



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 02:48 PM UTC

PDB ID : 5T62 / pdb_00005t62
EMDB ID : EMD-8362
Title : Nmd3 is a structural mimic of eIF5A, and activates the cpGTPase Lsg1 during 60S ribosome biogenesis: 60S-Nmd3-Tif6-Lsg1 Complex
Authors : Malyutin, A.G.; Musalgaonkar, S.; Patchett, S.; Frank, J.; Johnson, A.W.
Deposited on : 2016-09-01
Resolution : 3.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

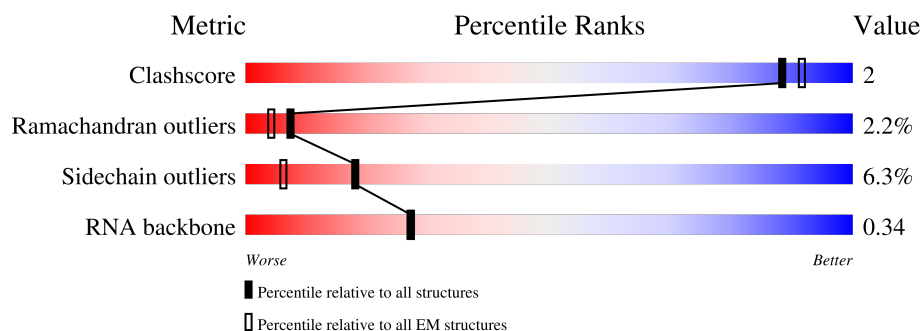
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



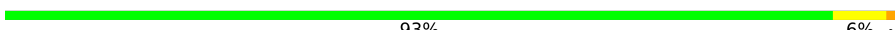
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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

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

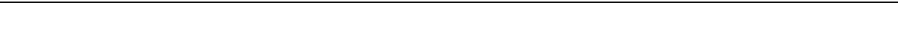
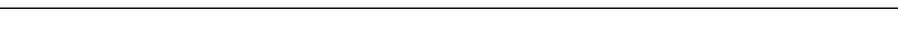
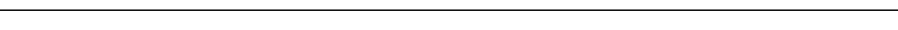
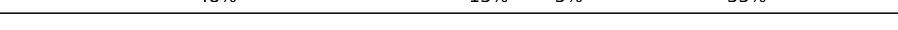
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Mol	Chain	Length	Quality of chain
8	G	297	 92% 8%
9	H	176	 83% 5% 11%
10	I	244	 82% 7% 9%
11	J	256	 80% 10% 9%
12	K	191	 89% 9% ..
13	L	221	 85% 10% 5%
14	M	174	 90% 7% ..
15	N	199	 84% 12% ..
16	O	138	 89% 8% ..
17	a	204	 91% 7% .
18	b	199	 93% 6%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

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Mol	Chain	Length	Quality of chain
33	q	113	 86% 10% . .
34	r	130	 89% 7% . .
35	s	107	 89% 7% . .
36	t	121	 83% 9% 7%
37	u	120	 88% 10% . .
38	v	100	 91% 8% .
39	w	88	 81% 17% . .
40	x	78	 94% 5% .
41	y	51	 90% 8% .
42	z	128	 37% . 59%
43	Q	106	 87% 11% . .
44	R	92	 88% 11% .
45	S	217	 96% . .
46	V	524	 48% 13% 5% . 33%
47	W	651	 33% 11% . 53%

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

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

2 Entry composition

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

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

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

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

There are 19 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a RNA chain called TPA_inf: Saccharomyces cerevisiae S288C chromosome XII, complete sequence.

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

- Molecule 3 is a RNA chain called 5S Ribosomal RNA.

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

- Molecule 4 is a RNA chain called 5.8S Ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	c	183	Total	C	N	O		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		0	0
			1521	935	326	260			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 45 is a protein called Ribosomal Protein uL1.

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

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

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

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

There are 77 discrepancies between the modelled and reference sequences:

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

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

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

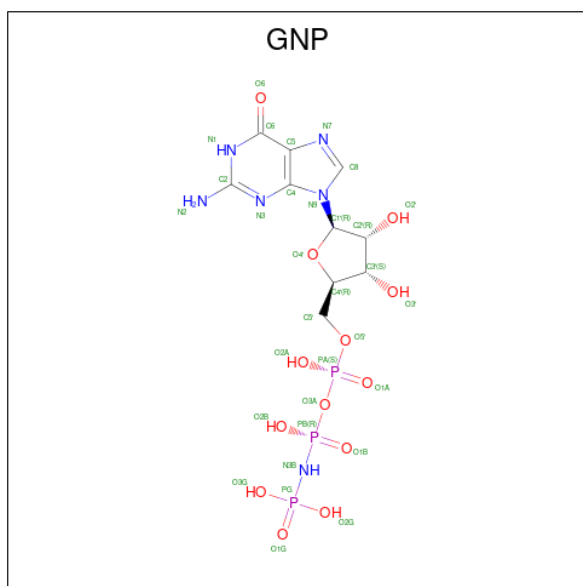
- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

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

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

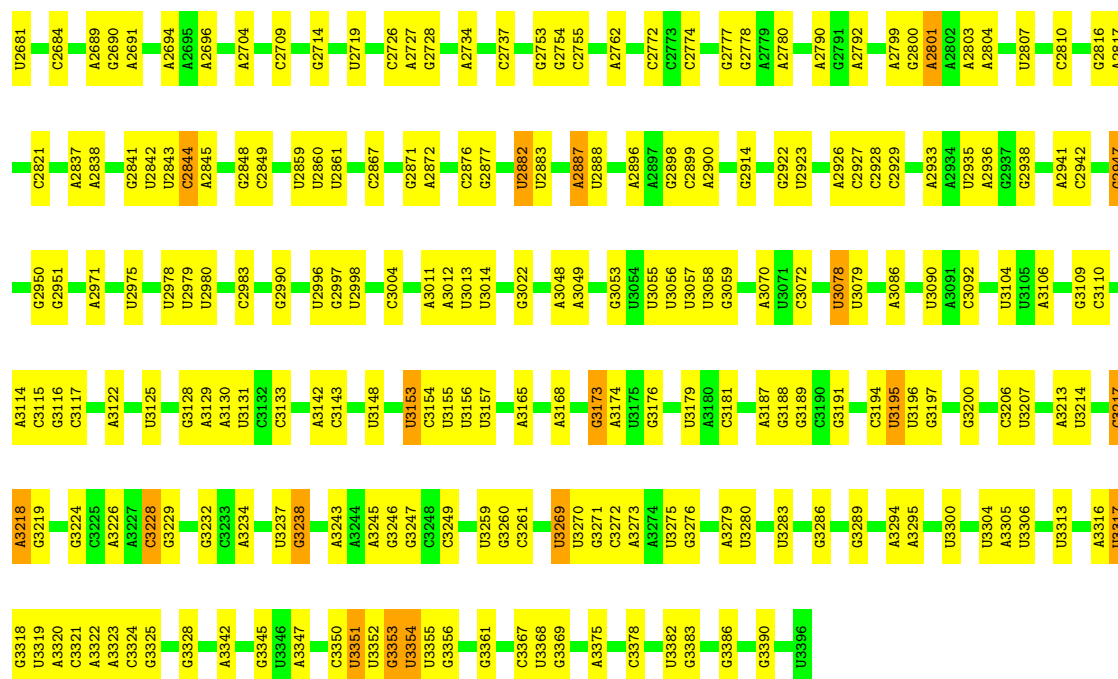


Mol	Chain	Residues	Atoms					AltConf
50	W	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 51 is water.

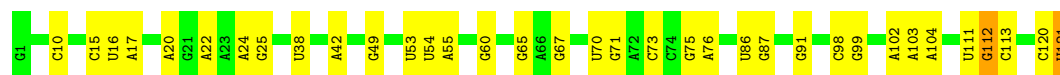
Mol	Chain	Residues	Atoms		AltConf
51	A	5	Total	O	0
			5	5	
51	e	1	Total	O	0
			1	1	

