



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 14, 2017 – 02:48 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 : 3.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

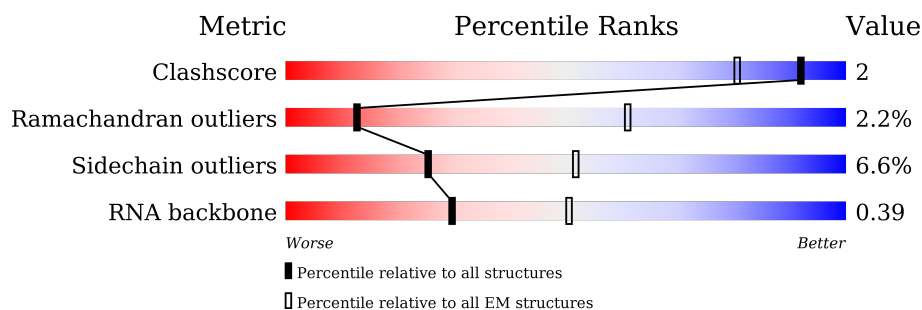
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 Å.

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













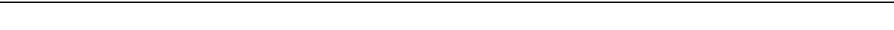

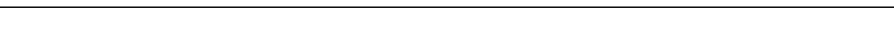
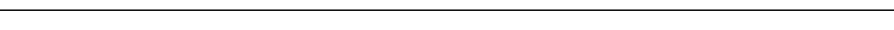



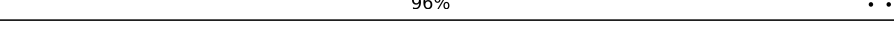


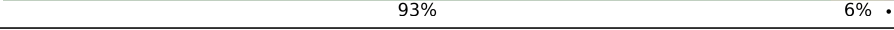
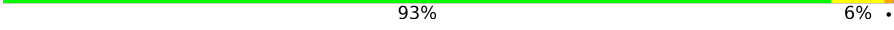



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

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

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Mol	Chain	Length	Quality of chain
9	H	176	 83% 6% 11%
10	I	244	 82% 8% 9%
11	J	256	 80% 10% 9%
12	K	191	 88% 10% .
13	L	221	 85% 10% 5%
14	M	174	 90% 7% . .
15	N	199	 85% 11% . .
16	O	138	 88% 10% . .
17	a	204	 95% 5%
18	b	199	 96% . .
19	c	184	 93% 6% .
20	d	186	 95% 5% .
21	e	189	 94% 6% .
22	f	172	 92% 8%
23	g	160	 91% 8% . .
24	h	121	 79% . 17%
25	i	137	 96% . .
26	j	155	 61% . 37%
27	k	142	 79% 6% 15%
28	l	127	 93% 6% . .
29	m	136	 93% 6% . .
30	n	149	 88% 11% . .
31	o	59	 88% 8% . .
32	p	105	 90% . 8%
33	q	113	 89% 7% .

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

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

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

## 2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 131766 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Eukaryotic translation initiation factor 6.

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

There are 19 discrepancies between the modelled and reference sequences:

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

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

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

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

chromosome XII sequence.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 45 is a protein called Ribosomal Protein uL1.

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

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

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

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

There are 77 discrepancies between the modelled and reference sequences:

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

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

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

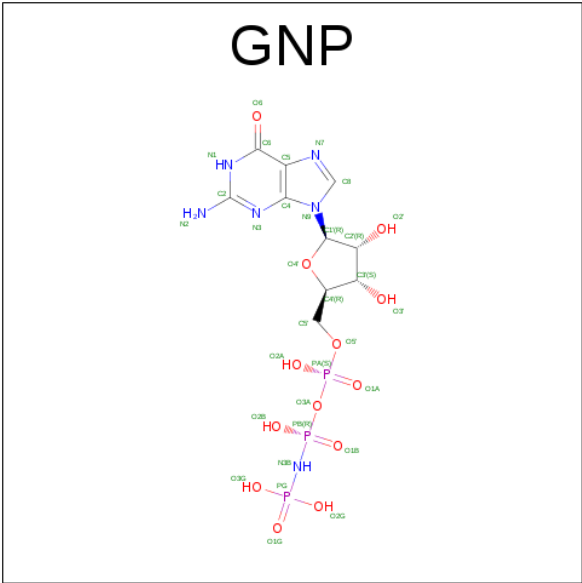
- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 50 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



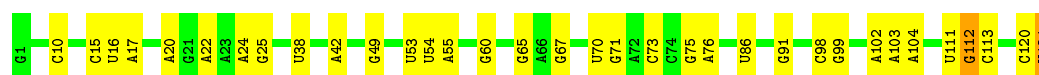


G2898	A2762	G2621	U2514	U2446	A2309	C2197	G1954	A1798	G1661	U1553	G1392	U1267	C1175
C2899	C2772	G2624	A2515	A2447	U2310	A2198	U1955	C1803	G1662	U1554	A1393	A1270	C1176
A2900	C2773	C2625	G2522	G2448	A2311	G	A	G1804	C1663	U1555	A1394	A1271	G1177
G2914	C2774	A2626	G2522	A2449	A2312	U	G	C1805	G1664	U1556	A1399	A1274	G1178
G2922	G2777	G2627	C2531	G2450	A2313	C	U	G1808	C1665	A1557	G1400	C1275	A1179
U2923	G2778	A2628	U2532	G2452	U2314	U	G	G1808	G1666	G1560	G1409	U1276	A1180
A2926	A2779	A2635	G2533	U2453	G2315	C	A	G1812	G1674	G1561	G1409	U1277	U1181
C2927	A2780	A2636	U2537	G2454	A2332	U	G	G1812	G1678	G1562	G1414	C1276	C1189
C2928	A2790	U2641	U2538	U2455	G2335	G	G	A1813	G1678	U1563	U1415	C1279	A1190
C2929	G2793	U2644	C2539	G2457	U2336	C	C	A1814	U1682	U1564	U1416	G1285	U1191
A2933	A2792	C2644	U2540	A2458	C2337	U	U	U1815	U1683	G1565	C1416	A1286	C1192
U2934	G2793	C2644	U2541	A2459	C2337	C	U	A1816	A1683	A1566	A1419	A1287	A1200
A2935	A2799	G2648	U2542	U2460	A2372	U	G	U1820	A1696	U1568	C1420	U1288	A1201
A2936	G2800	U2652	U2543	A2461	A2373	A	G	U1821	A1697	U1569	G1430	G1289	U1208
U2937	A2801	U2652	U2544	G2463	C2374	U	U	A1839	U1703	A1571	G1434	A1291	U1208
G2938	A2802	U2652	U2544	U2464	C2375	A	A	U1840	U1716	U1572	G1434	A1291	U1208
A2941	A2803	U2655	C2548	A2468	U2379	A2093	G	U1841	U1717	G1573	C1437	A1303	A1212
C2942	C2810	G2657	G2549	G2469	G2385	A2096	C	A1842	U1718	G1576	A1446	A1304	A1217
G2947	G2816	G2674	U2551	C2470	U2388	A2100	G	G1845	U1724	C1577	A1446	G1306	U1218
G2950	A2817	G2677	C2552	U2471	U2388	C2101	C	C1849	C1725	C1578	G1450	G1307	C1219
G2951	C2821	G2677	U2553	C2472	G2393	U2102	C	A1850	G1733	U1579	G1455	A1308	G1222
A2971	A2837	U2681	A2554	G2473	C2397	G2111	U	G1858	G1734	A1583	U1460	G1313	A1223
U2975	C2838	C2684	G2555	G2475	A2401	U2112	G	A1864	G1735	A1587	A1460	G1314	A1224
U2978	G2841	A2689	A2561	C2476	A2402	C2118	G	A1867	A1741	A1588	G1466	U1315	A1225
U2979	U2842	G2690	U2562	C2477	C2403	G2119	U	A1871	G1747	A1589	G1480	G1319	G1230
U2980	C2844	A2691	C2566	U2480	G2404	G2121	A	U1880	G1748	A1599	A1481	U1325	A1231
C2983	A2845	U2694	A2569	G2483	C2406	G2122	C	U1886	A1750	A1605	A1482	U1329	G1232
G2990	G2848	A2696	U2570	A2484	C2407	G2122	U	A1886	G1751	C1615	A1489	A1330	G1236
U2996	U2859	U2860	U2571	A2485	U2410	A2131	G	A1886	A1760	A1619	C1496	U1334	A1240
G2997	U2861	G2877	C2572	G2486	U2411	U2140	G	A1893	C1761	U1620	C1496	U1334	U1241
U2998	G2867	G2714	G2573	U2487	G2412	U2141	C	U1895	U1765	U1501	U1501	U1348	G1242
C3004	G2871	U2719	U2574	C2488	G2418	A2142	U	A1906	G1766	C1502	C1502	G1349	G1243
A3011	A2872	C2726	G2575	C2489	A2419	A2143	C	A1909	G1770	A1503	A1503	A1351	A1244
U3013	C2876	A2727	G2576	A2490	G2425	A2144	U	G1906	G1770	U1627	C1508	U1352	A1245
U3014	G2877	G2728	C2577	A2491	G2426	G2157	G	C1907	G1775	U1628	C1508	A1352	A1246
G3022	U2882	A2734	U2581	A2494	U2428	A2158	U	A1908	G1775	U1629	C1508	U1353	U1247
A3048	A2883	C2737	C2594	C2495	G2429	A2159	C	A1909	G1780	U1630	G1521	A1355	C1248
A3049	U2887	G2753	G2602	U2505	U2430	C2163	U	C1917	G1784	C1631	C1527	U1356	G1249
G3053	U2888	G2754	G2606	U2506	G2441	G2169	C	A1936	U1785	A1642	C1531	U1357	U1253
U3054	A2896	C2755	G2607	C2507	A2442	G2185	U	A1936	C1788	A1643	C1532	C1364	C1257
U3055	A2897	A2897	G2614	U2508	A2443	G2187	G	A1951	G1790	C1644	U1533	U1382	U1258
				U2513	A2445	U2191	U	G1952	G1796	U1645	G1536	U1382	G1262
						C2192	U	G1952	G1796	C1657	A1537	C1385	A1263
						C2196	G	G1952	G1796	G1658	G1547	A1386	G1264
							A	G1952	G1796	C1660		C1391	G1266



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

Chain B: 72% 26% .



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

Chain C: 73% 27% .



- Molecule 5: 60S ribosomal protein L2-A

Chain D: 91% 8% .



- Molecule 6: 60S ribosomal protein L3

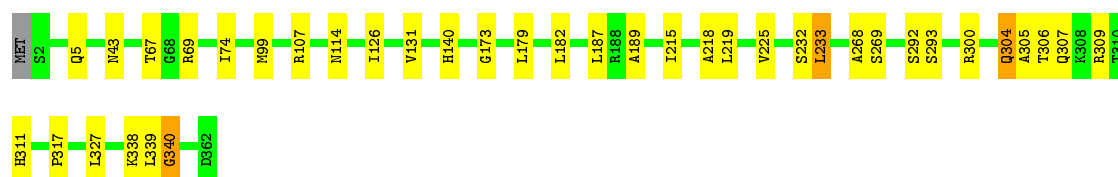
Chain E: 90% 10% .



- Molecule 7: 60S ribosomal protein L4-A

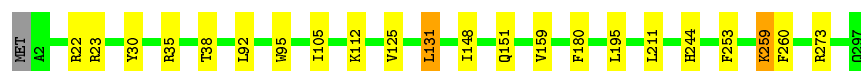
Chain F: 89% 10% .





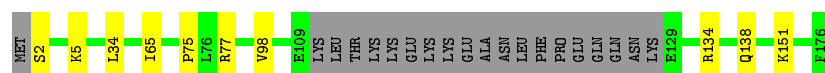
- Molecule 8: 60S ribosomal protein L5

Chain G: 92% 7%



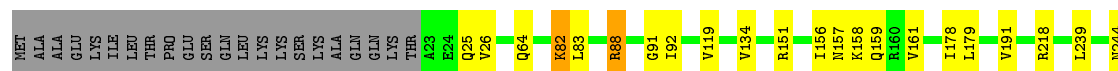
- Molecule 9: 60S ribosomal protein L6-A

Chain H: 83% 6% 11%



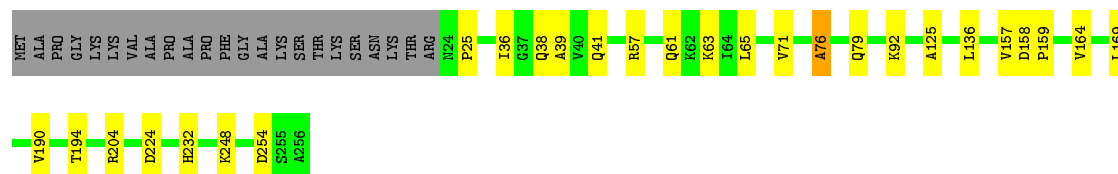
- Molecule 10: 60S ribosomal protein L7-A

Chain I: 82% 8% 9%



- Molecule 11: 60S ribosomal protein L8-A

Chain J: 80% 10% 9%



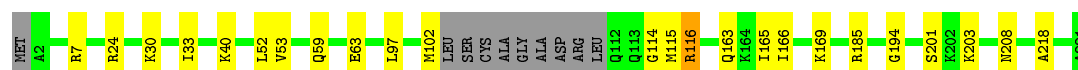
- Molecule 12: 60S ribosomal protein L9-A

Chain K: 88% 10% 2%



- Molecule 13: 60S ribosomal protein L10

Chain L: 85% 10% 5%




- Molecule 14: 60S ribosomal protein L11-A

Chain M:  90% 7% ..



