29
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	26
25	i	134/137 (98%)	124 (92%)	9 (7%)	1 (1%)	19	51
26	j	96/155 (62%)	81 (84%)	12 (12%)	3 (3%)	3	19
27	k	119/142 (84%)	107 (90%)	11 (9%)	1 (1%)	16	48
28	l	124/127 (98%)	115 (93%)	7 (6%)	2 (2%)	8	31
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	48
35	s	104/107 (97%)	95 (91%)	7 (7%)	2 (2%)	6	27
36	t	110/121 (91%)	102 (93%)	6 (6%)	2 (2%)	7	29
37	u	117/120 (98%)	109 (93%)	4 (3%)	4 (3%)	3	17
38	v	97/100 (97%)	88 (91%)	8 (8%)	1 (1%)	13	42
39	w	85/88 (97%)	77 (91%)	6 (7%)	2 (2%)	5	22
40	x	75/78 (96%)	67 (89%)	5 (7%)	3 (4%)	2	14
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	26
43	Q	103/106 (97%)	88 (85%)	10 (10%)	5 (5%)	2	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%)	8	24

5 of 155 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	E	351	LEU

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Mol	Chain	Res	Type
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%)	70	84
5	D	193/196 (98%)	181 (94%)	12 (6%)	15	43
6	E	320/323 (99%)	300 (94%)	20 (6%)	15	42
7	F	288/289 (100%)	276 (96%)	12 (4%)	25	56
8	G	244/245 (100%)	231 (95%)	13 (5%)	19	48
9	H	134/153 (88%)	130 (97%)	4 (3%)	36	64
10	I	186/205 (91%)	177 (95%)	9 (5%)	21	51
11	J	187/208 (90%)	171 (91%)	16 (9%)	8	31
12	K	171/171 (100%)	157 (92%)	14 (8%)	9	33
13	L	177/187 (95%)	161 (91%)	16 (9%)	8	29
14	M	147/150 (98%)	139 (95%)	8 (5%)	18	47
15	N	154/159 (97%)	141 (92%)	13 (8%)	9	32
16	O	107/109 (98%)	100 (94%)	7 (6%)	14	41
17	a	175/176 (99%)	167 (95%)	8 (5%)	23	52
18	b	160/162 (99%)	154 (96%)	6 (4%)	28	59
19	c	140/146 (96%)	130 (93%)	10 (7%)	12	39
20	d	150/151 (99%)	144 (96%)	6 (4%)	27	58
21	e	153/154 (99%)	146 (95%)	7 (5%)	23	52
22	f	156/156 (100%)	145 (93%)	11 (7%)	12	39
23	g	136/137 (99%)	125 (92%)	11 (8%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	h	87/107 (81%)	85 (98%)	2 (2%)	45	70
25	i	104/105 (99%)	101 (97%)	3 (3%)	37	65
26	j	57/129 (44%)	57 (100%)	0	100	100
27	k	104/118 (88%)	96 (92%)	8 (8%)	10	35
28	l	109/110 (99%)	102 (94%)	7 (6%)	14	42
29	m	115/116 (99%)	109 (95%)	6 (5%)	19	48
30	n	118/119 (99%)	108 (92%)	10 (8%)	8	32
31	o	46/47 (98%)	43 (94%)	3 (6%)	14	41
32	p	81/88 (92%)	78 (96%)	3 (4%)	29	59
33	q	92/97 (95%)	87 (95%)	5 (5%)	18	47
34	r	109/111 (98%)	101 (93%)	8 (7%)	11	37
35	s	90/91 (99%)	83 (92%)	7 (8%)	10	35
36	t	95/103 (92%)	89 (94%)	6 (6%)	15	42
37	u	104/105 (99%)	96 (92%)	8 (8%)	10	35
38	v	81/82 (99%)	77 (95%)	4 (5%)	21	51
39	w	70/71 (99%)	63 (90%)	7 (10%)	6	24
40	x	68/69 (99%)	65 (96%)	3 (4%)	24	54
41	y	45/46 (98%)	44 (98%)	1 (2%)	47	71
42	z	47/116 (40%)	44 (94%)	3 (6%)	14	42
43	Q	90/91 (99%)	85 (94%)	5 (6%)	17	46
44	R	71/72 (99%)	67 (94%)	4 (6%)	17	46
46	V	291/473 (62%)	254 (87%)	37 (13%)	3	15
47	W	209/502 (42%)	171 (82%)	38 (18%)	1	6
All	All	5838/6672 (88%)	5455 (93%)	383 (7%)	16	41

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

Mol	Chain	Res	Type
30	n	4	ARG
39	w	24	ARG
30	n	115	LYS
35	s	31	LYS
43	Q	35	LEU

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

Mol	Chain	Res	Type
37	u	108	GLN
47	W	442	GLN
40	x	67	GLN
47	W	209	ASN
47	W	500	ASN

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	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	2258	2	18,21,22	1.40	2 (11%)	21,30,33	2.10	5 (23%)
2	PSU	A	2264	2	18,21,22	1.34	2 (11%)	21,30,33	2.14	6 (28%)
2	PSU	A	2260	2	18,21,22	1.36	2 (11%)	21,30,33	2.08	4 (19%)
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	2258	2	-	2/7/25/26	0/2/2/2
2	PSU	A	2264	2	-	1/7/25/26	0/2/2/2
2	PSU	A	2260	2	-	0/7/25/26	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'
2	A	2264	PSU	C2'-C1'-C5-C4
2	A	2266	PSU	O4'-C1'-C5-C4

There are no ring outliers.