A2561	C2476	G2401	G2261	C2118	A1867	G1747	A1605	A1482	U1329	U1122	A1009
A2562	G2477	A2402	A2262	G2121	U1871	G1748	A1606	G1483	A1330	U1123	G1010
G2563	C2478	G2403	U2263	A	U	A1749	C1615	A1489	U1334	U1124	G1013
G2564	C2479	A2404	U2264	U	U	A1750	C1616	A1490	U1335	U1125	U1014
U2565	A2481	C2405	C2265	G	U	G1751	A1619	G1496	U1336	A1129	U1015
C2566	U2482	C2406	U2266	C	U	A1760	U1620	U1501	U1337	A1130	G1016
U2569	G2483	C2407	U2267	U	U	C1761	G1623	C1502	U1338	G1131	C1017
U2571	A2484	U2410	U2268	G	G	U1765	U1627	A1503	U1339	G1140	U1018
A2572	A2485	U2411	A2270	U	A	G1766	C1628	A1504	U1340	G1141	G1019
G2573	U2486	G2412	A2271	C	U	U1767	U1629	A1505	U1341	G1142	U1024
G2574	U2487	G2413	A2272	U	U	G1770	U1630	G1508	U1342	G1143	A1025
G2575	G2488	U2414	A2273	G	U	U1775	U1631	G1509	U1343	G1144	A1026
G2576	C2489	G2415	U2274	C	U	U1776	C1632	G1510	U1344	G1145	U1027
C2577	A2490	A2416	G2281	U	U	G1777	A1633	G1511	U1345	A1153	G1029
U2581	G2425	U2417	A2282	G	U	U1778	A1634	C1512	U1346	G1157	A1030
U2582	U2426	U2418	U2283	U	U	G1779	C1635	U1513	U1347	A1158	C1031
G2585	G2427	U2419	C2284	G	U	U1780	A1636	G1514	U1348	A1159	G1035
G2586	U2428	U2420	U2285	U	U	G1781	U1637	U1515	U1349	A1160	C1037
A2593	C2435	U2421	G2286	C	U	U1782	A1638	G1516	U1350	C1175	U1040
C2594	G2436	U2422	U2287	U	U	C1783	U1639	A1517	U1351	G1176	U1041
U2602	U2437	G2423	G2288	G	U	G1784	U1640	G1518	U1352	G1177	A1047
U2505	G2440	U2424	U2289	U	U	U1785	A1641	U1519	U1353	G1178	A1048
U2506	A2441	U2425	G2290	C	U	U1786	U1642	U1520	U1354	A1179	A1049
C2507	G2442	U2426	C2291	U	U	G1787	A1643	G1521	U1355	U1180	U1050
U2508	U2443	G2427	G2292	G	U	C1788	U1644	G1522	U1356	U1181	U1051
U2513	A2444	U2428	C2293	C	U	G1789	U1645	U1523	U1357	G1189	A1190
U2514	U2445	U2429	U2294	U	U	G1790	G1657	G1524	U1358	C1192	G1063
A2515	G2446	U2430	G2295	U	U	U1791	G1658	U1525	U1359	A1195	A1065
G2522	A2447	U2431	U2296	A	U	G1792	U1659	U1526	U1360	C1196	U1069
C2531	U2448	U2432	G2297	C	U	U1793	C1660	U1527	U1361	U1200	U1070
U2532	G2449	A2433	C2298	C	U	G1794	G1661	U1528	U1362	C1201	G1072
U2537	U2450	U2434	U2299	U	U	U1795	U1662	U1529	U1363	U1208	U1081
C2538	G2451	G2435	G2300	G	U	G1796	C1663	A1530	U1364	A1212	A1093
U2539	U2452	U2436	U2301	U	U	U1797	U1664	U1531	U1365	U1094	U1095
A2541	A2453	U2437	A2312	C	U	A1798	G1665	U1532	U1366	A1217	U1096
U2542	G2454	U2438	U2313	U	U	U1799	G1666	U1533	U1367	C1218	G1097
U2543	U2455	U2439	U2314	C	U	G1800	G1667	U1534	U1368	A1219	A1098
U2544	G2456	U2440	G2315	U	U	U1801	U1668	U1535	U1369	G1222	A1099
A2547	U2457	U2441	U2316	A	U	G1802	A1696	A1536	U1370	A1223	U1100
C2548	A2458	U2442	A2317	U	U	U1803	U1697	U1537	U1371	C1224	G1101
G2549	U2459	U2443	U2318	C	U	A1804	U1703	U1538	U1372	A1225	A1102
U2550	G2460	U2444	G2319	G	U	U1805	U1704	U1539	U1373	G1230	A1103
U2551	A2461	U2445	U2320	U	U	C1806	U1705	U1540	U1374	A1231	G1104
U2552	U2462	U2446	U2321	C	U	U1807	U1706	U1541	U1375	G1232	G1117
C2552	G2463	U2447	U2322	U	U	G1808	U1707	U1542	U1376	U1325	
U2553	U2464	U2448	A2093	G	U	U1809	U1708	U1543	U1377		
U2554	A2465	U2449	U2094	C	U	U1810	U1709	U1544	U1378		
A2554	G2466	U2450	G2095	U	U	A1811	U1710	U1545	U1379		
U2555	U2467	U2451	A2096	U	U	U1812	U1711	U1546	U1380		
U2556	A2468	U2452	A2100	G	U	U1813	U1712	U1547	U1381		
G2557	G2469	U2453	C2101	C	U	A1814	U1713	U1548	U1382		
U2558	U2470	U2454	U2102	U	U	U1815	U1714	U1549	U1383		
A2574	C2471	U2455	U2103	C	U	A1816	U1715	U1550	U1384		
U2553	U2472	U2456	G2111	U	U	U1817	U1716	U1551	U1385		
G2554	G2473	U2457	U2112	G	U	G1818	U1717	U1552	U1386		
G2555	U2474	U2458	A2113	U	U	U1819	U1718	U1553	U1387		
G2556	G2475	U2459	C2114	C	U	U1820	U1719	U1554	U1388		
		U2260	A2397	G	U	U1821	U1720	U1555	U1389		
						U1822	U1721	U1556	U1390		
						U1823	U1722	U1557	U1391		
						U1824	U1723	U1558	U1392		
						U1825	U1724	U1559	U1393		
						U1826	U1725	U1560	U1394		
						U1827	U1726	U1561	U1395		
						U1828	U1727	U1562	U1396		
						U1829	U1728	U1563	U1397		
						U1830	U1729	U1564	U1398		
						U1831	U1730	U1565	U1399		
						U1832	U1731	U1566	U1400		
						U1833	U1732	U1567	U1401		
						U1834	U1733	U1568	U1402		
						U1835	U1734	U1569	U1403		
						U1836	U1735	U1570	U1404		
						U1837	U1736	U1571	U1405		
						U1838	U1737	U1572	U1406		
						U1839	U1738	U1573	U1407		
						U1840	U1739	U1574	U1408		
						U1841	U1740	U1575	U1409		
						U1842	U1741	U1576	U1410		
						U1843	U1742	U1577	U1411		
						U1844	U1743	U1578	U1412		
						U1845	U1744	U1579	U1413		
						U1846	U1745	U1580	U1414		
						U1847	U1746	U1581	U1415		
						U1848	U1747	U1582	U1416		
						U1849	U1748	U1583	U1417		
						U1850	U1749	U1584	U1418		
						U1851	U1750	U1585	U1419		
						U1852	U1751	U1586	U1420		
						U1853	U1752	U1587	U1421		
						U1854	U1753	U1588	U1422		
						U1855	U1754	U1589	U1423		
						U1856	U1755	U1590	U1424		
						U1857	U1756	U1591	U1425		
						U1858	U1757	U1592	U1426		
						U1859	U1758	U1593	U1427		
						U1860	U1759	U1594	U1428		
						U1861	U1760	U1595	U1429		
						U1862	U1761	U1596	U1430		
						U1863	U1762	U1597	U1431		
						U1864	U1763	U1598	U1432		
						U1865	U1764	U1599	U1433		
						U1866	U1765	U1600	U1434		
						U1867	U1766	U1601	U1435		
						U1868	U1767	U1602	U1436		
						U1869	U1768	U1603	U1437		
						U1870	U1769	U1604	U1438		
						U1871	U1770	U1605	U1439		
						U1872	U1771	U1606	U1440		
						U1873	U1772	U1607	U1441		
						U1874	U1773	U1608	U1442		
						U1875	U1774	U1609	U1443		
						U1876	U1775	U1610	U1444		
						U1877	U1776	U1611	U1445		
						U1878	U1777	U1612	U1446		
						U1879	U1778	U1613	U1447		
						U1880	U1779	U1614	U1448		
						U1881	U1780	U1615	U1449		
						U1882	U1781	U1616	U1450		
						U1883	U1782	U1617	U1451		
						U1884	U1783	U1618	U1452		
						U1885	U1784	U1619	U1453		
						U1886	U1785	U1620	U1454		
						U1887	U1786	U1621	U1455		
						U1888	U1787	U1622	U1456		
						U1889	U1788	U1623	U1457		
						U1890	U1789	U1624	U1458		
						U1891	U1790	U1625	U1459		
						U1892	U1791	U1626	U1460		
						U1893	U1792	U1627	U1461		
						U1894	U1793	U1628	U1462		
						U1895	U1794	U1629	U1463		
						U1896	U1795	U1630	U1464		
						U1897	U1796	U1631	U1465		
						U1898	U1797	U1632	U1466		
						U1899	U1798	U1633	U1467		
						U1900	U1799				



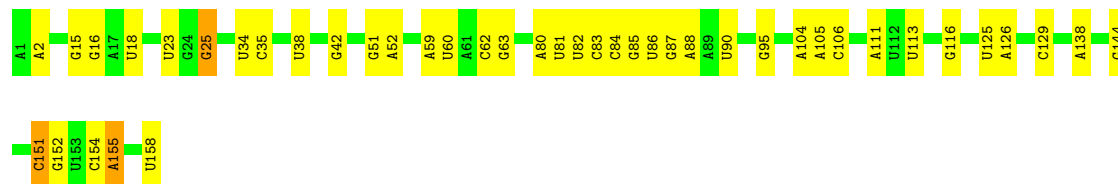
• Molecule 3: 5S Ribosomal RNA

Chain B: 71% 27% .



• Molecule 4: 5.8S Ribosomal RNA

Chain C: 73% 25% .



• Molecule 5: 60S ribosomal protein L2-A

Chain D: 92% 7% .



• Molecule 6: 60S ribosomal protein L3

Chain E: 88% 11% .

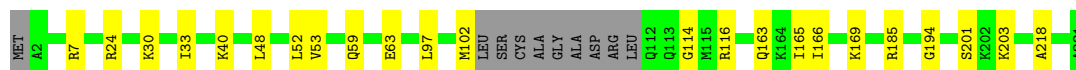






- Molecule 13: 60S ribosomal protein L10

Chain L: 85% 10% 5%



- Molecule 14: 60S ribosomal protein L11-A

Chain M: 90% 7% ..



- Molecule 15: 60S ribosomal protein L13-A

Chain N: 84% 12% ..



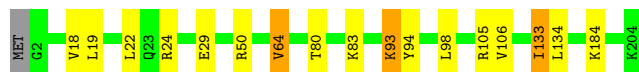
- Molecule 16: 60S ribosomal protein L14-A

Chain O: 89% 8% ..



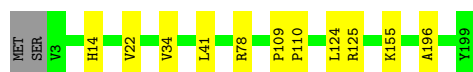
- Molecule 17: 60S ribosomal protein L15-A

Chain a: 91% 7% .



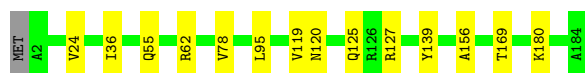
- Molecule 18: 60S ribosomal protein L16-A

Chain b: 93% 6% .