- Molecule 15: 60S ribosomal protein L13-A

Chain N:  85% 11% ..



- Molecule 16: 60S ribosomal protein L14-A

Chain O:  88% 10% ..



- Molecule 17: 60S ribosomal protein L15-A

Chain a:  95% 5%



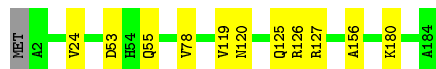
- Molecule 18: 60S ribosomal protein L16-A

Chain b:  96% ..



- Molecule 19: 60S ribosomal protein L17-A

Chain c:  93% 6% .



- Molecule 20: 60S ribosomal protein L18-A

Chain d:  95% 5% .



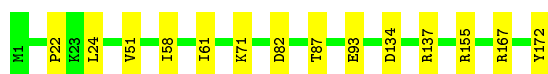
- Molecule 21: 60S ribosomal protein L19-A

Chain e:  94% 6%




- Molecule 22: 60S ribosomal protein L20-A

Chain f:  92% 8%




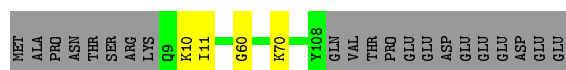
- Molecule 23: 60S ribosomal protein L21-A

Chain g:  91% 8%



- Molecule 24: 60S ribosomal protein L22-A

Chain h:  79% 17%



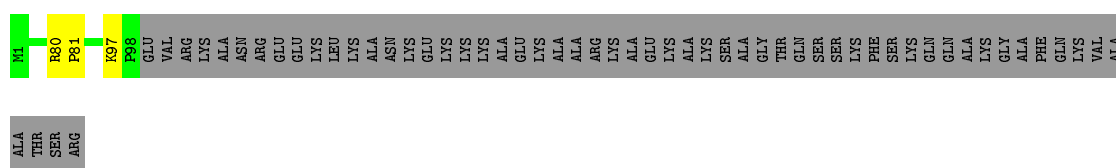
- Molecule 25: 60S ribosomal protein L23-A

Chain i:  96%




- Molecule 26: 60S ribosomal protein L24-A

Chain j:  61% 37%




- Molecule 27: 60S ribosomal protein L25

Chain k:  79% 6% 15%



- Molecule 28: 60S ribosomal protein L26-A

Chain l:  93% 6% ..




- Molecule 29: 60S ribosomal protein L27-A

Chain m:  93% 6% ..




- Molecule 30: 60S ribosomal protein L28

Chain n:  88% 11% ..




- Molecule 31: 60S ribosomal protein L29

Chain o:  88% 8% ..




- Molecule 32: 60S ribosomal protein L30

Chain p:  90% 8% .




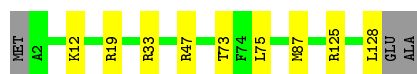
- Molecule 33: 60S ribosomal protein L31-A

Chain q:  89% 7% .




- Molecule 34: 60S ribosomal protein L32

Chain r:  91% 7% .



- Molecule 35: 60S ribosomal protein L33-A

Chain s:  91% 8% .



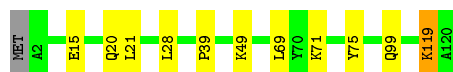
- Molecule 36: 60S ribosomal protein L34-A

Chain t: 86% 7% 7%



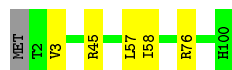
- Molecule 37: 60S ribosomal protein L35-A

Chain u: 90% 8% ..



- Molecule 38: 60S ribosomal protein L36-A

Chain v: 94% 5% .



- Molecule 39: 60S ribosomal protein L37-A

Chain w: 88% 11% .



- Molecule 40: 60S ribosomal protein L38

Chain x: 91% 8% .



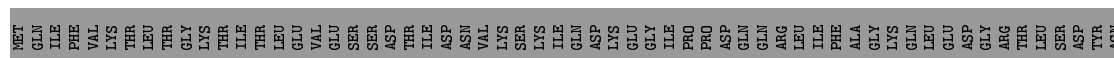
- Molecule 41: 60S ribosomal protein L39

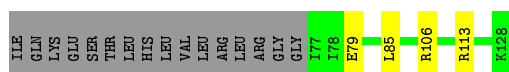
Chain y: 94% . .



- Molecule 42: Ubiquitin-60S ribosomal protein L40

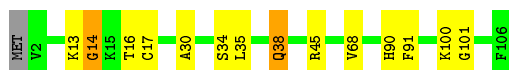
Chain z: 38% . 59%





- Molecule 43: 60S ribosomal protein L42-A

Chain Q: 86% 11% ..



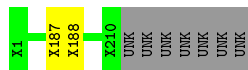
- Molecule 44: 60S ribosomal protein L43-A

Chain R: 90% 9% .



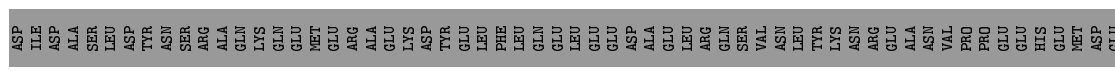
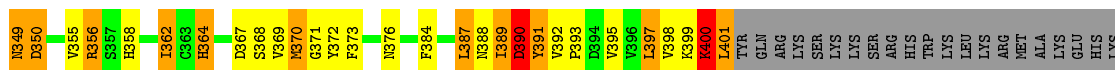
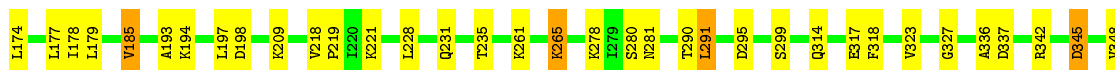
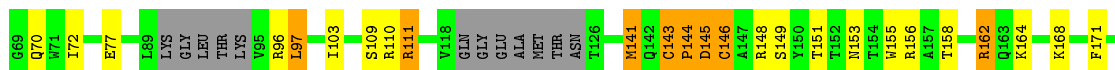
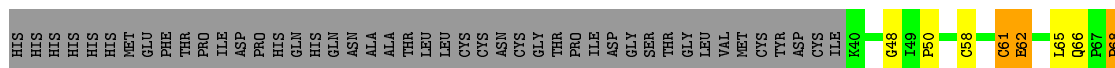
- Molecule 45: Ribosomal Protein uL1

Chain S: 96% ..



- Molecule 46: 60S ribosomal export protein NMD3

Chain V: 48% 13% 5% 33%



- Molecule 47: Large subunit GTPase 1

Chain W: 34% 10% 53%



HIS	ASN	PHE	H440	T339	R246	GLY	ASN	ASN	TRP	ASN
HIS	ALA	ASP	K444	Y344	W249	ASN	LEU	LEU	VAL	TRP
HIS	GLU	ARG	SER	P345	N346	ALA	LEU	LEU	VAL	LEU
HIS	ASP	PRO	ARG	N347	Y347	LYS	ARG	ARG	ARG	ARG
	ASP	THR	ASP	G348	S259	GLN	SER	SER	VAL	SER
	ARG	ARG	GLU	K349	F260	ARG	VAL	VAL	THR	THR
	ASP	LYS	GLY	T353	L265	LEU	GLN	GLN	GLU	GLU
	PHE	GLN	ASN	G362	A266	ALA	SER	SER	THR	SER
	VAL	VAL	GLY	S363	ARG	LEU	ALA	ALA	ALA	ALA
	GLN	ASN	I454	S366		LEU	ASP	ASP	LEU	LEU
	ASN	ALA	P455			ILE	ILE	ASP	ASP	ASP
	VAL	ALA	T456			VAL	PRO	PHE	GLU	GLU
	GLU	LYS	A457	G369	LEU	GLN	LEU	LEU	LEU	PHE
	ALA	ALA	L461	K370	GLU	ARG	ARG	SER	LEU	LEU
	ARG	LYS		T371	GLY	THR	THR	THR	SER	SER
	LEU	GLY	T472	K372	GLY	ALA	ALA	ALA	ALA	ALA
	SER	ILE	Q473	H373	GLY	LEU	LEU	LEU	LEU	LEU
	THR	ILE			GLY	GLY	GLY	GLY	GLY	GLY
	PRO	ILE	S477	T376	GLY	GLY	GLY	GLY	GLY	GLY
	PHE	VAL	A478	I377	GLY	GLY	GLY	GLY	GLY	GLY
	HIS	ASP	D479	K376	GLY	GLY	GLY	GLY	GLY	GLY
	LYS	LEU	E480	S380	GLY	GLY	GLY	GLY	GLY	GLY
	VAL	ALA	P481	D381	GLY	GLY	GLY	GLY	GLY	GLY
	GLN	ARG	R482		GLY	GLY	GLY	GLY	GLY	GLY
	ASN	ASP			GLY	GLY	GLY	GLY	GLY	GLY
	ASP	LEU	R485	N384	GLY	GLY	GLY	GLY	GLY	GLY
	SER	ASN		L385	GLY	GLY	GLY	GLY	GLY	GLY
	ALA	GLN	L487	C386	GLY	GLY	GLY	GLY	GLY	GLY
	GLY	LEU	Y488	D387	GLY	GLY	GLY	GLY	GLY	GLY
	LYS	THR	V489	C388	GLY	GLY	GLY	GLY	GLY	GLY
	ARG	PHE			GLY	GLY	GLY	GLY	GLY	GLY
	HIS	SER			GLY	GLY	GLY	GLY	GLY	GLY
	ASN	ALA	P502	F386	GLY	GLY	GLY	GLY	GLY	GLY
	LYS	HIS	P503	ALA	GLY	GLY	GLY	GLY	GLY	GLY
	LYS	THR	UNK	TYR	GLY	GLY	GLY	GLY	GLY	GLY
	LYS	ASN	LEU	ASN	GLY	GLY	GLY	GLY	GLY	GLY
	LYS	GLY	GLU	K400	GLY	GLY	GLY	GLY	GLY	GLY
	LYS	ASP	ASP		GLY	GLY	GLY	GLY	GLY	GLY
	LYS	THR	ASP	C405	GLY	GLY	GLY	GLY	GLY	GLY
	ASN	GLN	THR	M406	GLY	GLY	GLY	GLY	GLY	GLY
	ALA	LYS	PRO	G407	GLY	GLY	GLY	GLY	GLY	GLY
	LYS	GLU	TYR	V408	GLY	GLY	GLY	GLY	GLY	GLY
	SER	ALA	THR	L409	GLY	GLY	GLY	GLY	GLY	GLY
	LYS	LYS	ARG		GLY	GLY	GLY	GLY	GLY	GLY
	VAL	SER	GLU	Q413	GLY	GLY	GLY	GLY	GLY	GLY
	PHE	VAL	GLU		GLY	GLY	GLY	GLY	GLY	GLY
	SER	THR	CYS	G422	GLY	GLY	GLY	GLY	GLY	GLY
	ILE	HIS	GLU		GLY	GLY	GLY	GLY	GLY	GLY
	GLY	GLY	GLU	I428	GLY	GLY	GLY	GLY	GLY	GLY
	ASN	GLY	PHE	P429	GLY	GLY	GLY	GLY	GLY	GLY
	ASN	LYS	ASN	K430	GLY	GLY	GLY	GLY	GLY	GLY
	ALA	GLN	LYS	Y431	GLY	GLY	GLY	GLY	GLY	GLY
	ALA	ALA	ASP	Y432	GLY	GLY	GLY	GLY	GLY	GLY
	ALA	ALA	LEU		GLY	GLY	GLY	GLY	GLY	GLY
	LEU	LEU	TYR	I436	GLY	GLY	GLY	GLY	GLY	GLY
	GLU	TYR	VAL	Y437	GLY	GLY	GLY	GLY	GLY	GLY

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	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	Not provided, Not provided	Depositor
Microscope	FEI TECNAI F30, FEI TITAN KRIOS	Depositor
Voltage (kV)	300, 300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided, Not provided	Depositor
Minimum defocus (nm)	1500, Not provided	Depositor
Maximum defocus (nm)	4000, Not provided	Depositor
Magnification	31000, Not provided	Depositor
Image detector	Not provided, Not provided, Not provided	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

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

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	J	0	1
30	n	0	1
31	o	0	1
All	All	0	3

There are no bond length outliers.