No monomer is involved in short contacts.

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	29,34,34	1.67	3 (10%)	33,54,54	1.85	7 (21%)

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	-	6/14/38/38	0/3/3/3

All (3) 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	W	701	GNP	C5-C6	4.19	1.48	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	W	701	GNP	C2-N3-C4	5.24	121.14	115.48
50	W	701	GNP	C2-N1-C6	4.44	122.14	115.96
50	W	701	GNP	C5-C6-N1	-4.03	118.04	123.42
50	W	701	GNP	N3-C2-N1	-3.33	122.98	127.21
50	W	701	GNP	C4-C5-N7	-2.53	106.67	109.34

There are no chirality outliers.

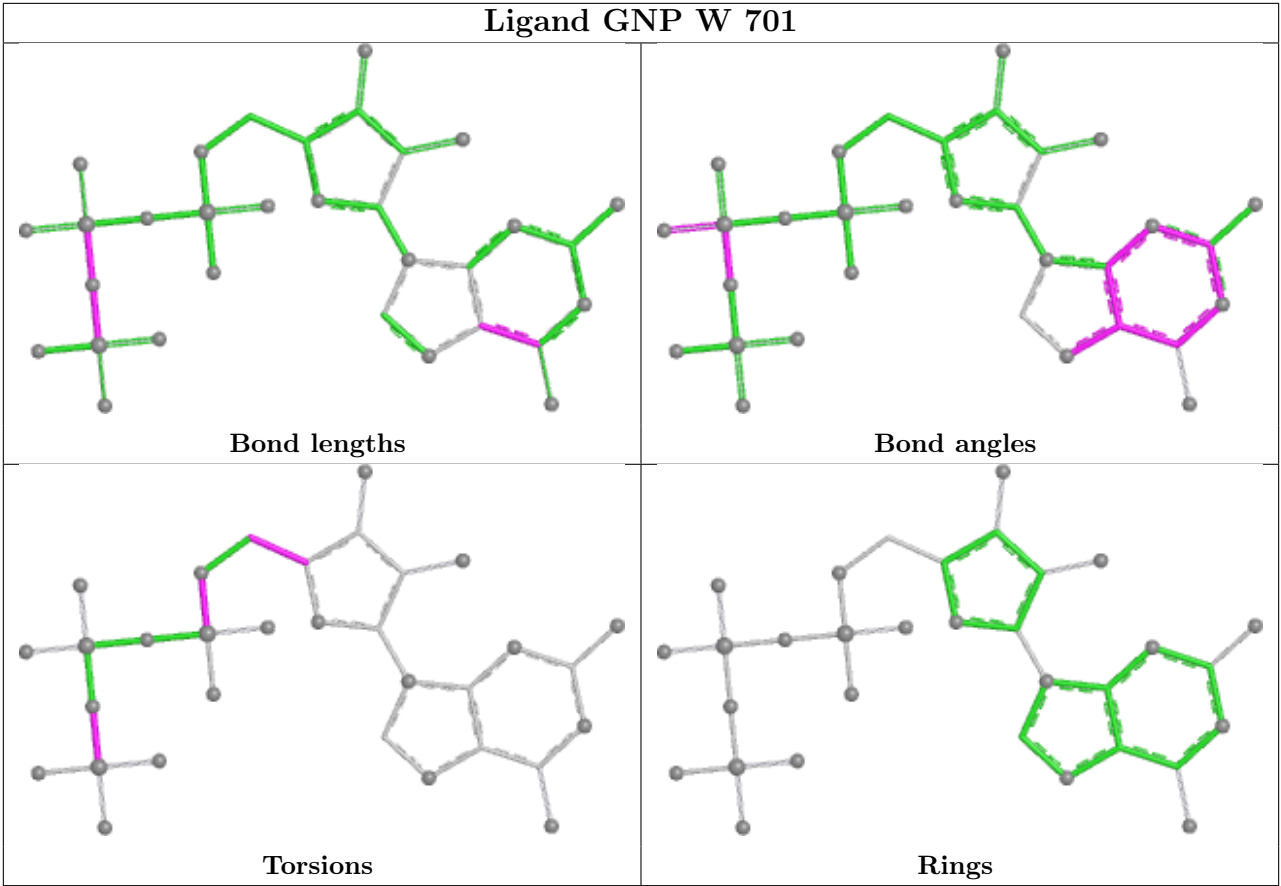
5 of 6 torsion outliers are listed below:

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.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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