- Molecule 19: 60S ribosomal protein L17-A

Chain c: 92% 8% .



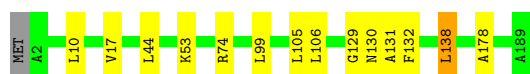
- Molecule 20: 60S ribosomal protein L18-A

Chain d: 93% 6% ..



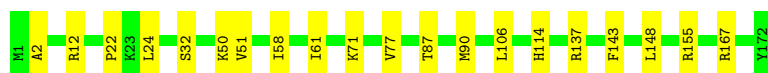
- Molecule 21: 60S ribosomal protein L19-A

Chain e: 92% 7% ..



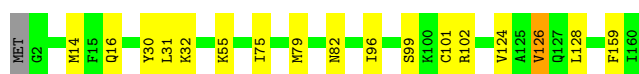
- Molecule 22: 60S ribosomal protein L20-A

Chain f: 88% 12%



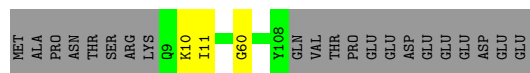
- Molecule 23: 60S ribosomal protein L21-A

Chain g: 89% 10% ..



- Molecule 24: 60S ribosomal protein L22-A

Chain h: 80% 17%



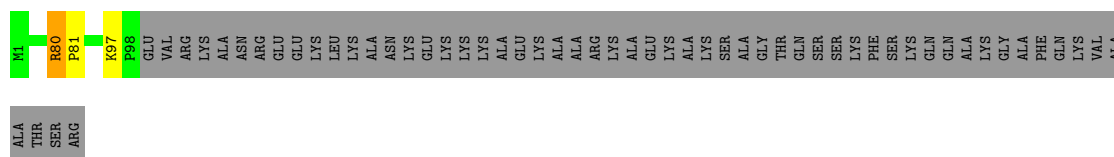
- Molecule 25: 60S ribosomal protein L23-A

Chain i: 92% 7% .



- Molecule 26: 60S ribosomal protein L24-A

Chain j: 61% .. 37%



- Molecule 27: 60S ribosomal protein L25

Chain k: 75% 10% 15%



- Molecule 28: 60S ribosomal protein L26-A

Chain l: 92% 5%



- Molecule 29: 60S ribosomal protein L27-A

Chain m: 90% 8%



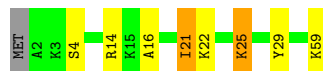
- Molecule 30: 60S ribosomal protein L28

Chain n: 83% 15%



- Molecule 31: 60S ribosomal protein L29

Chain o: 85% 10%



- Molecule 32: 60S ribosomal protein L30

Chain p: 88% 5% 8%



- Molecule 33: 60S ribosomal protein L31-A

Chain q:  86% 10% ..



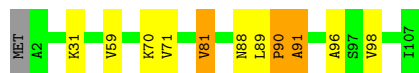
- Molecule 34: 60S ribosomal protein L32

Chain r:  89% 7% ..



- Molecule 35: 60S ribosomal protein L33-A

Chain s:  89% 7% ..



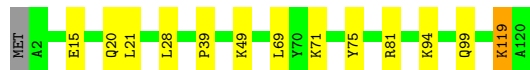
- Molecule 36: 60S ribosomal protein L34-A

Chain t:  83% 9% 7%



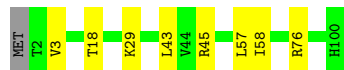
- Molecule 37: 60S ribosomal protein L35-A

Chain u:  88% 10% ..



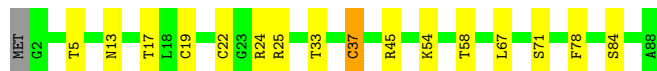
- Molecule 38: 60S ribosomal protein L36-A

Chain v:  91% 8% .



- Molecule 39: 60S ribosomal protein L37-A

Chain w:  81% 17% ..



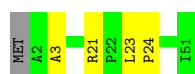
- Molecule 40: 60S ribosomal protein L38

Chain x:  94% 5%



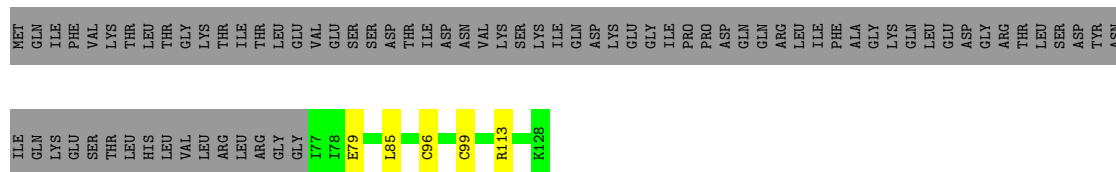
- Molecule 41: 60S ribosomal protein L39

Chain y:  90% 8%



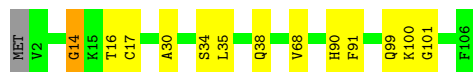
- Molecule 42: Ubiquitin-60S ribosomal protein L40

Chain z:  37% 59%



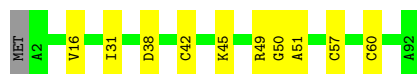
- Molecule 43: 60S ribosomal protein L42-A

Chain Q:  87% 11%

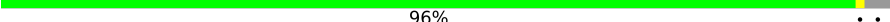


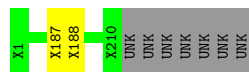
- Molecule 44: 60S ribosomal protein L43-A