All (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
2	A	3078	U	C4'-C3'-O3'	5.08	123.17	113.00
8	G	131	LEU	CA-CB-CG	5.05	126.91	115.30
39	w	11	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	n	1173	0	1215	0	0
31	o	462	0	491	0	0
32	p	743	0	797	0	0
33	q	876	0	912	0	0
34	r	1020	0	1090	0	0
35	s	850	0	880	0	0
36	t	880	0	945	0	0
37	u	969	0	1078	0	0
38	v	771	0	849	0	0
39	w	681	0	685	0	0
40	x	612	0	682	0	0
41	y	436	0	475	0	0
42	z	417	0	459	0	0
43	Q	847	0	918	4	0
44	R	694	0	738	2	0
45	S	1050	0	246	1	0
46	V	2713	0	2644	70	0
47	W	2236	0	2029	67	0
48	A	148	0	0	0	0
48	B	5	0	0	0	0
48	C	2	0	0	0	0
48	D	1	0	0	0	0
48	W	1	0	0	0	0
48	a	1	0	0	0	0
48	c	1	0	0	0	0
48	i	1	0	0	0	0
49	A	2	0	0	0	0
50	W	32	0	13	12	0
51	A	5	0	0	0	0
51	e	1	0	0	0	0
All	All	131766	0	95620	356	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (356) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2410:U:O4	2:A:2801:A:N1	1.61	1.33
47:W:349:LYS:HG2	50:W:701:GNP:O2B	1.32	1.30
2:A:2264:PSU:O2'	2:A:2265:C:H6	0.96	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:2258:PSU:H1'	47:W:193:ARG:NH1	1.56	1.18
2:A:1093:A:N3	2:A:1096:U:N3	1.92	1.16
2:A:2263:C:H2'	2:A:2264:PSU:H5'	1.23	1.16
2:A:1097:G:O2'	2:A:1098:A:OP2	1.62	1.14
47:W:371:THR:HG21	47:W:387:ASP:OD2	1.49	1.11
2:A:681:U:O2	2:A:696:C:N4	1.84	1.09
2:A:2252:A:N6	2:A:2264:PSU:C2	2.21	1.06
2:A:2264:PSU:O2'	2:A:2265:C:C6	1.75	1.02
2:A:1093:A:C2	2:A:1096:U:N3	2.29	1.00
47:W:209:ASN:ND2	47:W:212:LEU:HB3	1.76	1.00
2:A:1093:A:N9	2:A:1096:U:O4	1.96	0.98
2:A:2258:PSU:H1'	47:W:193:ARG:HH11	1.17	0.93
2:A:1190:A:N1	2:A:1315:U:O4	2.02	0.93
2:A:1093:A:C4	2:A:1096:U:O4	2.22	0.92
46:V:389:ILE:HG22	46:V:389:ILE:O	1.67	0.92
46:V:337:ASP:OD2	46:V:356:ARG:HG3	1.70	0.90
2:A:2258:PSU:C1'	47:W:193:ARG:NH1	2.36	0.88
2:A:2263:C:H2'	2:A:2264:PSU:C5'	2.03	0.87
2:A:2252:A:N6	2:A:2264:PSU:N1	2.21	0.86
2:A:1093:A:C4	2:A:1096:U:C4	2.64	0.85
47:W:349:LYS:CG	50:W:701:GNP:O2B	2.23	0.85
2:A:78:U:H5''	2:A:78:U:C6	2.11	0.84
2:A:2513:U:O2'	2:A:2514:U:P	2.35	0.84
2:A:2266:PSU:O2'	2:A:2267:C:O5'	1.95	0.83
2:A:2266:PSU:HO2'	2:A:2267:C:P	2.02	0.82
2:A:1093:A:C4	2:A:1096:U:N3	2.46	0.82
2:A:2263:C:C2'	2:A:2264:PSU:H5'	2.08	0.81
2:A:2257:C:C6	2:A:2257:C:H5''	2.16	0.80
2:A:2410:U:O4	2:A:2801:A:C2	2.35	0.80
46:V:367:ASP:CG	46:V:400:LYS:NZ	2.35	0.80
2:A:2252:A:N6	2:A:2264:PSU:HN1	1.79	0.79
5:D:126:LEU:HD13	5:D:150:LEU:HD21	1.62	0.79
2:A:2261:G:OP1	47:W:373:HIS:CE1	2.36	0.79
47:W:366:SER:HA	50:W:701:GNP:O3'	1.82	0.79
2:A:2264:PSU:O2'	2:A:2265:C:H5''	1.82	0.79
46:V:367:ASP:CG	46:V:400:LYS:HZ2	1.85	0.79
2:A:1093:A:C2	2:A:1096:U:C2	2.71	0.77
2:A:2267:C:H6	2:A:2267:C:H5''	1.49	0.77
46:V:372:TYR:CE1	46:V:398:VAL:CG2	2.68	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:V:372:TYR:CE1	46:V:398:VAL:HG21	2.20	0.76
2:A:1097:G:HO2'	2:A:1098:A:P	2.08	0.76
47:W:209:ASN:HD21	47:W:212:LEU:HB3	1.50	0.76
46:V:367:ASP:OD2	46:V:400:LYS:NZ	2.19	0.75
47:W:428:ILE:HG22	47:W:429:PRO:HD2	1.68	0.74
47:W:266:LEU:O	47:W:266:LEU:HD23	1.88	0.74
2:A:2513:U:O2'	2:A:2514:U:H2'	1.87	0.73
2:A:2261:G:OP1	47:W:373:HIS:NE2	2.20	0.73
2:A:2513:U:O2'	2:A:2514:U:OP1	2.06	0.73
2:A:1481:A:O2'	2:A:1858:A:H1'	1.89	0.73
2:A:2254:U:N3	2:A:2259:A:C2	2.56	0.72
2:A:2264:PSU:C2'	2:A:2265:C:C6	2.73	0.72
47:W:237:LYS:HG3	50:W:701:GNP:N2	2.04	0.71
47:W:211:LEU:HD21	47:W:252:TYR:OH	1.89	0.71
46:V:372:TYR:HE1	46:V:398:VAL:CG2	2.03	0.71
46:V:368:SER:O	46:V:401:LEU:C	2.28	0.71
2:A:2266:PSU:C6	2:A:2266:PSU:H3'	2.27	0.70
2:A:2410:U:C4	2:A:2801:A:N1	2.54	0.70
47:W:366:SER:HA	50:W:701:GNP:HO3'	1.53	0.70
46:V:389:ILE:CG2	46:V:389:ILE:O	2.40	0.69
47:W:210:PRO:HD2	47:W:249:TRP:CZ2	2.29	0.68
47:W:371:THR:CG2	47:W:387:ASP:OD2	2.35	0.68
2:A:1097:G:O2'	2:A:1098:A:P	2.50	0.68
47:W:363:SER:HB2	47:W:370:LYS:HE2	1.76	0.68
2:A:1093:A:C1'	2:A:1096:U:O4	2.42	0.67
12:K:41:ILE:HD11	12:K:67:ALA:HB1	1.74	0.67
2:A:2249:G:O2'	2:A:2250:G:O5'	2.11	0.67
46:V:350:ASP:OD2	46:V:350:ASP:N	2.27	0.67
2:A:399:A:HO2'	2:A:403:C:HO2'	1.43	0.67
46:V:109:SER:O	46:V:111:ARG:N	2.28	0.67
46:V:261:LYS:O	46:V:265:LYS:HG3	1.95	0.66
46:V:323:VAL:HG13	46:V:336:ALA:HB1	1.76	0.66
46:V:384:PHE:O	46:V:387:LEU:HB2	1.95	0.66
46:V:401:LEU:HD22	46:V:401:LEU:O	1.96	0.66
46:V:61:CYS:O	46:V:62:GLU:HB2	1.96	0.66
46:V:401:LEU:HD13	46:V:401:LEU:O	1.96	0.66
2:A:2252:A:H61	2:A:2264:PSU:HN1	1.28	0.66
2:A:1093:A:N3	2:A:1096:U:C4	2.63	0.65
2:A:2841:G:C6	2:A:2844:C:H5	2.14	0.65
46:V:231:GLN:O	46:V:231:GLN:HG3	1.97	0.64
2:A:2513:U:O2'	2:A:2514:U:O5'	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:W:428:ILE:HG22	47:W:429:PRO:CD	2.28	0.64
2:A:2256:A:H3'	2:A:2257:C:H5''	1.79	0.63
2:A:2513:U:H4'	2:A:2514:U:OP1	1.98	0.63
2:A:1093:A:C2	2:A:1096:U:O2	2.51	0.63
47:W:379:LEU:HB2	47:W:385:LEU:HD21	1.79	0.63
2:A:78:U:OP1	2:A:78:U:H4'	1.99	0.62
46:V:373:PHE:HD1	46:V:395:VAL:HG22	1.64	0.62
46:V:369:VAL:HG12	46:V:400:LYS:HA	1.81	0.62
2:A:640:U:OP1	15:N:21:ARG:NH2	43.49	0.62
47:W:209:ASN:HD22	47:W:212:LEU:HD23	1.64	0.62
46:V:342:ARG:HB2	46:V:345:ASP:HB2	1.81	0.61
2:A:1661:G:H2'	2:A:1662:G:C8	2.34	0.61
46:V:65:LEU:HD22	46:V:141:MET:CE	2.31	0.61
47:W:241:LEU:CD1	47:W:499:VAL:HG11	2.32	0.60
47:W:371:THR:O	47:W:371:THR:HG22	2.01	0.60
46:V:348:VAL:O	46:V:349:ASN:CB	2.49	0.60
46:V:392:VAL:HG13	46:V:393:PRO:HD2	1.82	0.60
47:W:194:VAL:HG11	47:W:388:CYS:SG	2.42	0.60
46:V:144:PRO:O	46:V:148:ARG:HD3	2.02	0.59
6:E:215:ILE:HD12	6:E:338:LEU:HD12	1.84	0.59
46:V:362:ILE:HG13	46:V:362:ILE:O	2.00	0.59
47:W:344:TYR:CD2	47:W:408:VAL:HG21	2.37	0.59
2:A:2266:PSU:H6	2:A:2266:PSU:H3'	1.65	0.59
2:A:2267:C:C6	2:A:2267:C:H5''	2.36	0.58
2:A:1093:A:C8	2:A:1096:U:O4	2.56	0.58
2:A:2249:G:O2'	2:A:2250:G:P	2.61	0.58
46:V:392:VAL:CG1	46:V:393:PRO:HD2	2.34	0.58
47:W:237:LYS:HG3	50:W:701:GNP:C2	2.33	0.58
2:A:2258:PSU:H6	2:A:2258:PSU:O5'	1.87	0.58
2:A:2268:U:H5'	2:A:2269:U:OP2	2.04	0.58
46:V:372:TYR:HE1	46:V:398:VAL:HG21	1.62	0.58
2:A:2266:PSU:C3'	2:A:2266:PSU:C6	2.85	0.57
8:G:148:ILE:HG13	8:G:159:VAL:HG11	1.85	0.57
46:V:291:LEU:HD11	46:V:358:HIS:CB	2.34	0.57
47:W:209:ASN:HD21	47:W:212:LEU:CB	2.18	0.57
2:A:78:U:C5'	2:A:78:U:C6	2.85	0.56
47:W:212:LEU:HD12	47:W:212:LEU:O	2.06	0.56
2:A:2263:C:C2'	2:A:2264:PSU:C5'	2.78	0.56
2:A:706:A:H2'	2:A:707:U:O4'	2.06	0.56
46:V:146:CYS:O	46:V:149:SER:OG	2.15	0.55
47:W:209:ASN:ND2	47:W:212:LEU:CB	2.62	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1097:G:C2'	2:A:1098:A:OP2	2.52	0.55
46:V:162:ARG:NH2	46:V:193:ALA:HB3	2.21	0.55
47:W:349:LYS:N	50:W:701:GNP:O2B	2.37	0.55
46:V:388:ASN:HB3	46:V:391:TYR:HB2	1.88	0.55
46:V:318:PHE:CE2	46:V:342:ARG:HG2	2.41	0.55
2:A:3217:C:O2	2:A:3217:C:C2'	2.56	0.54
47:W:265:ALA:O	47:W:266:LEU:HB3	2.07	0.54
47:W:472:THR:HG22	47:W:479:ASP:HB3	1.89	0.54
46:V:143:CYS:O	46:V:145:ASP:N	2.40	0.54
47:W:376:THR:CG2	47:W:384:MET:SD	2.96	0.54
47:W:266:LEU:HD13	50:W:701:GNP:N1	2.23	0.54
2:A:2258:PSU:C1'	47:W:193:ARG:HH12	2.19	0.54
2:A:1189:C:N3	2:A:1315:U:O2	2.41	0.53
2:A:1573:G:H2'	2:A:1573:G:N3	2.23	0.53
3:B:121:U:O4'	3:B:121:U:O2	2.27	0.53
2:A:1286:A:N3	2:A:1287:A:H1'	2.23	0.53
2:A:1093:A:N3	2:A:1096:U:H3	1.45	0.53
46:V:261:LYS:NZ	46:V:265:LYS:HD3	2.23	0.53
2:A:681:U:H2'	2:A:696:C:N4	2.23	0.53
47:W:385:LEU:HD23	47:W:385:LEU:N	2.24	0.53
5:D:104:LEU:CD2	5:D:158:ILE:HD11	2.38	0.52
2:A:2249:G:HO2'	2:A:2250:G:P	2.33	0.52
46:V:348:VAL:O	46:V:349:ASN:HB3	2.09	0.52
2:A:1093:A:N3	2:A:1096:U:C2	2.75	0.52
47:W:502:PRO:HB2	47:W:503:PRO:CD	2.40	0.52
2:A:2257:C:H2'	2:A:2257:C:O2	2.09	0.52
47:W:376:THR:O	47:W:377:ILE:HD13	2.10	0.52
2:A:590:G:O2'	7:F:309:ARG:NH1	2.42	0.52
2:A:2257:C:H6	2:A:2257:C:H5''	1.69	0.52
46:V:144:PRO:O	46:V:148:ARG:CD	2.57	0.52
47:W:266:LEU:CD2	47:W:266:LEU:N	2.73	0.51
2:A:681:U:O2	2:A:696:C:C4	2.60	0.51
13:L:53:VAL:HG21	13:L:166:ILE:HD12	1.91	0.51
2:A:2251:G:C2	2:A:2266:PSU:O4	2.64	0.51
8:G:30:TYR:HB3	8:G:38:THR:HG22	10.70	0.51
2:A:3153:U:O4'	2:A:3153:U:O2	2.29	0.51
2:A:1329:U:H1'	2:A:1330:A:OP1	2.11	0.51
2:A:2490:C:H1'	2:A:2491:A:N7	2.27	0.50
2:A:2947:G:N3	6:E:250:ALA:HB1	2.25	0.50
46:V:401:LEU:HD22	46:V:401:LEU:C	2.29	0.50
47:W:379:LEU:CB	47:W:385:LEU:HD21	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2163:C:O2'	5:D:11:GLY:HA3	2.11	0.50
47:W:200:LEU:HB3	47:W:339:ILE:HG22	1.93	0.50
2:A:2636:A:N1	2:A:2641:U:O4	2.45	0.50
8:G:180:PHE:HB3	8:G:195:LEU:HD13	1.94	0.50
47:W:265:ALA:N	50:W:701:GNP:O6	2.43	0.50
2:A:103:G:OP1	15:N:70:ARG:NH2	2.42	0.50
2:A:2249:G:C8	2:A:2249:G:H3'	2.47	0.50
2:A:436:A:H2'	2:A:437:G:O4'	2.12	0.50
46:V:355:VAL:HG21	46:V:395:VAL:O	2.12	0.50
47:W:346:ASN:OD1	50:W:701:GNP:H4'	2.11	0.50
12:K:124:ARG:HB3	12:K:164:ILE:HD12	1.94	0.49
47:W:376:THR:HG21	47:W:384:MET:SD	2.53	0.49
2:A:2410:U:H3	2:A:2801:A:H61	1.60	0.49
2:A:2252:A:N1	2:A:2264:PSU:N1	2.60	0.49
44:R:42:CYS:SG	44:R:57:CYS:SG	3.11	0.49
47:W:237:LYS:HD2	50:W:701:GNP:N3	2.27	0.49
2:A:2185:G:O2'	2:A:2314:U:OP2	2.26	0.49
2:A:2635:A:C2	2:A:2641:U:C5	3.00	0.49
3:B:112:G:H2'	3:B:113:C:C6	2.48	0.49
2:A:2266:PSU:H2'	2:A:2267:C:C6	2.48	0.49
10:I:88:ARG:NH1	10:I:91:GLY:O	2.46	0.48
2:A:2264:PSU:O2'	2:A:2265:C:C5'	2.58	0.48
43:Q:90:HIS:NE2	46:V:314:GLN:OE1	2.43	0.48
47:W:214:ARG:HH12	47:W:258:ILE:HD13	1.78	0.48
7:F:338:LYS:O	7:F:340:GLY:N	2.46	0.48
2:A:2636:A:H61	2:A:2641:U:H3	1.61	0.48
7:F:126:ILE:HD11	7:F:233:LEU:HD13	1.95	0.48
46:V:61:CYS:O	46:V:62:GLU:CB	2.60	0.48
46:V:70:GLN:NE2	46:V:70:GLN:N	2.60	0.48
2:A:1554:U:C4'	2:A:1555:U:O5'	2.61	0.48
46:V:70:GLN:H	46:V:70:GLN:CD	2.17	0.48
2:A:2264:PSU:O4	2:A:2264:PSU:H2'	2.13	0.48
2:A:1717:U:H2'	2:A:1718:G:C8	2.48	0.48
6:E:168:LYS:O	6:E:319:ASN:ND2	2.47	0.48
2:A:1190:A:N1	2:A:1315:U:C4	2.78	0.48
47:W:211:LEU:HD13	47:W:211:LEU:O	2.13	0.48
47:W:237:LYS:CG	50:W:701:GNP:N2	2.73	0.47
46:V:68:PRO:HB2	46:V:70:GLN:OE1	2.13	0.47
10:I:151:ARG:HD2	10:I:244:ASN:HD22	1.79	0.47
47:W:211:LEU:CD2	47:W:252:TYR:OH	2.59	0.47
2:A:2624:G:OP1	46:V:162:ARG:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:41:ILE:O	12:K:41:ILE:HD13	2.13	0.47
2:A:1784:G:H2'	2:A:1785:U:O4'	2.14	0.47
2:A:315:C:N4	2:A:316:U:O4	2.48	0.47
10:I:88:ARG:HA	10:I:134:VAL:HG12	1.95	0.47
1:X:107:VAL:HG13	1:X:118:HIS:HB2	1.97	0.47
7:F:219:LEU:HD22	7:F:225:VAL:HG11	1.96	0.47
46:V:218:VAL:HG22	46:V:219:PRO:HD2	1.96	0.47
2:A:681:U:C2'	2:A:696:C:N4	2.78	0.47
2:A:2483:G:N2	2:A:2486:A:N7	2.62	0.47
12:K:86:TYR:CE2	12:K:151:VAL:HG22	2.50	0.47
47:W:502:PRO:HB2	47:W:503:PRO:HD3	1.96	0.47
2:A:2312:A:O2'	2:A:2315:G:N3	2.41	0.46
2:A:3214:U:O2	2:A:3214:U:O4'	2.31	0.46
2:A:2947:G:C2	6:E:250:ALA:HB1	2.51	0.46
46:V:174:LEU:O	46:V:178:ILE:HG22	2.15	0.46
46:V:399:LYS:O	46:V:400:LYS:O	2.33	0.46
47:W:480:GLU:N	47:W:481:PRO:CD	2.79	0.46
2:A:2257:C:C6	2:A:2257:C:C5'	2.95	0.46
47:W:214:ARG:HG2	47:W:215:SER:N	2.31	0.46
1:X:106:ASN:ND2	1:X:150:SER:OG	2.48	0.46
16:O:68:LEU:HD21	16:O:93:LYS:HD2	1.97	0.46
2:A:2922:G:O6	46:V:235:THR:OG1	2.34	0.46
2:A:2887:A:H2'	2:A:2887:A:N3	2.30	0.46
2:A:1839:A:O2'	2:A:1840:U:H5''	2.16	0.46
5:D:126:LEU:HD13	5:D:150:LEU:CD2	2.42	0.46
46:V:323:VAL:CG1	46:V:336:ALA:HB1	2.46	0.46
10:I:156:ILE:HD12	10:I:161:VAL:HG21	1.98	0.46
1:X:102:SER:OG	1:X:103:ALA:N	2.48	0.46
2:A:2249:G:C2'	2:A:2250:G:O5'	2.63	0.45
2:A:2295:A:N3	2:A:2929:C:O2'	2.49	0.45
2:A:824:C:H2'	2:A:825:U:O5'	2.16	0.45
2:A:1175:C:O5'	2:A:1175:C:H6	1.99	0.45
6:E:188:ILE:HD12	6:E:189:SER:N	2.32	0.45
2:A:2264:PSU:O2'	2:A:2265:C:O4'	2.35	0.45
2:A:681:U:O2	2:A:696:C:C5	2.70	0.45
47:W:222:VAL:HG11	47:W:231:ASN:HB3	1.98	0.45
2:A:979:U:C2	2:A:980:A:C2	3.05	0.45
46:V:96:ARG:O	46:V:97:LEU:CB	2.64	0.45
2:A:2271:A:N7	2:A:2272:G:C6	2.85	0.45
46:V:364:HIS:CB	46:V:367:ASP:OD2	2.64	0.45
2:A:2196:C:HO2'	2:A:2270:A:H8	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1100:U:H2'	2:A:1101:G:O4'	2.16	0.44
2:A:2841:G:C6	2:A:2844:C:C5	3.02	0.44
2:A:687:U:OP2	15:N:36:ARG:NH2	2.50	0.44
2:A:1658:G:H2'	2:A:1659:U:O4'	2.17	0.44
2:A:1696:A:H2'	2:A:1697:A:C8	2.52	0.44
2:A:2876:C:H2'	2:A:2877:G:O4'	2.17	0.44
14:M:14:ILE:HD12	14:M:14:ILE:N	2.32	0.44
2:A:681:U:H2'	2:A:696:C:H42	1.81	0.44
46:V:367:ASP:CB	46:V:400:LYS:HZ2	2.30	0.44
47:W:432:TYR:CE2	47:W:436:ILE:HD11	2.52	0.44
47:W:213:PHE:CE2	47:W:347:VAL:CG2	3.00	0.44
2:A:2256:A:H3'	2:A:2257:C:H6	1.82	0.44
2:A:1895:A:O2'	2:A:3053:G:H4'	2.17	0.44
2:A:662:U:H2'	2:A:663:C:C6	2.52	0.44
2:A:1018:G:N7	2:A:1035:G:N2	2.66	0.44
46:V:280:SER:OG	46:V:281:ASN:N	2.49	0.44
2:A:2267:C:H6	2:A:2267:C:C5'	2.26	0.44
46:V:162:ARG:HH22	46:V:193:ALA:HB3	1.82	0.44
47:W:370:LYS:O	47:W:371:THR:HB	2.18	0.44
47:W:473:GLN:HB2	47:W:473:GLN:HE21	1.56	0.44
2:A:2249:G:C8	2:A:2249:G:C3'	3.01	0.43
2:A:2257:C:H5'	2:A:2258:PSU:HN1	1.83	0.43
2:A:2488:A:OP2	2:A:2490:C:N4	2.50	0.43
2:A:2882:U:H2'	2:A:2883:U:O4'	2.18	0.43
2:A:787:G:H2'	2:A:788:C:C6	2.53	0.43
2:A:831:G:O2'	2:A:1864:A:N3	2.46	0.43
2:A:3106:A:N6	2:A:3128:G:O2'	2.50	0.43
2:A:3354:U:O2	2:A:3354:U:O4'	2.35	0.43
47:W:454:ILE:HB	47:W:455:PRO:CD	2.48	0.43
2:A:1804:A:H2'	2:A:1805:C:C6	2.54	0.43
2:A:324:A:C6	2:A:325:A:N6	2.87	0.43
15:N:165:SER:O	15:N:167:PHE:N	2.51	0.43
44:R:50:GLY:O	44:R:51:ALA:HB3	2.18	0.43
46:V:291:LEU:HD11	46:V:358:HIS:HB2	2.01	0.43
4:C:154:C:H2'	4:C:155:A:O4'	2.19	0.43
7:F:215:ILE:HA	7:F:218:ALA:HB3	2.01	0.43
43:Q:14:GLY:O	43:Q:16:THR:N	2.48	0.43
2:A:1176:C:H2'	2:A:1177:G:N2	2.34	0.43
16:O:55:ARG:NH2	16:O:76:ALA:O	2.51	0.43
2:A:435:C:H2'	2:A:436:A:C8	2.53	0.43
2:A:651:G:C6	2:A:652:G:C6	3.06	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:256:HIS:HA	6:E:257:PRO:C	2.39	0.42
46:V:317:GLU:HA	46:V:370:MET:HE3	2.01	0.42
2:A:1093:A:C1'	2:A:1096:U:C4	3.02	0.42
2:A:1225:A:C2	2:A:3116:G:C4	3.07	0.42
2:A:3322:A:H2'	2:A:3323:A:C8	2.54	0.42
7:F:304:GLN:O	7:F:306:THR:N	2.52	0.42
47:W:363:SER:CB	47:W:370:LYS:HE2	2.46	0.42
10:I:82:LYS:HA	10:I:119:VAL:HB	1.99	0.42
11:J:158:ASP:HB3	11:J:159:PRO:HD3	2.01	0.42
46:V:290:THR:O	46:V:291:LEU:C	2.57	0.42
1:X:28:VAL:HG13	1:X:52:THR:HG23	2.01	0.42
2:A:1482:A:H4'	2:A:1483:G:OP2	2.19	0.42
2:A:2191:U:H2'	2:A:2192:C:O4'	2.19	0.42
2:A:2926:A:H2'	2:A:2927:C:O4'	2.19	0.42
12:K:28:VAL:HG22	12:K:33:THR:HG22	2.01	0.42
43:Q:38:GLN:HA	43:Q:38:GLN:HE21	1.85	0.42
46:V:155:TRP:CZ3	46:V:158:THR:OG1	2.72	0.42
2:A:2435:G:N7	2:A:2593:A:H2'	2.34	0.42
2:A:3237:U:H2'	2:A:3238:G:O4'	2.19	0.42
3:B:16:U:H2'	3:B:17:A:O4'	2.19	0.42
43:Q:68:VAL:HG11	43:Q:91:PHE:CE1	2.54	0.42
46:V:355:VAL:HG22	46:V:356:ARG:O	2.20	0.42
46:V:65:LEU:HD22	46:V:141:MET:HE1	2.02	0.42
46:V:70:GLN:CD	46:V:70:GLN:N	2.73	0.42
2:A:2293:C:O2'	47:W:473:GLN:NE2	2.51	0.42
47:W:205:VAL:HG13	47:W:213:PHE:HB2	2.01	0.42
2:A:2513:U:C4'	2:A:2514:U:OP1	2.66	0.42
1:X:102:SER:HG	1:X:103:ALA:H	1.68	0.42
2:A:2244:A:OP1	5:D:243:THR:OG1	2.38	0.41
11:J:71:VAL:HG21	11:J:76:ALA:HB2	2.00	0.41
13:L:59:GLN:HE22	13:L:97:LEU:HD21	1.85	0.41
45:S:187:UNK:O	45:S:188:UNK:CB	2.67	0.41
47:W:213:PHE:CD2	47:W:347:VAL:HG21	2.55	0.41
2:A:2290:C:O2'	47:W:413:GLN:NE2	2.54	0.41
46:V:371:GLY:HA3	46:V:397:LEU:HA	2.01	0.41
2:A:2434:U:O4'	2:A:2434:U:O2	2.38	0.41
2:A:979:U:N3	2:A:980:A:C2	2.88	0.41
46:V:58:CYS:HB2	46:V:143:CYS:HB3	2.00	0.41
3:B:15:C:C2	3:B:16:U:C5	3.09	0.41
2:A:2448:G:H2'	2:A:2449:A:O4'	2.21	0.41
2:A:1093:A:H2	2:A:1096:U:O2	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3305:A:H2'	2:A:3306:U:O4'	2.21	0.41
2:A:824:C:C2'	2:A:825:U:O5'	2.68	0.41
47:W:422:GLY:HA2	47:W:457:ALA:HB2	2.03	0.41
2:A:526:C:N3	2:A:527:A:N6	2.69	0.41
2:A:1190:A:N3	2:A:1190:A:H2'	2.36	0.41
3:B:24:A:H2'	3:B:25:G:O4'	2.21	0.41
47:W:209:ASN:ND2	47:W:212:LEU:HD23	2.32	0.41
2:A:1093:A:O4'	2:A:1096:U:O4	2.39	0.41
12:K:41:ILE:HD11	12:K:67:ALA:CB	2.45	0.41
46:V:162:ARG:NH1	46:V:198:ASP:OD2	2.54	0.41
15:N:47:ALA:CB	15:N:48:PRO:CD	2.99	0.40
46:V:387:LEU:HD13	46:V:392:VAL:HG22	2.03	0.40
2:A:1420:C:OP2	7:F:189:ALA:O	2.39	0.40
2:A:2252:A:H61	2:A:2264:PSU:O2	1.30	0.40
46:V:364:HIS:HB2	46:V:367:ASP:OD2	2.22	0.40
2:A:1129:A:H2'	2:A:1130:A:C8	2.57	0.40
2:A:2256:A:H3'	2:A:2257:C:C5'	2.49	0.40
4:C:15:G:C6	4:C:16:G:N1	2.90	0.40
2:A:664:U:H5'	7:F:107:ARG:HA	2.04	0.40
2:A:1385:C:HO2'	9:H:2:SER:N	2.19	0.40
2:A:2266:PSU:H4'	2:A:2267:C:OP1	2.21	0.40
6:E:218:ILE:HG12	6:E:276:THR:HG23	2.02	0.40
9:H:75:PRO:HA	9:H:138:GLN:HE22	1.86	0.40
46:V:151:THR:O	46:V:153:ASN:N	2.52	0.40
47:W:461:LEU:HD13	47:W:480:GLU:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	222/264 (84%)	202 (91%)	20 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	D	250/254 (98%)	226 (90%)	22 (9%)	2 (1%)	24	62
6	E	384/387 (99%)	346 (90%)	31 (8%)	7 (2%)	11	46
7	F	359/362 (99%)	311 (87%)	32 (9%)	16 (4%)	3	21
8	G	294/297 (99%)	265 (90%)	25 (8%)	4 (1%)	14	50
9	H	152/176 (86%)	133 (88%)	16 (10%)	3 (2%)	9	43
10	I	220/244 (90%)	200 (91%)	14 (6%)	6 (3%)	6	35
11	J	231/256 (90%)	207 (90%)	17 (7%)	7 (3%)	5	33
12	K	189/191 (99%)	169 (89%)	17 (9%)	3 (2%)	12	48
13	L	207/221 (94%)	186 (90%)	16 (8%)	5 (2%)	7	38
14	M	167/174 (96%)	143 (86%)	19 (11%)	5 (3%)	5	33
15	N	191/199 (96%)	168 (88%)	18 (9%)	5 (3%)	7	36
16	O	134/138 (97%)	119 (89%)	10 (8%)	5 (4%)	4	27
17	a	201/204 (98%)	188 (94%)	11 (6%)	2 (1%)	19	58
18	b	195/199 (98%)	184 (94%)	11 (6%)	0	100	100
19	c	181/184 (98%)	163 (90%)	17 (9%)	1 (1%)	30	68
20	d	183/186 (98%)	162 (88%)	18 (10%)	3 (2%)	12	48
21	e	186/189 (98%)	173 (93%)	9 (5%)	4 (2%)	8	41
22	f	170/172 (99%)	156 (92%)	11 (6%)	3 (2%)	11	46
23	g	157/160 (98%)	141 (90%)	13 (8%)	3 (2%)	10	45
24	h	98/121 (81%)	79 (81%)	17 (17%)	2 (2%)	9	43
25	i	134/137 (98%)	124 (92%)	9 (7%)	1 (1%)	26	66
26	j	96/155 (62%)	81 (84%)	12 (12%)	3 (3%)	5	32
27	k	119/142 (84%)	107 (90%)	11 (9%)	1 (1%)	24	62
28	l	124/127 (98%)	115 (93%)	7 (6%)	2 (2%)	12	48
29	m	133/136 (98%)	111 (84%)	18 (14%)	4 (3%)	5	33
30	n	146/149 (98%)	126 (86%)	13 (9%)	7 (5%)	3	20
31	o	56/59 (95%)	48 (86%)	5 (9%)	3 (5%)	2	17
32	p	95/105 (90%)	88 (93%)	7 (7%)	0	100	100
33	q	107/113 (95%)	98 (92%)	6 (6%)	3 (3%)	6	34
34	r	125/130 (96%)	121 (97%)	3 (2%)	1 (1%)	24	62
35	s	104/107 (97%)	95 (91%)	7 (7%)	2 (2%)	10	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	t	110/121 (91%)	102 (93%)	6 (6%)	2 (2%)	11	46
37	u	117/120 (98%)	109 (93%)	4 (3%)	4 (3%)	5	29
38	v	97/100 (97%)	88 (91%)	8 (8%)	1 (1%)	19	58
39	w	85/88 (97%)	77 (91%)	6 (7%)	2 (2%)	7	38
40	x	75/78 (96%)	67 (89%)	5 (7%)	3 (4%)	4	24
41	y	48/51 (94%)	44 (92%)	3 (6%)	1 (2%)	9	42
42	z	50/128 (39%)	47 (94%)	2 (4%)	1 (2%)	9	43
43	Q	103/106 (97%)	88 (85%)	10 (10%)	5 (5%)	3	19
44	R	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
46	V	344/524 (66%)	302 (88%)	27 (8%)	15 (4%)	3	22
47	W	231/651 (36%)	198 (86%)	25 (11%)	8 (4%)	4	29
All	All	6959/7997 (87%)	6240 (90%)	564 (8%)	155 (2%)	13	41