Chain R:  88% 11%



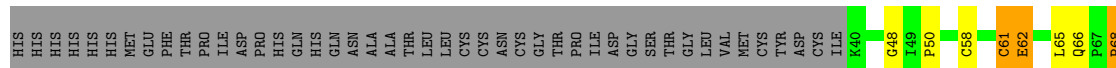
- Molecule 45: Ribosomal Protein uL1

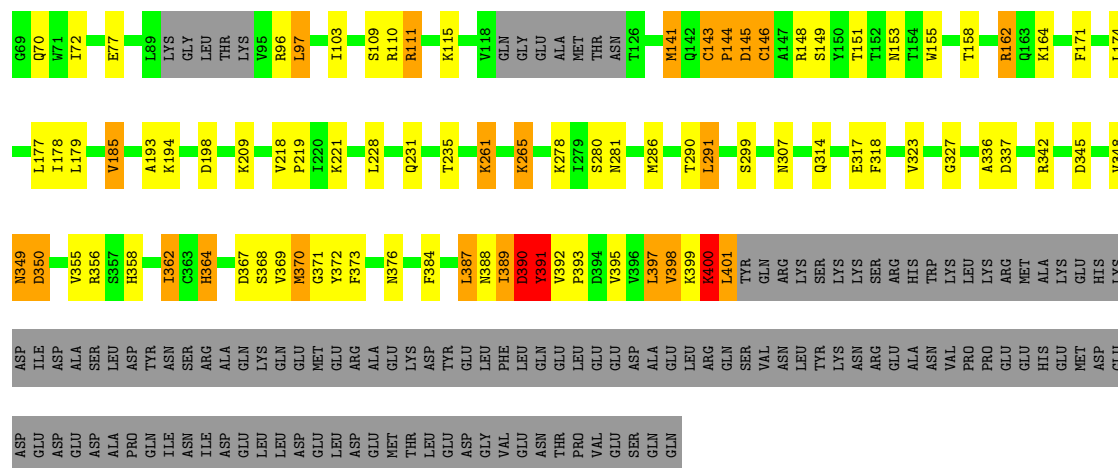
Chain S:  96%



- Molecule 46: 60S ribosomal export protein NMD3

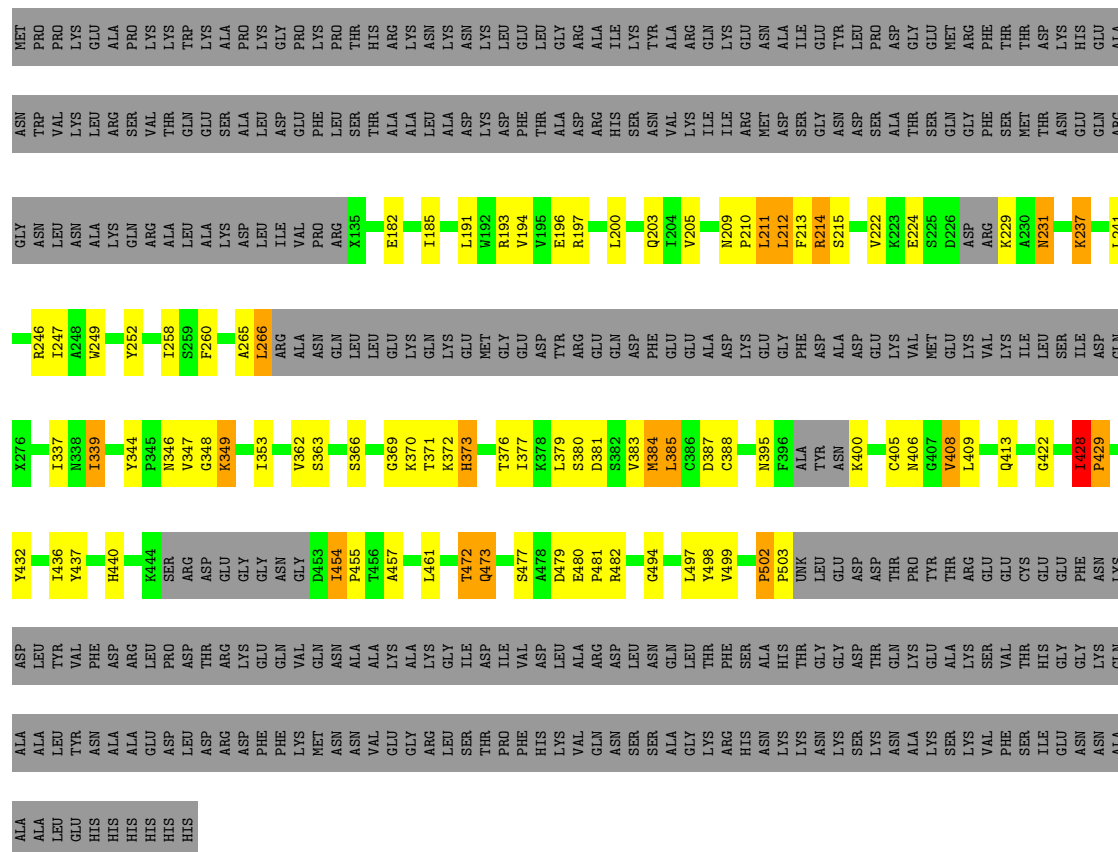
Chain V:  48% 13% 5% 33%





• Molecule 47: Large subunit GTPase 1

Chain W: 33% 11% 53%



4 Experimental information

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	q	0.58	0/890	0.76	0/1196
34	r	0.58	0/1041	0.81	1/1394 (0.1%)
35	s	0.56	0/868	0.81	3/1168 (0.3%)
36	t	0.62	0/890	0.85	0/1189
37	u	0.63	0/978	0.88	0/1301
38	v	0.65	0/778	0.87	0/1034
39	w	0.71	0/696	0.93	1/923 (0.1%)
40	x	0.61	0/618	0.72	0/826
41	y	0.57	0/443	0.81	0/588
42	z	0.60	0/423	0.79	0/562
43	Q	0.61	0/860	0.74	0/1136
44	R	0.67	0/701	0.87	0/934
46	V	0.63	0/2766	0.94	5/3759 (0.1%)
47	W	0.70	0/1950	0.98	2/2640 (0.1%)
All	All	0.49	0/139979	0.77	70/206037 (0.0%)

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

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

There are no bond length outliers.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	j	80	ARG	CA-C-N	9.53	131.76	119.84
26	j	80	ARG	C-N-CA	9.53	131.76	119.84
2	A	3078	U	C4'-C3'-O3'	9.18	123.17	109.40
18	b	109	PRO	CA-C-N	8.93	129.58	120.38
18	b	109	PRO	C-N-CA	8.93	129.58	120.38
18	b	110	PRO	N-CA-C	8.65	121.25	110.70
2	A	979	U	C2'-C3'-O3'	8.40	122.10	109.50
2	A	65	A	C4'-C3'-O3'	8.29	121.83	109.40
2	A	3269	U	C4'-C3'-O3'	8.16	121.64	109.40
2	A	2496	C	C4'-C3'-O3'	7.73	121.00	109.40
46	V	398	VAL	N-CA-C	7.68	118.48	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	169	U	C4'-C3'-O3'	7.62	120.83	109.40
2	A	3218	A	C4'-C3'-O3'	7.53	120.69	109.40
2	A	3228	C	C4'-C3'-O3'	7.51	120.67	109.40
2	A	1576	G	C2'-C3'-O3'	7.51	120.76	109.50
2	A	1716	U	C2'-C3'-O3'	7.37	120.56	109.50
46	V	391	TYR	N-CA-C	-7.37	104.14	113.72
2	A	2112	U	C2'-C3'-O3'	7.25	120.38	109.50
46	V	50	PRO	N-CA-CB	7.11	109.94	103.33
47	W	369	GLY	N-CA-C	7.01	129.79	113.18
46	V	143	CYS	C-N-CD	-6.95	96.51	125.00
2	A	1815	U	C2'-C3'-O3'	6.84	119.75	109.50
17	a	93	LYS	N-CA-C	6.82	122.70	113.97
2	A	2541	U	C2'-C3'-O3'	6.68	119.53	109.50
35	s	89	LEU	CA-C-N	6.57	127.08	119.47
35	s	89	LEU	C-N-CA	6.57	127.08	119.47
2	A	1064	A	C2'-C3'-O3'	6.46	119.20	109.50
2	A	3317	U	C4'-C3'-O3'	6.33	118.90	109.40
2	A	2209	U	C2'-C3'-O3'	6.32	118.98	109.50
46	V	261	LYS	N-CA-C	6.28	117.78	111.07
2	A	2593	A	C4'-C3'-O3'	6.18	118.67	109.40
39	w	37	CYS	N-CA-C	6.15	118.06	111.36
2	A	3353	G	C4'-C3'-O3'	6.14	118.62	109.40
35	s	90	PRO	N-CA-C	6.12	122.68	113.81
2	A	2101	C	C2'-C3'-O3'	6.05	118.58	109.50
22	f	12	ARG	N-CA-C	5.90	117.37	110.41
2	A	2101	C	C4'-C3'-O3'	5.89	118.23	109.40
2	A	1355	A	C2'-C3'-O3'	5.80	118.20	109.50
2	A	2593	A	C2'-C3'-O3'	5.79	118.19	109.50
2	A	2537	U	C2'-C3'-O3'	5.79	118.19	109.50
2	A	2453	U	C4'-C3'-O3'	5.77	118.06	109.40
2	A	1352	A	C2'-C3'-O3'	5.73	118.10	109.50
2	A	599	C	C2'-C3'-O3'	5.69	122.23	113.70
1	X	102	SER	N-CA-C	5.64	115.83	107.88
2	A	1103	A	C2'-C3'-O3'	5.61	117.92	109.50
2	A	1562	C	C4'-C3'-O3'	5.60	117.81	109.40
2	A	1142	G	C4'-C3'-O3'	-5.59	104.61	113.00
2	A	3195	U	C4'-C3'-O3'	5.53	117.70	109.40
2	A	3013	U	C4'-C3'-O3'	-5.51	104.74	113.00
17	a	64	VAL	N-CA-C	5.37	114.93	108.06
12	K	151	VAL	N-CA-C	-5.36	106.47	111.45
2	A	780	A	C2'-C3'-O3'	5.31	117.47	109.50
2	A	115	A	C2'-C3'-O3'	-5.31	105.73	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	W	494	GLY	N-CA-C	5.31	119.31	112.83
2	A	2281	A	C4'-C3'-O3'	5.30	117.36	109.40
2	A	1816	A	C3'-C2'-O2'	5.30	118.66	110.70
2	A	3351	U	C4'-C3'-O3'	5.28	117.32	109.40
2	A	1196	C	C2'-C3'-O3'	5.27	117.40	109.50
2	A	873	C	C2'-C3'-O3'	-5.23	105.86	113.70
2	A	2636	A	C4'-C3'-O3'	-5.22	105.16	113.00
2	A	1194	G	C4'-C3'-O3'	-5.22	105.17	113.00
2	A	1355	A	C4'-C3'-O3'	5.19	117.19	109.40
1	X	28	VAL	N-CA-C	5.19	115.41	110.53
2	A	2807	U	C4'-C3'-O3'	-5.18	105.22	113.00
2	A	711	A	C4'-C3'-O3'	-5.17	105.25	113.00
2	A	959	C	C2'-C3'-O3'	-5.09	106.06	113.70
2	A	2655	U	C4'-C3'-O3'	5.09	117.03	109.40
2	A	1858	A	C4'-C3'-O3'	5.08	117.03	109.40
34	r	40	SER	N-CA-C	5.08	118.15	110.64
2	A	2501	U	C3'-C2'-O2'	5.02	118.23	110.70

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	1633	0	1596	11	0
2	A	68535	0	34438	193	0
3	B	2579	0	1304	5	0
4	C	3353	0	1695	4	0
5	D	1914	0	1981	6	0
6	E	3075	0	3142	7	0
7	F	2748	0	2859	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	2375	0	2325	4	0
9	H	1239	0	1326	1	0
10	I	1784	0	1862	6	0
11	J	1804	0	1877	2	0
12	K	1518	0	1587	7	0
13	L	1705	0	1736	2	0
14	M	1353	0	1383	2	0
15	N	1543	0	1608	6	0
16	O	1053	0	1149	4	0
17	a	1720	0	1779	4	0
18	b	1555	0	1659	2	0
19	c	1420	0	1437	4	0
20	d	1441	0	1543	3	0
21	e	1521	0	1617	3	0
22	f	1445	0	1487	5	0
23	g	1276	0	1323	7	0
24	h	796	0	812	0	0
25	i	1003	0	1048	7	0
26	j	699	0	640	0	0
27	k	964	0	1025	5	0
28	l	993	0	1081	3	0
29	m	1092	0	1155	4	0
30	n	1173	0	1215	10	0
31	o	462	0	491	2	0
32	p	743	0	797	2	0
33	q	876	0	912	2	0
34	r	1020	0	1090	2	0
35	s	850	0	880	3	0
36	t	880	0	945	3	0
37	u	969	0	1078	1	0
38	v	771	0	849	1	0
39	w	681	0	685	5	0
40	x	612	0	682	0	0
41	y	436	0	475	1	0
42	z	417	0	459	1	0
43	Q	847	0	918	4	0
44	R	694	0	738	2	0
45	S	1050	0	246	1	0
46	V	2713	0	2644	71	0
47	W	2236	0	2029	67	0
48	A	148	0	0	0	0
48	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	C	2	0	0	0	0
48	D	1	0	0	0	0
48	W	1	0	0	0	0
48	a	1	0	0	0	0
48	c	1	0	0	0	0
48	i	1	0	0	0	0
49	A	2	0	0	0	0
50	W	32	0	13	12	0
51	A	5	0	0	0	0
51	e	1	0	0	0	0
All	All	131766	0	95620	436	0