All (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
21	e	131	ALA
23	g	124	VAL
26	j	81	PRO
30	n	78	LEU
33	q	61	LYS
43	Q	30	ALA
46	V	72	ILE
46	V	97	LEU
46	V	110	ARG
46	V	144	PRO
46	V	185	VAL
46	V	389	ILE
46	V	400	LYS
47	W	348	GLY
47	W	498	TYR
6	E	187	SER
6	E	347	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	E	348	ARG
7	F	182	LEU
7	F	269	SER
7	F	293	SER
7	F	305	ALA
10	I	178	ILE
14	M	10	ARG
14	M	95	ASN
14	M	114	ILE
15	N	76	THR
16	O	8	LYS
16	O	29	ALA
20	d	41	ASP
20	d	98	LYS
26	j	97	LYS
28	l	84	LYS
30	n	66	ALA
35	s	88	ASN
36	t	77	GLY
46	V	77	GLU
46	V	390	ASP
47	W	454	ILE
7	F	140	HIS
7	F	173	GLY
7	F	232	SER
7	F	233	LEU
7	F	268	ALA
8	G	259	LYS
8	G	260	PHE
10	I	158	LYS
11	J	25	PRO
11	J	36	ILE
15	N	166	ALA
22	f	167	ARG
23	g	159	PHE
31	o	25	LYS
35	s	91	ALA
37	u	39	PRO
38	v	3	VAL
40	x	18	ALA
43	Q	34	SER
46	V	62	GLU

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Mol	Chain	Res	Type
46	V	194	LYS
47	W	380	SER
47	W	502	PRO
5	D	144	ASN
7	F	292	SER
7	F	311	HIS
8	G	253	PHE
9	H	5	LYS
11	J	39	ALA
11	J	79	GLN
11	J	125	ALA
12	K	2	LYS
12	K	22	SER
12	K	110	LYS
13	L	24	ARG
13	L	116	ARG
13	L	218	ALA
14	M	117	ASP
15	N	66	ASN
16	O	9	ALA
19	c	156	ALA
20	d	162	ALA
21	e	53	LYS
22	f	24	LEU
27	k	50	ALA
28	l	126	LEU
29	m	59	ALA
30	n	56	VAL
30	n	117	ARG
31	o	29	TYR
33	q	82	GLU
34	r	12	LYS
37	u	75	TYR
40	x	33	LYS
40	x	34	ALA
41	y	3	ALA
42	z	79	GLU
43	Q	17	CYS
46	V	349	ASN
47	W	381	ASP
47	W	428	ILE
5	D	125	ALA

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Mol	Chain	Res	Type
6	E	155	ALA
7	F	5	GLN
9	H	151	LYS
10	I	25	GLN
14	M	108	GLU
15	N	75	PHE
17	a	94	TYR
21	e	178	ALA
22	f	22	PRO
24	h	11	ILE
29	m	17	ARG
30	n	47	LYS
31	o	21	ILE
37	u	99	GLN
37	u	119	LYS
39	w	78	PHE
46	V	68	PRO
6	E	317	ILE
7	F	131	VAL
7	F	317	PRO
7	F	339	LEU
8	G	125	VAL
10	I	26	VAL
29	m	124	ALA
30	n	15	VAL
33	q	7	VAL
36	t	46	ASP
39	w	84	SER
47	W	429	PRO
6	E	141	GLY
11	J	164	VAL
24	h	60	GLY
25	i	3	GLY
46	V	327	GLY
7	F	340	GLY
13	L	114	GLY
26	j	80	ARG
46	V	48	GLY
9	H	98	VAL
21	e	129	GLY
29	m	125	GLY
10	I	191	VAL

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Mol	Chain	Res	Type
13	L	194	GLY
16	O	6	ILE
16	O	52	GLY
30	n	116	GLY
43	Q	14	GLY
23	g	126	VAL
43	Q	101	GLY