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

All (436) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2410:U:O4	2:A:2801:A:N1	1.61	1.33
47:W:349:LYS:HG2	50:W:701:GNP:O2B	1.32	1.30
2:A:2264:PSU:O2'	2:A:2265:C:H6	0.96	1.28
2:A:2252:A:N6	2:A:2264:PSU:O2	1.69	1.24
46:V:388:ASN:O	46:V:390:ASP:N	1.73	1.20
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
46:V:367:ASP:CG	46:V:400:LYS:NZ	2.35	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
46:V:367:ASP:CG	46:V:400:LYS:HZ2	1.85	0.83
2:A:2266:PSU:HO2'	2:A:2267:C:P	2.02	0.82
20:d:71:LEU:HD13	20:d:99:THR:HG21	1.61	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
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
2:A:1093:A:C2	2:A:1096:U:C2	2.71	0.77
2:A:2267:C:H5''	2:A:2267:C:H6	1.49	0.77
46:V:372:TYR:CE1	46:V:398:VAL:CG2	2.68	0.77
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:368:SER:O	46:V:401:LEU:C	2.28	0.75
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:HD23	47:W:266:LEU:O	1.88	0.74
1:X:106:ASN:ND2	25:i:131:SER:O	2.19	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:H2'	1.87	0.73
16:O:38:ILE:HD11	22:f:148:LEU:HD23	1.69	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
1:X:102:SER:OG	25:i:134:GLY:O	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:W:366:SER:HA	50:W:701:GNP:HO3'	1.52	0.70
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
46:V:389:ILE:O	46:V:389:ILE:CG2	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
29:m:24:VAL:HG11	29:m:87:LEU:HD23	1.76	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
22:f:77:VAL:HG11	22:f:106:LEU:HD13	1.76	0.66
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:401:LEU:O	46:V:401:LEU:HD13	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
46:V:61:CYS:O	46:V:62:GLU:HB2	1.96	0.64
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:H4'	2:A:78:U:OP1	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	30:n:21:ARG:NH2	2.32	0.62
21:e:106:LEU:HD13	21:e:138:LEU:HD11	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:192:VAL:HG21	25:i:128:ARG:NE	2.16	0.61
47:W:241:LEU:CD1	47:W:499:VAL:HG11	2.32	0.60
1:X:102:SER:HA	25:i:135:VAL:HA	1.82	0.60
47:W:371:THR:HG22	47:W:371:THR:O	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:O	46:V:362:ILE:HG13	2.00	0.59
47:W:344:TYR:CD2	47:W:408:VAL:HG21	2.37	0.59
15:N:2:ALA:HB1	30:n:33:GLY:O	2.03	0.59
17:a:18:VAL:HG13	17:a:19:LEU:HD12	1.85	0.59
2:A:2266:PSU:H3'	2:A:2266:PSU:H6	1.65	0.59
2:A:2267:C:H5''	2:A:2267:C:C6	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
21:e:105:LEU:HD12	21:e:138:LEU:HD13	1.83	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
46:V:388:ASN:C	46:V:390:ASP:N	2.58	0.58
2:A:2266:PSU:C6	2:A:2266:PSU:C3'	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
2:A:1427:U:OP2	30:n:4:ARG:NH2	2.38	0.57
47:W:209:ASN:HD21	47:W:212:LEU:CB	2.18	0.57
35:s:71:VAL:HG13	35:s:81:VAL:HG13	1.87	0.56
2:A:78:U:C6	2:A:78:U:C5'	2.85	0.56
47:W:212:LEU:O	47:W:212:LEU:HD12	2.06	0.56
2:A:2263:C:C2'	2:A:2264:PSU:C5'	2.78	0.56
27:k:105:VAL:HG11	27:k:126:LEU:HD22	1.87	0.56
23:g:14:MET:HE1	23:g:55:LYS:HB2	1.86	0.56
2:A:706:A:H2'	2:A:707:U:O4'	2.06	0.56
46:V:401:LEU:C	46:V:401:LEU:HD22	2.29	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:266:LEU:HD13	50:W:701:GNP:N1	2.23	0.54
47:W:376:THR:CG2	47:W:384:MET:SD	2.96	0.54
2:A:2258:PSU:C1'	47:W:193:ARG:HH12	2.19	0.54
39:w:19:CYS:SG	39:w:37:CYS:SG	3.06	0.54
2:A:1189:C:N3	2:A:1315:U:O2	2.41	0.53
2:A:1573:G:N3	2:A:1573:G:H2'	2.23	0.53
39:w:54:LYS:O	39:w:58:THR:HG23	2.08	0.53
3:B:121:U:O2	3:B:121:U:O4'	2.27	0.53
2:A:1286:A:N3	2:A:1287:A:H1'	2.23	0.53
2:A:2312:A:O2'	2:A:2315:G:N3	2.41	0.53
2:A:1093:A:N3	2:A:1096:U:H3	1.45	0.53
22:f:2:ALA:HB3	22:f:32:SER:HB3	1.91	0.53
31:o:16:ALA:HB1	31:o:21:ILE:HD11	1.89	0.53
46:V:70:GLN:CD	46:V:70:GLN:H	2.17	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
46:V:65:LEU:HD22	46:V:141:MET:HE1	1.90	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:H5''	2:A:2257:C:H6	1.69	0.52
23:g:14:MET:HE1	23:g:55:LYS:CB	2.40	0.52
46:V:144:PRO:O	46:V:148:ARG:CD	2.57	0.52
47:W:266:LEU:N	47:W:266:LEU:CD2	2.73	0.51
30:n:104:THR:HG21	30:n:112:ILE:HD11	1.92	0.51
2:A:40:A:N7	30:n:29:PRO:O	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2251:G:C2	2:A:2266:PSU:O4	2.64	0.51
8:G:38:THR:HG22	23:g:30:TYR:HB3	1.91	0.51
23:g:99:SER:HG	23:g:101:CYS:HG	1.58	0.51
33:q:14:ILE:HD12	33:q:39:PHE:CG	2.45	0.51
2:A:662:U:OP1	30:n:8:THR:HG21	2.11	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
47:W:379:LEU:CB	47:W:385:LEU:HD21	2.41	0.50
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:1639:C:OP2	36:t:74:ARG:NH2	2.45	0.50
2:A:436:A:H2'	2:A:437:G:O4'	2.12	0.50
2:A:2249:G:C8	2:A:2249:G:H3'	2.47	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
30:n:3:SER:O	30:n:6:THR:HG22	2.13	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
17:a:18:VAL:HG13	17:a:19:LEU:CD1	2.42	0.49
30:n:77:LYS:O	30:n:79:TRP:N	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:261:LYS:HZ2	46:V:265:LYS:HD3	1.79	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:618:C:H5'	19:c:169:THR:HG22	1.95	0.48
2:A:1190:A:N1	2:A:1315:U:C4	2.78	0.48
2:A:1393:A:OP1	34:r:125:ARG:NH2	2.46	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
22:f:90:MET:HE1	22:f:114:HIS:NE2	2.29	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
46:V:317:GLU:HA	46:V:370:MET:HE3	1.97	0.47
47:W:211:LEU:CD2	47:W:252:TYR:OH	2.59	0.47
6:E:256:HIS:HA	6:E:257:PRO:C	2.39	0.47
23:g:82:ASN:HA	31:o:21:ILE:HD13	1.94	0.47
2:A:2624:G:OP1	46:V:162:ARG:HD3	2.15	0.47
12:K:41:ILE:HD13	12:K:41:ILE:O	2.13	0.47
2:A:1784:G:H2'	2:A:1785:U:O4'	2.14	0.47
41:y:23:LEU:HD22	41:y:24:PRO:HD2	1.96	0.47
1:X:107:VAL:HG13	1:X:118:HIS:HB2	1.97	0.47
2:A:315:C:N4	2:A:316:U:O4	2.48	0.47
7:F:219:LEU:HD22	7:F:225:VAL:HG11	1.96	0.47
10:I:88:ARG:HA	10:I:134:VAL:HG12	1.95	0.47
12:K:4:ILE:HD12	22:f:143:PHE:CE1	2.50	0.47
46:V:70:GLN:CD	46:V:70:GLN:N	2.73	0.47
46:V:290:THR:O	46:V:291:LEU:C	2.57	0.47
35:s:90:PRO:O	35:s:91:ALA:HB3	2.14	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
42:z:96:CYS:SG	42:z:99:CYS:SG	3.05	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:239:G:OP1	37:u:94:LYS:NZ	2.46	0.46
47:W:480:GLU:N	47:W:481:PRO:CD	2.79	0.46
1:X:106:ASN:ND2	1:X:150:SER:OG	2.48	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
2:A:2922:G:O6	46:V:235:THR:OG1	2.34	0.46
16:O:68:LEU:HD21	16:O:93:LYS:HD2	1.97	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
29:m:24:VAL:CG1	29:m:87:LEU:HD23	2.45	0.46
46:V:323:VAL:CG1	46:V:336:ALA:HB1	2.46	0.46
1:X:102:SER:OG	1:X:103:ALA:N	2.48	0.46
10:I:156:ILE:HD12	10:I:161:VAL:HG21	1.98	0.46
2:A:824:C:H2'	2:A:825:U:O5'	2.16	0.45
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: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:3173:G:C2	35:s:96:ALA:HB2	2.51	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
1:X:102:SER:CB	25:i:134:GLY:O	2.64	0.45
2:A:979:U:C2	2:A:980:A:C2	3.05	0.45
19:c:36:ILE:CD1	19:c:95:LEU:HD11	2.46	0.45
46:V:96:ARG:O	46:V:97:LEU:CB	2.64	0.45
2:A:1002:A:N1	2:A:1050:U:O2'	2.45	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
30:n:112:ILE:HB	30:n:130:VAL:HG12	1.98	0.45
2:A:2196:C:HO2'	2:A:2270:A:H8	1.63	0.45
2:A:687:U:OP2	15:N:36:ARG:NH2	2.50	0.44
2:A:901:G:OP1	39:w:13:ASN:ND2	2.50	0.44
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
32:p:26:GLY:O	32:p:30:THR:HG23	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:216:G:OP1	28:l:16:ARG:NH1	2.50	0.44
2:A:681:U:H2'	2:A:696:C:H42	1.81	0.44
20:d:161:LYS:O	20:d:162:ALA:HB3	2.17	0.44
28:l:56:VAL:CG2	28:l:70:ILE:HD11	2.47	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:662:U:H2'	2:A:663:C:C6	2.52	0.44
2:A:1895:A:O2'	2:A:3053:G:H4'	2.17	0.44
2:A:2256:A:H3'	2:A:2257:C:H6	1.82	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:HE21	47:W:473:GLN:HB2	1.56	0.44
2:A:1097:G:C8	23:g:128:LEU:HD13	2.53	0.43
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:1157:G:O2'	2:A:1169:A:N3	2.49	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
1:X:192:VAL:HG21	25:i:128:ARG:HE	1.83	0.43
2:A:324:A:C6	2:A:325:A:N6	2.87	0.43
2:A:1804:A:H2'	2:A:1805:C:C6	2.54	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
8:G:37:VAL:HG12	23:g:31:LEU:HD21	2.00	0.43
27:k:86:VAL:HG21	27:k:95:ILE:HG12	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
2:A:1845:G:O2'	39:w:5:THR:HG22	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:q:29:ALA:HB3	33:q:30:PRO:HD3	2.01	0.43
2:A:651:G:C6	2:A:652:G:C6	3.06	0.42
4:C:25:G:N7	28:l:13:ARG:NH2	2.67	0.42
2:A:361:A:O3'	39:w:45:ARG:NH2	2.52	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
1:X:28:VAL:HG13	1:X:52:THR:HG23	2.01	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
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:HE21	43:Q:38:GLN:HA	1.85	0.42
15:N:106:GLN:HB3	38:v:18:THR:HG23	2.01	0.42
46:V:155:TRP:CZ3	46:V:158:THR:OG1	2.72	0.42
2:A:2293:C:O2'	47:W:473:GLN:NE2	2.51	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
2:A:289:A:N3	17:a:93:LYS:HG2	2.35	0.42
21:e:130:ASN:O	21:e:132:PHE:N	2.53	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
32:p:30:THR:HG21	32:p:89:VAL:HG22	2.01	0.42
36:t:56:THR:O	36:t:57:LEU:HD23	2.20	0.42
10:I:158:LYS:O	10:I:159:GLN:C	2.63	0.42
14:M:12:LEU:HD12	14:M:131:MET:HE3	2.01	0.42
17:a:133:ILE:HD12	17:a:134:LEU:N	2.35	0.42
27:k:63:ILE:HD13	27:k:63:ILE:C	2.45	0.42
1:X:102:SER:HA	25:i:134:GLY:C	2.44	0.42
20:d:71:LEU:CD1	20:d:99:THR:HG21	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:W:213:PHE:CD2	47:W:347:VAL:HG21	2.55	0.41
2:A:412:G:OP1	19:c:62:ARG:NH1	2.52	0.41
2:A:2290:C:O2'	47:W:413:GLN:NE2	2.54	0.41
16:O:108:ARG:NH2	18:b:196:ALA:O	2.54	0.41
46:V:371:GLY:HA3	46:V:397:LEU:HA	2.01	0.41
2:A:979:U:N3	2:A:980:A:C2	2.88	0.41
2:A:2434:U:O2	2:A:2434:U:O4'	2.38	0.41
46:V:58:CYS:HB2	46:V:143:CYS:HB3	2.00	0.41
2:A:2355:G:H4'	19:c:139:TYR:CE2	2.56	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
29:m:16:GLY:O	29:m:18:TYR:N	2.54	0.41
2:A:824:C:C2'	2:A:825:U:O5'	2.68	0.41
2:A:1093:A:H2	2:A:1096:U:O2	2.00	0.41
2:A:3305:A:H2'	2:A:3306:U:O4'	2.21	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:H2'	2:A:1190:A:N3	2.36	0.41
3:B:24:A:H2'	3:B:25:G:O4'	2.21	0.41
27:k:105:VAL:CG1	27:k:126:LEU:HD22	2.49	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
18:b:14:HIS:CE1	18:b:124:LEU:HD13	2.56	0.40
29:m:14:VAL:HG21	36:t:90:ILE:HD11	2.02	0.40
2:A:1145:G:OP1	34:r:44:ARG:NH1	2.52	0.40
5:D:204:MET:HE3	5:D:209:HIS:HB2	2.03	0.40
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:664:U:H5'	7:F:107:ARG:HA	2.04	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
4:C:151:C:C4	27:k:24:LEU:HD11	2.57	0.40
2:A:785:G:O6	30:n:77:LYS:NZ	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	222/264 (84%)	202 (91%)	20 (9%)	0	100	100
5	D	250/254 (98%)	226 (90%)	22 (9%)	2 (1%)	16	47
6	E	384/387 (99%)	346 (90%)	31 (8%)	7 (2%)	6	28
7	F	359/362 (99%)	311 (87%)	32 (9%)	16 (4%)	2	12
8	G	294/297 (99%)	265 (90%)	25 (8%)	4 (1%)	9	34
9	H	152/176 (86%)	133 (88%)	16 (10%)	3 (2%)	6	25
10	I	220/244 (90%)	200 (91%)	14 (6%)	6 (3%)	4	20
11	J	231/256 (90%)	207 (90%)	17 (7%)	7 (3%)	3	19
12	K	189/191 (99%)	169 (89%)	17 (9%)	3 (2%)	7	30
13	L	207/221 (94%)	186 (90%)	16 (8%)	5 (2%)	4	22
14	M	167/174 (96%)	143 (86%)	19 (11%)	5 (3%)	3	19
15	N	191/199 (96%)	168 (88%)	18 (9%)	5 (3%)	4	21
16	O	134/138 (97%)	119 (89%)	10 (8%)	5 (4%)	2	15
17	a	201/204 (98%)	188 (94%)	11 (6%)	2 (1%)	12	41
18	b	195/199 (98%)	184 (94%)	11 (6%)	0	100	100
19	c	181/184 (98%)	163 (90%)	17 (9%)	1 (1%)	21	52
20	d	183/186 (98%)	162 (88%)	18 (10%)	3 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	e	186/189 (98%)	173 (93%)	9 (5%)	4 (2%)	5	24
22	f	170/172 (99%)	156 (92%)	11 (6%)	3 (2%)	6	28
23	g	157/160 (98%)	141 (90%)	13 (8%)	3 (2%)	6	27
24	h	98/121 (81%)	79 (81%)	17 (17%)	2 (2%)	6	25
25	i	134/137 (98%)	124 (92%)	9 (7%)	1 (1%)	18	49
26	j	96/155 (62%)	81 (84%)	12 (12%)	3 (3%)	3	18
27	k	119/142 (84%)	107 (90%)	11 (9%)	1 (1%)	16	47
28	l	124/127 (98%)	115 (93%)	7 (6%)	2 (2%)	7	30
29	m	133/136 (98%)	111 (84%)	18 (14%)	4 (3%)	3	19
30	n	146/149 (98%)	126 (86%)	13 (9%)	7 (5%)	2	11
31	o	56/59 (95%)	48 (86%)	5 (9%)	3 (5%)	1	9
32	p	95/105 (90%)	88 (93%)	7 (7%)	0	100	100
33	q	107/113 (95%)	98 (92%)	6 (6%)	3 (3%)	4	20
34	r	125/130 (96%)	121 (97%)	3 (2%)	1 (1%)	16	47
35	s	104/107 (97%)	95 (91%)	7 (7%)	2 (2%)	6	27
36	t	110/121 (91%)	102 (93%)	6 (6%)	2 (2%)	6	28
37	u	117/120 (98%)	109 (93%)	4 (3%)	4 (3%)	3	16
38	v	97/100 (97%)	88 (91%)	8 (8%)	1 (1%)	12	41
39	w	85/88 (97%)	77 (91%)	6 (7%)	2 (2%)	4	22
40	x	75/78 (96%)	67 (89%)	5 (7%)	3 (4%)	2	13
41	y	48/51 (94%)	44 (92%)	3 (6%)	1 (2%)	5	25
42	z	50/128 (39%)	47 (94%)	2 (4%)	1 (2%)	6	25
43	Q	103/106 (97%)	88 (85%)	10 (10%)	5 (5%)	1	11
44	R	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
46	V	344/524 (66%)	302 (88%)	27 (8%)	15 (4%)	2	12
47	W	231/651 (36%)	198 (86%)	25 (11%)	8 (4%)	3	16
All	All	6959/7997 (87%)	6240 (90%)	564 (8%)	155 (2%)	7	24