### 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%)	80	90
5	D	193/196 (98%)	181 (94%)	12 (6%)	23	61
6	E	320/323 (99%)	300 (94%)	20 (6%)	22	60
7	F	288/289 (100%)	276 (96%)	12 (4%)	36	73
8	G	244/245 (100%)	231 (95%)	13 (5%)	28	66
9	H	134/153 (88%)	130 (97%)	4 (3%)	48	79
10	I	186/205 (91%)	177 (95%)	9 (5%)	31	70
11	J	187/208 (90%)	171 (91%)	16 (9%)	13	45
12	K	171/171 (100%)	157 (92%)	14 (8%)	14	48
13	L	177/187 (95%)	161 (91%)	16 (9%)	12	42
14	M	147/150 (98%)	139 (95%)	8 (5%)	27	66
15	N	154/159 (97%)	141 (92%)	13 (8%)	14	46
16	O	107/109 (98%)	100 (94%)	7 (6%)	21	59
17	a	175/176 (99%)	167 (95%)	8 (5%)	33	71
18	b	160/162 (99%)	154 (96%)	6 (4%)	40	75
19	c	140/146 (96%)	130 (93%)	10 (7%)	18	55
20	d	150/151 (99%)	144 (96%)	6 (4%)	38	74
21	e	153/154 (99%)	146 (95%)	7 (5%)	33	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	f	156/156 (100%)	145 (93%)	11 (7%)	18	55
23	g	136/137 (99%)	125 (92%)	11 (8%)	15	48
24	h	87/107 (81%)	85 (98%)	2 (2%)	58	83
25	i	104/105 (99%)	101 (97%)	3 (3%)	50	80
26	j	57/129 (44%)	57 (100%)	0	100	100
27	k	104/118 (88%)	96 (92%)	8 (8%)	16	51
28	l	109/110 (99%)	102 (94%)	7 (6%)	22	60
29	m	115/116 (99%)	109 (95%)	6 (5%)	29	67
30	n	118/119 (99%)	108 (92%)	10 (8%)	13	46
31	o	46/47 (98%)	43 (94%)	3 (6%)	21	59
32	p	81/88 (92%)	78 (96%)	3 (4%)	41	76
33	q	92/97 (95%)	87 (95%)	5 (5%)	27	66
34	r	109/111 (98%)	101 (93%)	8 (7%)	17	53
35	s	90/91 (99%)	83 (92%)	7 (8%)	16	50
36	t	95/103 (92%)	89 (94%)	6 (6%)	22	60
37	u	104/105 (99%)	96 (92%)	8 (8%)	16	51
38	v	81/82 (99%)	77 (95%)	4 (5%)	31	69
39	w	70/71 (99%)	63 (90%)	7 (10%)	9	36
40	x	68/69 (99%)	65 (96%)	3 (4%)	35	72
41	y	45/46 (98%)	44 (98%)	1 (2%)	60	84
42	z	47/116 (40%)	44 (94%)	3 (6%)	22	60
43	Q	90/91 (99%)	85 (94%)	5 (6%)	26	65
44	R	71/72 (99%)	67 (94%)	4 (6%)	26	65
46	V	291/473 (62%)	254 (87%)	37 (13%)	5	24
47	W	209/502 (42%)	171 (82%)	38 (18%)	2	9
All	All	5838/6672 (88%)	5455 (93%)	383 (7%)	25	59

All (383) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	74	THR
1	X	99	GLU
5	D	23	ARG

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Mol	Chain	Res	Type
5	D	48	ILE
5	D	52	SER
5	D	116	VAL
5	D	122	ASP
5	D	128	ARG
5	D	160	SER
5	D	207	VAL
5	D	223	SER
5	D	227	ARG
5	D	230	VAL
5	D	246	LEU
6	E	10	ARG
6	E	25	ILE
6	E	74	GLU
6	E	84	VAL
6	E	85	VAL
6	E	103	THR
6	E	162	VAL
6	E	169	THR
6	E	211	GLN
6	E	235	THR
6	E	238	LEU
6	E	242	THR
6	E	252	ILE
6	E	296	THR
6	E	305	ILE
6	E	318	LYS
6	E	328	ILE
6	E	331	ASN
6	E	332	ARG
6	E	382	THR
7	F	43	ASN
7	F	67	THR
7	F	69	ARG
7	F	74	ILE
7	F	99	MET
7	F	114	ASN
7	F	179	LEU
7	F	187	LEU
7	F	300	ARG
7	F	304	GLN
7	F	307	GLN

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Mol	Chain	Res	Type
7	F	327	LEU
8	G	22	ARG
8	G	23	ARG
8	G	35	ARG
8	G	92	LEU
8	G	95	TRP
8	G	105	ILE
8	G	112	LYS
8	G	131	LEU
8	G	151	GLN
8	G	211	LEU
8	G	244	HIS
8	G	259	LYS
8	G	273	ARG
9	H	34	LEU
9	H	65	ILE
9	H	77	ARG
9	H	134	ARG
10	I	64	GLN
10	I	82	LYS
10	I	83	LEU
10	I	88	ARG
10	I	92	ILE
10	I	157	ASN
10	I	179	LEU
10	I	218	ARG
10	I	239	LEU
11	J	38	GLN
11	J	41	GLN
11	J	57	ARG
11	J	61	GLN
11	J	63	LYS
11	J	65	LEU
11	J	92	LYS
11	J	136	LEU
11	J	169	LEU
11	J	190	VAL
11	J	194	THR
11	J	204	ARG
11	J	224	ASP
11	J	232	HIS
11	J	248	LYS

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Mol	Chain	Res	Type
11	J	254	ASP
12	K	5	GLN
12	K	21	LYS
12	K	23	ARG
12	K	41	ILE
12	K	49	ASN
12	K	69	ARG
12	K	76	ASP
12	K	118	LEU
12	K	139	ASN
12	K	151	VAL
12	K	161	LEU
12	K	162	GLN
12	K	164	ILE
12	K	166	ARG
13	L	7	ARG
13	L	30	LYS
13	L	33	ILE
13	L	40	LYS
13	L	52	LEU
13	L	63	GLU
13	L	102	MET
13	L	115	MET
13	L	116	ARG
13	L	163	GLN
13	L	165	ILE
13	L	169	LYS
13	L	185	ARG
13	L	201	SER
13	L	203	LYS
13	L	208	ASN
14	M	10	ARG
14	M	12	LEU
14	M	40	LEU
14	M	81	GLU
14	M	94	ARG
14	M	107	ASP
14	M	115	LYS
14	M	140	ARG
15	N	17	HIS
15	N	24	VAL
15	N	55	ARG

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Mol	Chain	Res	Type
15	N	67	ARG
15	N	69	VAL
15	N	76	THR
15	N	101	ARG
15	N	124	ILE
15	N	136	GLU
15	N	168	ARG
15	N	176	GLU
15	N	188	ARG
15	N	190	LYS
16	O	12	TRP
16	O	50	LYS
16	O	68	LEU
16	O	72	LEU
16	O	91	CYS
16	O	108	ARG
16	O	125	LYS
17	a	24	ARG
17	a	50	ARG
17	a	80	THR
17	a	98	LEU
17	a	106	VAL
17	a	117	ASN
17	a	133	ILE
17	a	175	ASN
18	b	22	VAL
18	b	34	VAL
18	b	37	ARG
18	b	78	ARG
18	b	125	ARG
18	b	155	LYS
19	c	24	VAL
19	c	53	ASP
19	c	55	GLN
19	c	78	VAL
19	c	119	VAL
19	c	120	ASN
19	c	125	GLN
19	c	126	ARG
19	c	127	ARG
19	c	180	LYS
20	d	39	ARG

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Mol	Chain	Res	Type
20	d	49	LEU
20	d	69	ARG
20	d	135	GLN
20	d	145	ASN
20	d	150	VAL
21	e	10	LEU
21	e	17	VAL
21	e	36	ASN
21	e	44	LEU
21	e	74	ARG
21	e	99	LEU
21	e	138	LEU
22	f	51	VAL
22	f	58	ILE
22	f	61	ILE
22	f	71	LYS
22	f	82	ASP
22	f	87	THR
22	f	93	GLU
22	f	134	ASP
22	f	137	ARG
22	f	155	ARG
22	f	172	TYR
23	g	12	ARG
23	g	32	LYS
23	g	75	ILE
23	g	79	MET
23	g	88	ARG
23	g	96	ILE
23	g	102	ARG
23	g	126	VAL
23	g	127	GLN
23	g	128	LEU
23	g	139	ARG
24	h	10	LYS
24	h	70	LYS
25	i	33	ASN
25	i	83	LYS
25	i	88	ARG
27	k	61	LYS
27	k	63	ILE
27	k	70	GLU

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Mol	Chain	Res	Type
27	k	115	ARG
27	k	133	LEU
27	k	135	ILE
27	k	137	ASN
27	k	142	ILE
28	l	4	GLN
28	l	13	ARG
28	l	37	LYS
28	l	50	ILE
28	l	53	ASP
28	l	74	TYR
28	l	126	LEU
29	m	14	VAL
29	m	17	ARG
29	m	34	LYS
29	m	120	GLU
29	m	121	ARG
29	m	126	LYS
30	n	4	ARG
30	n	7	LYS
30	n	10	LYS
30	n	34	MET
30	n	42	ARG
30	n	60	TYR
30	n	78	LEU
30	n	115	LYS
30	n	120	ASN
30	n	130	VAL
31	o	22	LYS
31	o	25	LYS
31	o	59	LYS
32	p	40	LYS
32	p	61	MET
32	p	83	LYS
33	q	16	LEU
33	q	35	GLU
33	q	55	LEU
33	q	79	ARG
33	q	86	LYS
34	r	19	ARG
34	r	33	ARG
34	r	47	ARG

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Mol	Chain	Res	Type
34	r	73	THR
34	r	75	LEU
34	r	87	MET
34	r	125	ARG
34	r	128	LEU
35	s	31	LYS
35	s	59	VAL
35	s	70	LYS
35	s	73	ARG
35	s	81	VAL
35	s	86	ARG
35	s	98	VAL
36	t	29	ILE
36	t	33	GLN
36	t	51	LEU
36	t	52	GLN
36	t	58	ARG
36	t	86	LYS
37	u	15	GLU
37	u	20	GLN
37	u	21	LEU
37	u	28	LEU
37	u	49	LYS
37	u	69	LEU
37	u	71	LYS
37	u	119	LYS
38	v	45	ARG
38	v	57	LEU
38	v	58	ILE
38	v	76	ARG
39	w	22	CYS
39	w	24	ARG
39	w	25	ARG
39	w	33	THR
39	w	37	CYS
39	w	67	LEU
39	w	71	SER
40	x	46	ARG
40	x	67	GLN
40	x	77	ARG
41	y	21	ARG
42	z	85	LEU

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Mol	Chain	Res	Type
42	z	106	ARG
42	z	113	ARG
43	Q	13	LYS
43	Q	35	LEU
43	Q	38	GLN
43	Q	45	ARG
43	Q	100	LYS
44	R	38	ASP
44	R	45	LYS
44	R	49	ARG
44	R	60	CYS
46	V	61	CYS
46	V	66	GLN
46	V	103	ILE
46	V	111	ARG
46	V	141	MET
46	V	145	ASP
46	V	146	CYS
46	V	156	ARG
46	V	162	ARG
46	V	164	LYS
46	V	168	LYS
46	V	171	PHE
46	V	177	LEU
46	V	179	LEU
46	V	185	VAL
46	V	197	LEU
46	V	209	LYS
46	V	221	LYS
46	V	228	LEU
46	V	265	LYS
46	V	278	LYS
46	V	291	LEU
46	V	295	ASP
46	V	299	SER
46	V	345	ASP
46	V	350	ASP
46	V	356	ARG
46	V	362	ILE
46	V	364	HIS
46	V	370	MET
46	V	376	ASN

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Mol	Chain	Res	Type
46	V	387	LEU
46	V	390	ASP
46	V	391	TYR
46	V	397	LEU
46	V	400	LYS
46	V	401	LEU
47	W	182	GLU
47	W	185	ILE
47	W	191	LEU
47	W	196	GLU
47	W	197	ARG
47	W	203	GLN
47	W	211	LEU
47	W	212	LEU
47	W	214	ARG
47	W	224	GLU
47	W	226	ASP
47	W	231	ASN
47	W	246	ARG
47	W	260	PHE
47	W	266	LEU
47	W	339	ILE
47	W	349	LYS
47	W	353	ILE
47	W	362	VAL
47	W	372	LYS
47	W	373	HIS
47	W	384	MET
47	W	385	LEU
47	W	400	LYS
47	W	405	CYS
47	W	406	ASN
47	W	409	LEU
47	W	413	GLN
47	W	428	ILE
47	W	431	TYR
47	W	437	TYR
47	W	440	HIS
47	W	472	THR
47	W	473	GLN
47	W	477	SER
47	W	482	ARG

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Mol	Chain	Res	Type
47	W	485	ARG
47	W	497	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
5	D	209	HIS
6	E	182	GLN
6	E	184	ASN
6	E	319	ASN
7	F	114	ASN
7	F	221	ASN
8	G	63	GLN
9	H	138	GLN
9	H	167	ASN
10	I	64	GLN
10	I	244	ASN
11	J	192	GLN
12	K	8	GLN
12	K	163	GLN
13	L	12	GLN
13	L	59	GLN
13	L	95	HIS
15	N	137	GLN
18	b	31	GLN
19	c	120	ASN
19	c	125	GLN
20	d	9	GLN
20	d	73	GLN
20	d	145	ASN
29	m	57	HIS
33	q	57	GLN
37	u	68	GLN
37	u	104	GLN
37	u	108	GLN
40	x	67	GLN
46	V	163	GLN
46	V	231	GLN
47	W	209	ASN
47	W	375	GLN
47	W	440	HIS
47	W	442	GLN