All (155) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	E	351	LEU
10	I	159	GLN

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	65 78
5	D	193/196 (98%)	184 (95%)	9 (5%)	23 55
6	E	320/323 (99%)	293 (92%)	27 (8%)	10 35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	F	288/289 (100%)	278 (96%)	10 (4%)	32	62
8	G	244/245 (100%)	230 (94%)	14 (6%)	18	49
9	H	134/153 (88%)	128 (96%)	6 (4%)	24	56
10	I	186/205 (91%)	178 (96%)	8 (4%)	26	57
11	J	187/208 (90%)	171 (91%)	16 (9%)	10	34
12	K	171/171 (100%)	159 (93%)	12 (7%)	14	41
13	L	177/187 (95%)	163 (92%)	14 (8%)	11	37
14	M	147/150 (98%)	141 (96%)	6 (4%)	27	59
15	N	154/159 (97%)	140 (91%)	14 (9%)	9	32
16	O	107/109 (98%)	103 (96%)	4 (4%)	30	61
17	a	175/176 (99%)	164 (94%)	11 (6%)	16	45
18	b	160/162 (99%)	154 (96%)	6 (4%)	29	60
19	c	140/146 (96%)	132 (94%)	8 (6%)	18	49
20	d	150/151 (99%)	144 (96%)	6 (4%)	28	60
21	e	153/154 (99%)	147 (96%)	6 (4%)	28	60
22	f	156/156 (100%)	148 (95%)	8 (5%)	21	52
23	g	136/137 (99%)	129 (95%)	7 (5%)	21	52
24	h	87/107 (81%)	86 (99%)	1 (1%)	65	78
25	i	104/105 (99%)	99 (95%)	5 (5%)	23	54
26	j	57/129 (44%)	57 (100%)	0	100	100
27	k	104/118 (88%)	95 (91%)	9 (9%)	9	34
28	l	109/110 (99%)	103 (94%)	6 (6%)	19	50
29	m	115/116 (99%)	109 (95%)	6 (5%)	21	51
30	n	118/119 (99%)	111 (94%)	7 (6%)	18	48
31	o	46/47 (98%)	42 (91%)	4 (9%)	9	34
32	p	81/88 (92%)	79 (98%)	2 (2%)	42	69
33	q	92/97 (95%)	86 (94%)	6 (6%)	15	44
34	r	109/111 (98%)	100 (92%)	9 (8%)	10	35
35	s	90/91 (99%)	85 (94%)	5 (6%)	19	49
36	t	95/103 (92%)	90 (95%)	5 (5%)	20	51
37	u	104/105 (99%)	95 (91%)	9 (9%)	9	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	v	81/82 (99%)	75 (93%)	6 (7%)	13	40
39	w	70/71 (99%)	63 (90%)	7 (10%)	7	29
40	x	68/69 (99%)	67 (98%)	1 (2%)	57	75
41	y	45/46 (98%)	44 (98%)	1 (2%)	45	71
42	z	47/116 (40%)	45 (96%)	2 (4%)	26	57
43	Q	90/91 (99%)	87 (97%)	3 (3%)	33	63
44	R	71/72 (99%)	65 (92%)	6 (8%)	10	35
46	V	291/473 (62%)	257 (88%)	34 (12%)	5	22
47	W	209/502 (42%)	168 (80%)	41 (20%)	1	6
All	All	5838/6672 (88%)	5469 (94%)	369 (6%)	18	45