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Mol	Chain	Res	Type
47	W	473	GLN
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%)

All (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
2	A	43	A
2	A	44	U
2	A	48	A
2	A	49	A
2	A	59	G
2	A	60	A
2	A	65	A
2	A	66	A
2	A	67	A
2	A	78	U
2	A	79	U
2	A	83	U
2	A	92	G
2	A	99	A
2	A	105	C
2	A	109	A
2	A	110	G
2	A	111	C
2	A	116	A
2	A	122	A
2	A	123	A
2	A	127	G

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Mol	Chain	Res	Type
2	A	131	C
2	A	136	G
2	A	137	G
2	A	156	G
2	A	157	A
2	A	160	G
2	A	161	G
2	A	162	G
2	A	166	C
2	A	167	U
2	A	168	U
2	A	170	G
2	A	171	G
2	A	173	G
2	A	175	C
2	A	182	U
2	A	190	U
2	A	191	U
2	A	192	C
2	A	193	C
2	A	206	G
2	A	210	U
2	A	211	A
2	A	213	A
2	A	218	G
2	A	219	A
2	A	232	G
2	A	240	U
2	A	241	G
2	A	243	G
2	A	245	U
2	A	246	U
2	A	249	U
2	A	250	U
2	A	252	U
2	A	262	U
2	A	264	G
2	A	266	A
2	A	269	G
2	A	286	U
2	A	295	A
2	A	305	U

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Mol	Chain	Res	Type
2	A	306	A
2	A	307	A
2	A	313	A
2	A	314	U
2	A	315	C
2	A	323	A
2	A	329	U
2	A	336	A
2	A	338	A
2	A	339	C
2	A	348	A
2	A	372	A
2	A	375	A
2	A	376	G
2	A	379	C
2	A	381	U
2	A	383	G
2	A	392	G
2	A	395	A
2	A	398	A
2	A	399	A
2	A	401	U
2	A	402	A
2	A	403	C
2	A	404	G
2	A	415	G
2	A	420	G
2	A	421	G
2	A	422	A
2	A	429	U
2	A	433	A
2	A	439	C
2	A	440	A
2	A	495	G
2	A	503	C
2	A	507	U
2	A	510	G
2	A	511	G
2	A	519	A
2	A	520	U
2	A	521	A
2	A	523	A

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Mol	Chain	Res	Type
2	A	526	C
2	A	529	A
2	A	532	A
2	A	534	U
2	A	536	U
2	A	541	U
2	A	543	C
2	A	546	C
2	A	547	G
2	A	548	G
2	A	549	U
2	A	551	A
2	A	553	U
2	A	555	U
2	A	556	U
2	A	557	A
2	A	559	A
2	A	560	G
2	A	578	A
2	A	579	G
2	A	588	G
2	A	589	A
2	A	598	A
2	A	599	C
2	A	600	G
2	A	603	A
2	A	604	G
2	A	607	A
2	A	611	A
2	A	616	G
2	A	620	U
2	A	621	A
2	A	622	A
2	A	634	C
2	A	636	C
2	A	649	A
2	A	660	A
2	A	677	A
2	A	681	U
2	A	683	U
2	A	684	G
2	A	689	U

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Mol	Chain	Res	Type
2	A	690	A
2	A	691	A
2	A	701	G
2	A	705	A
2	A	712	G
2	A	715	A
2	A	720	A
2	A	721	G
2	A	735	A
2	A	739	G
2	A	744	A
2	A	764	U
2	A	765	C
2	A	766	U
2	A	767	U
2	A	774	G
2	A	776	U
2	A	777	U
2	A	781	G
2	A	785	G
2	A	786	A
2	A	793	C
2	A	799	G
2	A	801	A
2	A	806	A
2	A	811	U
2	A	816	A
2	A	817	A
2	A	825	U
2	A	826	G
2	A	827	A
2	A	830	A
2	A	832	G
2	A	841	A
2	A	848	A
2	A	849	C
2	A	861	C
2	A	869	G
2	A	874	U
2	A	879	U
2	A	880	G
2	A	884	A

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Mol	Chain	Res	Type
2	A	894	G
2	A	896	A
2	A	897	U
2	A	907	G
2	A	908	G
2	A	911	C
2	A	914	A
2	A	916	G
2	A	917	A
2	A	921	A
2	A	923	C
2	A	924	G
2	A	925	A
2	A	937	G
2	A	939	U
2	A	941	G
2	A	944	C
2	A	959	C
2	A	960	U
2	A	961	C
2	A	978	G
2	A	979	U
2	A	980	A
2	A	981	U
2	A	982	C
2	A	984	G
2	A	994	G
2	A	1001	G
2	A	1002	A
2	A	1006	A
2	A	1009	A
2	A	1010	G
2	A	1013	G
2	A	1015	U
2	A	1017	C
2	A	1018	G
2	A	1019	G
2	A	1024	G
2	A	1025	A
2	A	1026	A
2	A	1029	G
2	A	1030	A

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Mol	Chain	Res	Type
2	A	1031	C
2	A	1036	A
2	A	1037	C
2	A	1040	A
2	A	1041	U
2	A	1047	A
2	A	1049	C
2	A	1051	U
2	A	1057	A
2	A	1063	G
2	A	1064	A
2	A	1065	A
2	A	1069	C
2	A	1071	U
2	A	1072	G
2	A	1081	U
2	A	1093	A
2	A	1094	U
2	A	1095	U
2	A	1097	G
2	A	1098	A
2	A	1099	A
2	A	1103	A
2	A	1104	G
2	A	1117	G
2	A	1122	U
2	A	1124	U
2	A	1129	A
2	A	1131	G
2	A	1140	G
2	A	1145	G
2	A	1153	A
2	A	1157	G
2	A	1159	A
2	A	1178	G
2	A	1179	A
2	A	1180	A
2	A	1181	U
2	A	1190	A
2	A	1192	C
2	A	1200	A
2	A	1201	C

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Mol	Chain	Res	Type
2	A	1208	U
2	A	1212	A
2	A	1213	G
2	A	1217	A
2	A	1219	C
2	A	1222	G
2	A	1223	A
2	A	1230	G
2	A	1232	C
2	A	1233	G
2	A	1236	G
2	A	1237	G
2	A	1240	A
2	A	1241	U
2	A	1242	G
2	A	1243	G
2	A	1244	A
2	A	1245	A
2	A	1246	G
2	A	1247	U
2	A	1248	C
2	A	1249	G
2	A	1253	U
2	A	1257	C
2	A	1258	U
2	A	1262	G
2	A	1263	A
2	A	1264	G
2	A	1265	U
2	A	1267	U
2	A	1270	A
2	A	1271	A
2	A	1274	A
2	A	1276	U
2	A	1278	A
2	A	1279	C
2	A	1285	G
2	A	1287	A
2	A	1289	G
2	A	1291	A
2	A	1303	A
2	A	1305	U

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Mol	Chain	Res	Type
2	A	1307	G
2	A	1309	U
2	A	1313	G
2	A	1315	U
2	A	1319	G
2	A	1325	U
2	A	1330	A
2	A	1334	U
2	A	1348	U
2	A	1349	G
2	A	1351	U
2	A	1352	A
2	A	1353	U
2	A	1356	U
2	A	1357	G
2	A	1364	C
2	A	1383	G
2	A	1386	A
2	A	1392	G
2	A	1393	A
2	A	1394	A
2	A	1399	A
2	A	1400	G
2	A	1409	G
2	A	1414	G
2	A	1416	C
2	A	1419	A
2	A	1430	U
2	A	1434	G
2	A	1437	C
2	A	1446	A
2	A	1450	G
2	A	1455	U
2	A	1460	A
2	A	1466	G
2	A	1481	A
2	A	1482	A
2	A	1489	A
2	A	1496	C
2	A	1501	U
2	A	1503	A
2	A	1508	C

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Mol	Chain	Res	Type
2	A	1521	G
2	A	1527	C
2	A	1531	C
2	A	1533	U
2	A	1536	G
2	A	1537	A
2	A	1547	G
2	A	1555	U
2	A	1556	C
2	A	1557	A
2	A	1560	G
2	A	1561	G
2	A	1562	C
2	A	1563	C
2	A	1564	U
2	A	1565	G
2	A	1566	A
2	A	1567	U
2	A	1568	U
2	A	1569	U
2	A	1570	U
2	A	1572	U
2	A	1576	G
2	A	1577	G
2	A	1578	C
2	A	1579	C
2	A	1582	C
2	A	1583	A
2	A	1587	A
2	A	1589	A
2	A	1599	G
2	A	1605	A
2	A	1615	C
2	A	1619	A
2	A	1620	U
2	A	1623	G
2	A	1627	U
2	A	1628	C
2	A	1629	U
2	A	1630	U
2	A	1632	A
2	A	1642	A

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Mol	Chain	Res	Type
2	A	1643	A
2	A	1645	U
2	A	1657	C
2	A	1658	G
2	A	1664	G
2	A	1666	G
2	A	1674	G
2	A	1678	G
2	A	1682	U
2	A	1683	A
2	A	1703	U
2	A	1716	U
2	A	1717	U
2	A	1724	U
2	A	1725	C
2	A	1733	G
2	A	1735	G
2	A	1741	A
2	A	1747	G
2	A	1749	A
2	A	1750	A
2	A	1751	G
2	A	1760	A
2	A	1761	C
2	A	1765	U
2	A	1766	G
2	A	1770	G
2	A	1775	G
2	A	1780	G
2	A	1788	C
2	A	1790	G
2	A	1795	U
2	A	1797	A
2	A	1798	A
2	A	1803	C
2	A	1808	G
2	A	1812	G
2	A	1814	A
2	A	1815	U
2	A	1816	A
2	A	1817	G
2	A	1820	U

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Mol	Chain	Res	Type
2	A	1821	U
2	A	1839	A
2	A	1841	A
2	A	1842	A
2	A	1845	G
2	A	1849	C
2	A	1850	A
2	A	1867	A
2	A	1871	U
2	A	1880	U
2	A	1886	A
2	A	1893	A
2	A	1895	A
2	A	1906	G
2	A	1908	A
2	A	1909	A
2	A	1917	C
2	A	1926	C
2	A	1930	A
2	A	1936	A
2	A	1951	C
2	A	1952	G
2	A	1953	G
2	A	1954	G
2	A	2096	A
2	A	2100	A
2	A	2101	C
2	A	2102	U
2	A	2111	G
2	A	2113	A
2	A	2114	C
2	A	2118	C
2	A	2121	G
2	A	2122	G
2	A	2131	A
2	A	2140	U
2	A	2142	A
2	A	2158	A
2	A	2169	G
2	A	2185	G
2	A	2187	G
2	A	2192	C

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Mol	Chain	Res	Type
2	A	2198	A
2	A	2205	U
2	A	2210	G
2	A	2221	G
2	A	2228	A
2	A	2239	G
2	A	2244	A
2	A	2246	G
2	A	2250	G
2	A	2253	G
2	A	2255	A
2	A	2256	A
2	A	2257	C
2	A	2258	PSU
2	A	2259	A
2	A	2262	A
2	A	2264	PSU
2	A	2266	PSU
2	A	2267	C
2	A	2268	U
2	A	2269	U
2	A	2270	A
2	A	2273	G
2	A	2274	U
2	A	2281	A
2	A	2282	U
2	A	2288	G
2	A	2298	U
2	A	2307	G
2	A	2308	C
2	A	2310	U
2	A	2313	A
2	A	2314	U
2	A	2315	G
2	A	2332	A
2	A	2335	G
2	A	2336	U
2	A	2337	C
2	A	2372	A
2	A	2373	A
2	A	2374	C
2	A	2375	G

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Mol	Chain	Res	Type
2	A	2379	U
2	A	2385	G
2	A	2388	U
2	A	2393	G
2	A	2397	A
2	A	2401	A
2	A	2402	A
2	A	2403	G
2	A	2404	A
2	A	2405	C
2	A	2407	C
2	A	2411	U
2	A	2412	G
2	A	2418	G
2	A	2419	A
2	A	2425	G
2	A	2428	U
2	A	2429	G
2	A	2434	U
2	A	2437	G
2	A	2440	G
2	A	2442	G
2	A	2444	C
2	A	2445	A
2	A	2446	U
2	A	2449	A
2	A	2450	G
2	A	2451	G
2	A	2452	G
2	A	2453	U
2	A	2454	G
2	A	2455	U
2	A	2457	G
2	A	2458	A
2	A	2459	A
2	A	2461	A
2	A	2463	G
2	A	2464	U
2	A	2468	A
2	A	2470	C
2	A	2472	U
2	A	2473	C