All (369) 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
5	D	45	VAL
5	D	48	ILE
5	D	101	VAL
5	D	116	VAL
5	D	207	VAL
5	D	227	ARG
5	D	230	VAL
5	D	246	LEU
6	E	10	ARG
6	E	25	ILE
6	E	30	LYS
6	E	43	LEU
6	E	56	ILE
6	E	74	GLU
6	E	84	VAL
6	E	85	VAL
6	E	90	VAL
6	E	103	THR
6	E	115	LYS
6	E	146	ARG
6	E	162	VAL
6	E	169	THR

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Mol	Chain	Res	Type
6	E	205	VAL
6	E	211	GLN
6	E	232	ARG
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	328	ILE
6	E	331	ASN
6	E	338	LEU
6	E	382	THR
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	307	GLN
7	F	313	LEU
7	F	327	LEU
8	G	22	ARG
8	G	23	ARG
8	G	35	ARG
8	G	41	LYS
8	G	58	LYS
8	G	92	LEU
8	G	95	TRP
8	G	105	ILE
8	G	112	LYS
8	G	131	LEU
8	G	146	LEU
8	G	151	GLN
8	G	173	VAL
8	G	211	LEU
9	H	34	LEU
9	H	35	VAL
9	H	65	ILE
9	H	77	ARG
9	H	151	LYS

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Mol	Chain	Res	Type
9	H	155	LEU
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	163	VAL
11	J	169	LEU
11	J	189	LEU
11	J	190	VAL
11	J	194	THR
11	J	224	ASP
11	J	232	HIS
11	J	248	LYS
12	K	5	GLN
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	164	ILE
12	K	166	ARG
13	L	7	ARG
13	L	30	LYS
13	L	33	ILE
13	L	40	LYS
13	L	48	LEU

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Mol	Chain	Res	Type
13	L	52	LEU
13	L	63	GLU
13	L	102	MET
13	L	163	GLN
13	L	165	ILE
13	L	169	LYS
13	L	185	ARG
13	L	201	SER
13	L	203	LYS
14	M	12	LEU
14	M	40	LEU
14	M	81	GLU
14	M	107	ASP
14	M	130	VAL
14	M	142	LYS
15	N	23	LYS
15	N	24	VAL
15	N	54	LEU
15	N	58	VAL
15	N	69	VAL
15	N	76	THR
15	N	86	THR
15	N	116	LEU
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	68	LEU
16	O	72	LEU
16	O	91	CYS
16	O	108	ARG
17	a	22	LEU
17	a	24	ARG
17	a	29	GLU
17	a	50	ARG
17	a	64	VAL
17	a	80	THR
17	a	83	LYS
17	a	98	LEU
17	a	105	ARG

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Mol	Chain	Res	Type
17	a	106	VAL
17	a	133	ILE
18	b	22	VAL
18	b	34	VAL
18	b	41	LEU
18	b	78	ARG
18	b	125	ARG
18	b	155	LYS
19	c	24	VAL
19	c	55	GLN
19	c	78	VAL
19	c	119	VAL
19	c	120	ASN
19	c	125	GLN
19	c	127	ARG
19	c	180	LYS
20	d	39	ARG
20	d	49	LEU
20	d	122	ILE
20	d	135	GLN
20	d	150	VAL
20	d	186	VAL
21	e	10	LEU
21	e	17	VAL
21	e	44	LEU
21	e	74	ARG
21	e	99	LEU
21	e	138	LEU
22	f	50	LYS
22	f	51	VAL
22	f	58	ILE
22	f	61	ILE
22	f	71	LYS
22	f	87	THR
22	f	137	ARG
22	f	155	ARG
23	g	16	GLN
23	g	32	LYS
23	g	75	ILE
23	g	79	MET
23	g	96	ILE
23	g	102	ARG

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Mol	Chain	Res	Type
23	g	126	VAL
24	h	10	LYS
25	i	33	ASN
25	i	71	LYS
25	i	73	VAL
25	i	83	LYS
25	i	88	ARG
27	k	26	VAL
27	k	63	ILE
27	k	70	GLU
27	k	96	LYS
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	56	VAL
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	7	LYS
30	n	34	MET
30	n	42	ARG
30	n	78	LEU
30	n	120	ASN
30	n	130	VAL
30	n	133	LEU
31	o	14	ARG
31	o	22	LYS
31	o	25	LYS
31	o	59	LYS
32	p	41	LEU
32	p	87	VAL
33	q	16	LEU

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Mol	Chain	Res	Type
33	q	35	GLU
33	q	55	LEU
33	q	79	ARG
33	q	82	GLU
33	q	86	LYS
34	r	8	LYS
34	r	19	ARG
34	r	33	ARG
34	r	44	ARG
34	r	47	ARG
34	r	73	THR
34	r	75	LEU
34	r	125	ARG
34	r	128	LEU
35	s	31	LYS
35	s	59	VAL
35	s	70	LYS
35	s	81	VAL
35	s	98	VAL
36	t	29	ILE
36	t	33	GLN
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	81	ARG
37	u	119	LYS
38	v	29	LYS
38	v	43	LEU
38	v	45	ARG
38	v	57	LEU
38	v	58	ILE
38	v	76	ARG
39	w	17	THR
39	w	22	CYS
39	w	24	ARG

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Mol	Chain	Res	Type
39	w	25	ARG
39	w	33	THR
39	w	67	LEU
39	w	71	SER
40	x	67	GLN
41	y	21	ARG
42	z	85	LEU
42	z	113	ARG
43	Q	35	LEU
43	Q	99	GLN
43	Q	100	LYS
44	R	16	VAL
44	R	31	ILE
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	115	LYS
46	V	141	MET
46	V	145	ASP
46	V	146	CYS
46	V	162	ARG
46	V	164	LYS
46	V	171	PHE
46	V	177	LEU
46	V	179	LEU
46	V	185	VAL
46	V	209	LYS
46	V	221	LYS
46	V	228	LEU
46	V	265	LYS
46	V	278	LYS
46	V	286	MET
46	V	291	LEU
46	V	299	SER
46	V	307	ASN
46	V	350	ASP
46	V	362	ILE

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Mol	Chain	Res	Type
46	V	364	HIS
46	V	370	MET
46	V	376	ASN
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	229	LYS
47	W	231	ASN
47	W	237	LYS
47	W	246	ARG
47	W	247	ILE
47	W	260	PHE
47	W	266	LEU
47	W	337	ILE
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	383	VAL
47	W	384	MET
47	W	385	LEU
47	W	395	ASN
47	W	400	LYS
47	W	405	CYS
47	W	406	ASN
47	W	408	VAL
47	W	409	LEU

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Mol	Chain	Res	Type
47	W	428	ILE
47	W	437	TYR
47	W	440	HIS
47	W	472	THR
47	W	473	GLN
47	W	477	SER
47	W	482	ARG
47	W	497	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	11	ASN
1	X	118	HIS
1	X	162	HIS
5	D	7	ASN
5	D	209	HIS
5	D	211	HIS
6	E	11	HIS
6	E	182	GLN
6	E	273	HIS
6	E	331	ASN
7	F	48	GLN
7	F	58	HIS
7	F	175	HIS
7	F	260	GLN
7	F	361	HIS
8	G	81	HIS
9	H	138	GLN
9	H	167	ASN
10	I	64	GLN
10	I	93	ASN
10	I	231	ASN
10	I	244	ASN
11	J	41	GLN
11	J	45	ASN
11	J	95	ASN
11	J	192	GLN
11	J	240	ASN
12	K	5	GLN
12	K	8	GLN
12	K	96	HIS

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Mol	Chain	Res	Type
12	K	139	ASN
12	K	156	GLN
12	K	162	GLN
13	L	12	GLN
13	L	51	HIS
13	L	59	GLN
13	L	95	HIS
13	L	123	HIS
13	L	163	GLN
14	M	20	ASN
15	N	19	GLN
15	N	99	HIS
15	N	103	ASN
16	O	59	ASN
17	a	86	ASN
17	a	182	ASN
18	b	182	ASN
19	c	55	GLN
19	c	116	HIS
19	c	120	ASN
19	c	133	HIS
19	c	137	ASN
19	c	145	HIS
20	d	9	GLN
20	d	73	GLN
20	d	78	ASN
20	d	145	ASN
21	e	68	GLN
21	e	166	ASN
22	f	63	GLN
22	f	89	ASN
23	g	5	HIS
23	g	66	ASN
23	g	134	GLN
24	h	52	ASN
24	h	87	ASN
24	h	101	ASN
26	j	32	GLN
26	j	59	HIS
27	k	85	GLN
27	k	117	ASN
28	l	42	GLN