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Mol	Chain	Res	Type
2	A	2474	G
2	A	2475	G
2	A	2477	G
2	A	2479	C
2	A	2481	G
2	A	2482	U
2	A	2483	G
2	A	2485	A
2	A	2488	A
2	A	2491	A
2	A	2494	A
2	A	2495	C
2	A	2496	C
2	A	2497	U
2	A	2498	U
2	A	2501	U
2	A	2502	A
2	A	2505	U
2	A	2506	U
2	A	2508	U
2	A	2513	U
2	A	2514	U
2	A	2515	A
2	A	2522	G
2	A	2531	C
2	A	2533	G
2	A	2537	U
2	A	2538	U
2	A	2539	C
2	A	2540	A
2	A	2541	U
2	A	2542	U
2	A	2543	U
2	A	2544	U
2	A	2547	A
2	A	2548	C
2	A	2549	G
2	A	2550	U
2	A	2552	C
2	A	2554	A
2	A	2555	G
2	A	2561	A

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Mol	Chain	Res	Type
2	A	2562	A
2	A	2564	G
2	A	2565	U
2	A	2566	C
2	A	2569	A
2	A	2570	U
2	A	2571	U
2	A	2572	C
2	A	2573	G
2	A	2575	G
2	A	2577	C
2	A	2581	U
2	A	2585	G
2	A	2586	G
2	A	2593	A
2	A	2594	C
2	A	2602	G
2	A	2606	G
2	A	2607	G
2	A	2614	G
2	A	2621	G
2	A	2626	A
2	A	2628	A
2	A	2635	A
2	A	2648	G
2	A	2652	U
2	A	2656	A
2	A	2657	A
2	A	2658	G
2	A	2674	A
2	A	2677	G
2	A	2681	U
2	A	2684	C
2	A	2689	A
2	A	2690	G
2	A	2691	A
2	A	2694	A
2	A	2696	A
2	A	2704	A
2	A	2709	C
2	A	2714	G
2	A	2719	U

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Mol	Chain	Res	Type
2	A	2726	C
2	A	2727	A
2	A	2728	G
2	A	2734	A
2	A	2737	C
2	A	2753	G
2	A	2754	G
2	A	2755	C
2	A	2762	A
2	A	2772	C
2	A	2774	C
2	A	2777	G
2	A	2778	G
2	A	2780	A
2	A	2790	A
2	A	2792	A
2	A	2799	A
2	A	2800	G
2	A	2801	A
2	A	2803	A
2	A	2810	C
2	A	2816	G
2	A	2817	A
2	A	2821	C
2	A	2837	A
2	A	2838	A
2	A	2842	U
2	A	2843	U
2	A	2844	C
2	A	2845	A
2	A	2848	G
2	A	2849	C
2	A	2860	U
2	A	2861	U
2	A	2867	C
2	A	2871	G
2	A	2872	A
2	A	2882	U
2	A	2887	A
2	A	2888	U
2	A	2896	A
2	A	2898	G

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Mol	Chain	Res	Type
2	A	2899	C
2	A	2900	A
2	A	2914	G
2	A	2923	U
2	A	2928	C
2	A	2933	A
2	A	2935	U
2	A	2936	A
2	A	2938	G
2	A	2941	A
2	A	2942	C
2	A	2947	G
2	A	2951	G
2	A	2971	A
2	A	2975	U
2	A	2978	U
2	A	2979	U
2	A	2980	U
2	A	2983	C
2	A	2990	G
2	A	2996	U
2	A	2997	G
2	A	2998	U
2	A	3004	C
2	A	3011	A
2	A	3012	A
2	A	3014	U
2	A	3022	G
2	A	3049	A
2	A	3056	U
2	A	3057	U
2	A	3058	U
2	A	3059	G
2	A	3070	A
2	A	3072	C
2	A	3078	U
2	A	3079	U
2	A	3086	A
2	A	3090	U
2	A	3092	C
2	A	3104	U
2	A	3109	G

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Mol	Chain	Res	Type
2	A	3110	C
2	A	3114	A
2	A	3115	C
2	A	3117	C
2	A	3122	A
2	A	3125	U
2	A	3129	A
2	A	3130	A
2	A	3131	U
2	A	3133	C
2	A	3142	A
2	A	3143	C
2	A	3148	U
2	A	3153	U
2	A	3154	C
2	A	3155	U
2	A	3156	U
2	A	3157	U
2	A	3165	A
2	A	3168	A
2	A	3173	G
2	A	3174	A
2	A	3176	G
2	A	3179	U
2	A	3181	C
2	A	3187	A
2	A	3188	G
2	A	3189	G
2	A	3191	G
2	A	3194	C
2	A	3196	U
2	A	3197	G
2	A	3200	G
2	A	3206	C
2	A	3207	U
2	A	3213	A
2	A	3217	C
2	A	3218	A
2	A	3219	G
2	A	3224	G
2	A	3226	A
2	A	3229	G

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Mol	Chain	Res	Type
2	A	3232	G
2	A	3234	A
2	A	3238	G
2	A	3243	A
2	A	3245	A
2	A	3246	G
2	A	3247	G
2	A	3249	C
2	A	3259	U
2	A	3260	G
2	A	3261	C
2	A	3269	U
2	A	3270	U
2	A	3271	G
2	A	3273	A
2	A	3275	U
2	A	3276	G
2	A	3279	A
2	A	3280	U
2	A	3283	U
2	A	3286	G
2	A	3289	G
2	A	3294	A
2	A	3295	A
2	A	3300	U
2	A	3304	U
2	A	3313	U
2	A	3316	A
2	A	3317	U
2	A	3318	G
2	A	3319	U
2	A	3320	A
2	A	3321	C
2	A	3324	C
2	A	3325	G
2	A	3328	G
2	A	3342	A
2	A	3345	G
2	A	3347	A
2	A	3350	C
2	A	3351	U
2	A	3352	U

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Mol	Chain	Res	Type
2	A	3353	G
2	A	3354	U
2	A	3355	U
2	A	3356	G
2	A	3361	G
2	A	3367	C
2	A	3368	U
2	A	3369	G
2	A	3375	A
2	A	3378	C
2	A	3382	U
2	A	3383	G
2	A	3386	G
2	A	3390	G
3	B	10	C
3	B	20	A
3	B	22	A
3	B	38	U
3	B	42	A
3	B	49	G
3	B	53	U
3	B	54	U
3	B	55	A
3	B	60	G
3	B	65	G
3	B	67	G
3	B	70	U
3	B	71	G
3	B	73	C
3	B	75	G
3	B	91	G
3	B	98	C
3	B	99	G
3	B	102	A
3	B	103	A
3	B	104	A
3	B	112	G
3	B	120	C
3	B	121	U
4	C	2	A
4	C	18	U
4	C	23	U

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Mol	Chain	Res	Type
4	C	25	G
4	C	34	U
4	C	35	C
4	C	38	U
4	C	42	G
4	C	51	G
4	C	52	A
4	C	59	A
4	C	60	U
4	C	62	C
4	C	63	G
4	C	80	A
4	C	81	U
4	C	82	U
4	C	83	C
4	C	84	C
4	C	86	U
4	C	87	G
4	C	88	A
4	C	90	U
4	C	95	G
4	C	104	A
4	C	105	A
4	C	106	C
4	C	111	A
4	C	113	U
4	C	116	G
4	C	125	U
4	C	126	A
4	C	129	C
4	C	138	A
4	C	144	G
4	C	151	C
4	C	152	G
4	C	155	A
4	C	158	U

All (106) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	65	A
2	A	66	A

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Mol	Chain	Res	Type
2	A	78	U
2	A	116	A
2	A	169	U
2	A	239	G
2	A	285	A
2	A	518	G
2	A	547	G
2	A	558	U
2	A	588	G
2	A	594	U
2	A	599	C
2	A	816	A
2	A	896	A
2	A	916	G
2	A	937	G
2	A	960	U
2	A	978	G
2	A	979	U
2	A	993	G
2	A	1064	A
2	A	1097	G
2	A	1103	A
2	A	1263	A
2	A	1308	A
2	A	1329	U
2	A	1352	A
2	A	1355	A
2	A	1391	C
2	A	1480	G
2	A	1482	A
2	A	1553	U
2	A	1554	U
2	A	1556	C
2	A	1562	C
2	A	1576	G
2	A	1643	A
2	A	1716	U
2	A	1795	U
2	A	1815	U
2	A	1816	A
2	A	1820	U
2	A	1841	A

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Mol	Chain	Res	Type
2	A	2101	C
2	A	2112	U
2	A	2144	A
2	A	2157	G
2	A	2158	A
2	A	2209	U
2	A	2249	G
2	A	2258	PSU
2	A	2266	PSU
2	A	2269	U
2	A	2281	A
2	A	2335	G
2	A	2385	G
2	A	2404	A
2	A	2418	G
2	A	2434	U
2	A	2453	U
2	A	2495	C
2	A	2496	C
2	A	2501	U
2	A	2505	U
2	A	2513	U
2	A	2537	U
2	A	2541	U
2	A	2585	G
2	A	2593	A
2	A	2627	C
2	A	2644	C
2	A	2655	U
2	A	2657	A
2	A	2727	A
2	A	2728	G
2	A	2754	G
2	A	2801	A
2	A	2803	A
2	A	2837	A
2	A	2843	U
2	A	2859	U
2	A	2950	G
2	A	2979	U
2	A	2983	C
2	A	3022	G

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Mol	Chain	Res	Type
2	A	3048	A
2	A	3055	U
2	A	3056	U
2	A	3057	U
2	A	3078	U
2	A	3195	U
2	A	3218	A
2	A	3228	C
2	A	3269	U
2	A	3272	C
2	A	3317	U
2	A	3350	C
2	A	3351	U
2	A	3353	G
3	B	76	A
3	B	86	U
3	B	111	U
4	C	80	A
4	C	82	U
4	C	85	G

## 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	15,21,22	1.64	2 (13%)	16,30,33	2.68	4 (25%)
2	PSU	A	2260	2	15,21,22	1.43	1 (6%)	16,30,33	2.06	3 (18%)
2	PSU	A	2264	2	15,21,22	1.46	1 (6%)	16,30,33	2.32	5 (31%)
2	PSU	A	2266	2	15,21,22	1.59	2 (13%)	16,30,33	2.78	4 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2258	PSU	C5-C1'	-4.93	1.47	1.52
2	A	2266	PSU	C5-C1'	-4.93	1.47	1.52
2	A	2264	PSU	C5-C1'	-4.70	1.48	1.52
2	A	2260	PSU	C5-C1'	-4.39	1.48	1.52
2	A	2258	PSU	C2'-C1'	-2.86	1.51	1.53
2	A	2266	PSU	C2'-C1'	-2.30	1.51	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2266	PSU	C5-C1'-C2'	-7.04	103.48	115.44
2	A	2258	PSU	C5-C1'-C2'	-6.89	103.73	115.44
2	A	2258	PSU	C5-C6-N1	-3.98	118.83	124.38
2	A	2260	PSU	C5-C6-N1	-3.83	119.04	124.38
2	A	2264	PSU	C5-C6-N1	-3.82	119.06	124.38
2	A	2266	PSU	C5-C6-N1	-3.73	119.18	124.38
2	A	2264	PSU	C5-C1'-C2'	-3.03	110.28	115.44
2	A	2260	PSU	C5-C1'-C2'	-2.07	111.92	115.44
2	A	2264	PSU	O3'-C3'-C4'	-2.05	104.88	111.01
2	A	2258	PSU	O3'-C3'-C4'	2.06	117.17	111.01
2	A	2266	PSU	O3'-C3'-C4'	2.17	117.48	111.01
2	A	2264	PSU	C3'-C2'-C1'	2.28	104.41	101.71
2	A	2258	PSU	C4-N3-C2	6.39	120.48	115.16
2	A	2260	PSU	C4-N3-C2	6.44	120.53	115.16
2	A	2266	PSU	C4-N3-C2	6.65	120.70	115.16
2	A	2264	PSU	C4-N3-C2	6.66	120.71	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 32 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 163 ligands modelled in this entry, 162 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
50	GNP	W	701	48	29,34,34	2.64	7 (24%)	28,54,54	1.39	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	GNP	W	701	48	-	0/16/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	W	701	GNP	C4-N9	-10.21	1.34	1.47
50	W	701	GNP	C8-N9	-3.85	1.34	1.47
50	W	701	GNP	C5-C6	-2.39	1.48	1.53
50	W	701	GNP	C2-N1	-2.22	1.34	1.44
50	W	701	GNP	C1'-N9	3.56	1.48	1.42
50	W	701	GNP	PB-N3B	4.27	1.75	1.63
50	W	701	GNP	PG-N3B	4.27	1.75	1.63

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	W	701	GNP	PA-O3A-PB	-3.56	119.78	132.71
50	W	701	GNP	C4-C5-N7	2.56	106.67	102.67
50	W	701	GNP	C8-N9-C4	3.19	108.42	104.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 12 short contacts:

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
47	W	2

All chain breaks are listed below:

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