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Mol	Chain	Res	Type
29	m	57	HIS
29	m	106	GLN
29	m	122	HIS
29	m	127	ASN
30	n	14	HIS
33	q	15	ASN
33	q	57	GLN
33	q	105	GLN
34	r	13	HIS
34	r	20	HIS
34	r	21	HIS
34	r	26	HIS
34	r	49	ASN
36	t	52	GLN
36	t	69	HIS
37	u	68	GLN
37	u	104	GLN
37	u	108	GLN
38	v	12	ASN
40	x	67	GLN
41	y	4	GLN
42	z	90	ASN
46	V	231	GLN
46	V	272	GLN
46	V	332	ASN
46	V	349	ASN
46	V	378	ASN
47	W	209	ASN
47	W	257	ASN
47	W	375	GLN
47	W	440	HIS
47	W	442	GLN
47	W	473	GLN
47	W	500	ASN

5.3.3 RNA ⓘ

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

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	3478/3675 (94%)	918 (26%)	106 (3%)

All (918) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	16	A
2	A	22	G
2	A	26	A
2	A	31	C
2	A	40	A
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	117	U
2	A	122	A
2	A	123	A
2	A	127	G
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
2	A	921	A
2	A	923	C
2	A	924	G
2	A	925	A
2	A	937	G
2	A	938	C
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	993	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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	2144	A
2	A	2145	A
2	A	2158	A
2	A	2159	U
2	A	2169	G
2	A	2185	G
2	A	2187	G
2	A	2192	C
2	A	2198	A
2	A	2205	U
2	A	2210	G
2	A	2221	G

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Mol	Chain	Res	Type
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
2	A	2379	U
2	A	2385	G
2	A	2388	U
2	A	2393	G

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Mol	Chain	Res	Type
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
2	A	2474	G
2	A	2475	G
2	A	2477	G
2	A	2479	C

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Mol	Chain	Res	Type
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
2	A	2562	A
2	A	2564	G
2	A	2565	U
2	A	2566	C

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Mol	Chain	Res	Type
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	2627	C
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
2	A	2726	C
2	A	2727	A
2	A	2728	G

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Mol	Chain	Res	Type
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	2804	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
2	A	2899	C
2	A	2900	A

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Mol	Chain	Res	Type
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	2950	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	3048	A
2	A	3049	A
2	A	3055	U
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

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Mol	Chain	Res	Type
2	A	3109	G
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

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Mol	Chain	Res	Type
2	A	3228	C
2	A	3229	G
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	3272	C
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

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Mol	Chain	Res	Type
2	A	3350	C
2	A	3351	U
2	A	3352	U
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	86	U
3	B	87	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

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Mol	Chain	Res	Type
3	B	120	C
3	B	121	U
4	C	2	A
4	C	18	U
4	C	23	U
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
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

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Mol	Chain	Res	Type
2	A	1841	A
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

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Mol	Chain	Res	Type
2	A	3022	G
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	2260	2	18,21,22	1.36	2 (11%)	21,30,33	2.08	4 (19%)
2	PSU	A	2264	2	18,21,22	1.34	2 (11%)	21,30,33	2.14	6 (28%)
2	PSU	A	2258	2	18,21,22	1.40	2 (11%)	21,30,33	2.10	5 (23%)
2	PSU	A	2266	2	18,21,22	1.38	2 (11%)	21,30,33	2.13	5 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	A	2260	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2264	2	-	1/7/25/26	0/2/2/2
2	PSU	A	2258	2	-	2/7/25/26	0/2/2/2
2	PSU	A	2266	2	-	1/7/25/26	0/2/2/2

All (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
2	A	2258	PSU	C4-N3	-2.72	1.33	1.38
2	A	2264	PSU	C4-N3	-2.71	1.33	1.38
2	A	2266	PSU	C4-N3	-2.68	1.33	1.38

All (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
2	A	2260	PSU	C4-N3-C2	-4.24	120.53	126.37
2	A	2266	PSU	C4-N3-C2	-4.11	120.70	126.37
2	A	2264	PSU	C4-N3-C2	-4.11	120.71	126.37
2	A	2266	PSU	O2-C2-N1	-3.80	118.87	122.79
2	A	2260	PSU	O2-C2-N1	-3.68	119.00	122.79
2	A	2264	PSU	O2-C2-N1	-3.61	119.07	122.79
2	A	2258	PSU	O2-C2-N1	-3.58	119.10	122.79
2	A	2258	PSU	C5-C6-N1	-2.39	118.83	122.14
2	A	2264	PSU	C3'-C2'-C1'	2.31	104.41	101.69
2	A	2260	PSU	C5-C6-N1	-2.24	119.04	122.14
2	A	2266	PSU	O3'-C3'-C4'	2.23	117.48	111.08
2	A	2264	PSU	C5-C6-N1	-2.22	119.06	122.14
2	A	2264	PSU	O3'-C3'-C4'	-2.16	104.88	111.08
2	A	2266	PSU	C5-C6-N1	-2.13	119.18	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2258	PSU	O3'-C3'-C4'	2.12	117.17	111.08

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.

3 monomers are involved in 32 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
50	GNP	W	701	48	34,34,34	1.62	5 (14%)	47,54,54	1.82	7 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	GNP	W	701	48	-	6/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

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

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	W	701	GNP	C5-C4-N3	-6.39	118.22	128.39
50	W	701	GNP	C2-N3-C4	5.13	121.14	112.30
50	W	701	GNP	N9-C4-N3	4.81	135.57	125.95
50	W	701	GNP	C6-C5-N7	3.05	135.85	130.29
50	W	701	GNP	C4-C5-N7	-2.53	106.67	110.67
50	W	701	GNP	O1B-PB-N3B	-2.21	108.52	111.77
50	W	701	GNP	O6-C6-C5	-2.12	120.93	126.53

There are no chirality outliers.

All (6) torsion outliers are listed below:

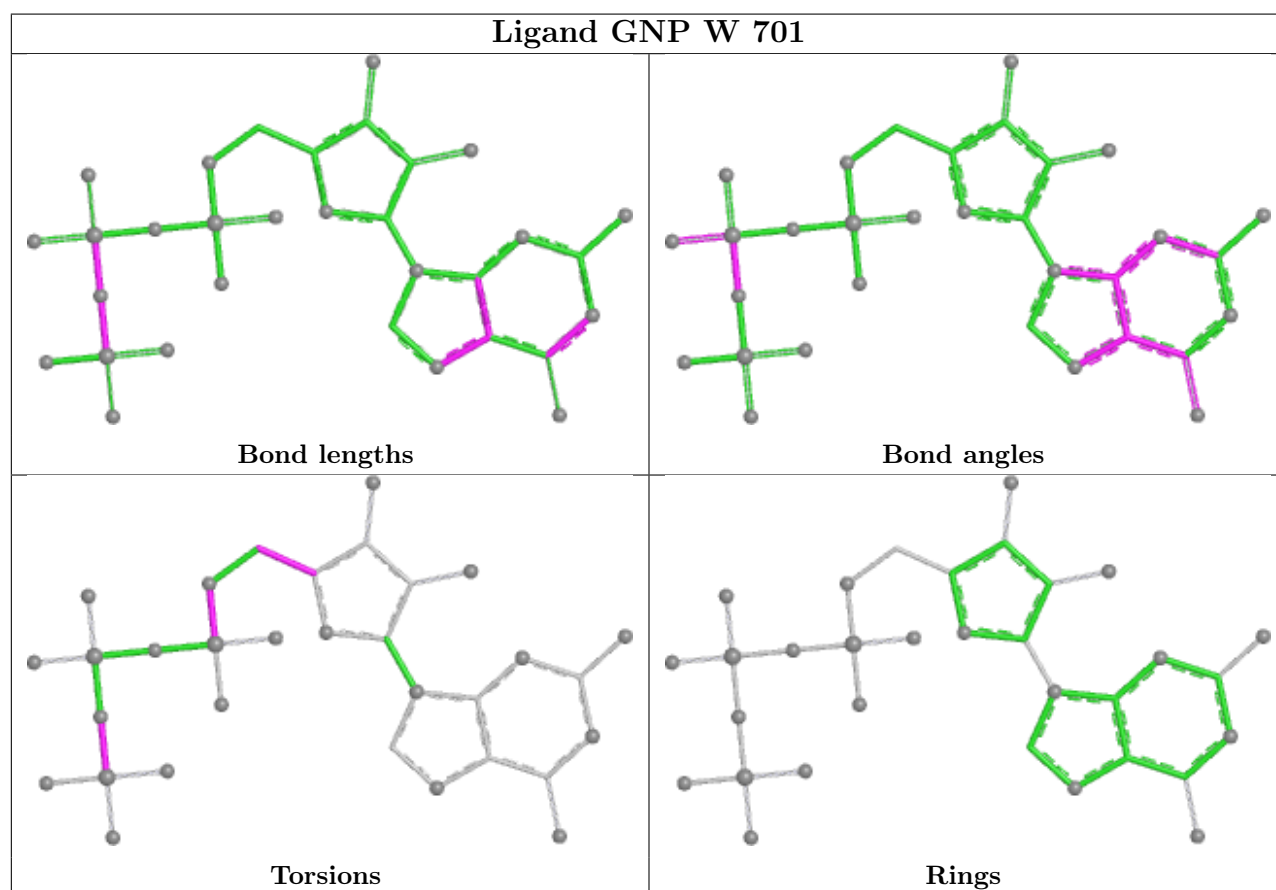
Mol	Chain	Res	Type	Atoms
50	W	701	GNP	PB-N3B-PG-O1G
50	W	701	GNP	C5'-O5'-PA-O3A
50	W	701	GNP	C5'-O5'-PA-O1A
50	W	701	GNP	C5'-O5'-PA-O2A
50	W	701	GNP	O4'-C4'-C5'-O5'
50	W	701	GNP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 12 short contacts:

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

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



5.7 Other polymers [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