



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

Nov 22, 2016 – 02:16 PM EST

PDB ID : 5LZS  
EMDB ID: : EMD-4130  
Title : Structure of the mammalian ribosomal elongation complex with aminoacyl-tRNA, eEF1A, and didemnin B  
Authors : Shao, S.; Murray, J.; Brown, A.; Taunton, J.; Ramakrishnan, V.; Hegde, R.S.  
Deposited on : 2016-10-02  
Resolution : 3.31 Å(reported)

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

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

A user guide is available at

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

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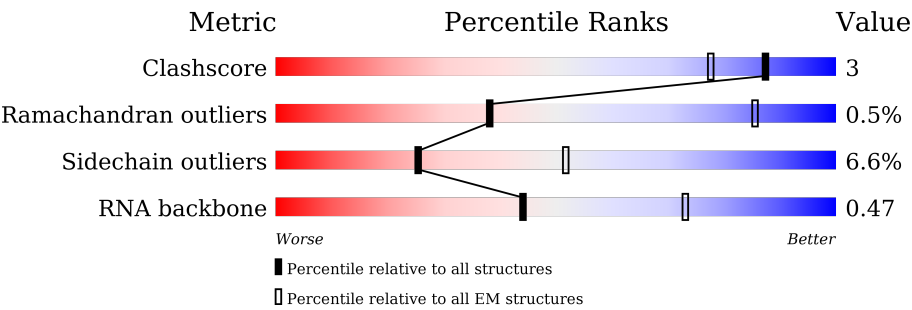
MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
EM map analysis : **NOT EXECUTED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028320

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.31 Å.

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




















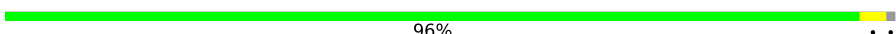






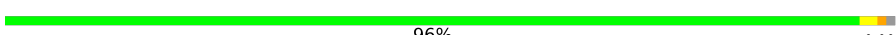
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	A	257	<div><div>79%16%..</div></div>
2	B	403	<div><div>86%11%..</div></div>
3	C	425	<div><div>75%9%.15%</div></div>
4	D	297	<div><div>88%11%.</div></div>
5	E	291	<div><div>66%7%.26%</div></div>
6	F	247	<div><div>79%11%.9%</div></div>
7	G	319	<div><div>62%11%27%</div></div>
8	H	192	<div><div>85%13%..</div></div>

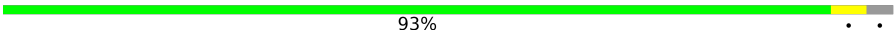

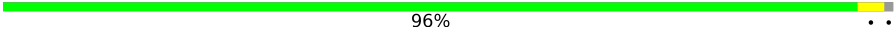
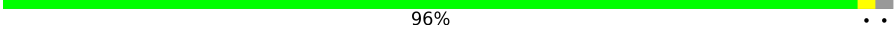


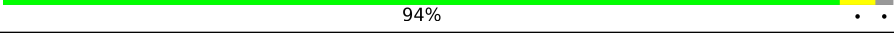
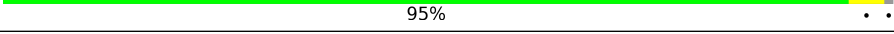


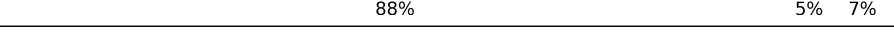
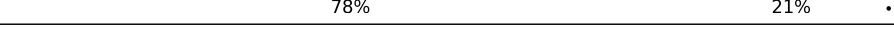
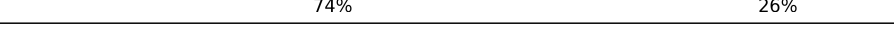


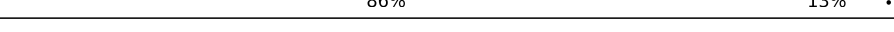









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Mol	Chain	Length	Quality of chain
9	I	214	 82% 11% . .
10	J	178	 89% 6% . .
11	L	211	 91% 9%
12	M	218	 56% 7% 37%
13	N	204	 86% 14%
14	O	203	 81% 16% . .
15	P	184	 71% 11% . 17%
16	Q	188	 88% 11% . .
17	R	196	 81% 9% . 8%
18	S	176	 86% 12% .
19	T	160	 88% 11% . .
20	U	128	 71% 5% . 23%
21	V	140	 81% 16% . . .
22	W	157	 62% . . 32%
23	X	156	 67% 9% 24%
24	Y	145	 83% 10% 8%
25	Z	136	 89% 10% .
26	a	148	 96% . .
27	b	245	 41% . 58%
28	c	115	 82% . 15%
29	d	125	 77% 9% 14%
30	e	135	 88% 7% 5%
31	f	110	 92% 6% . .
32	g	116	 93% 5% .
33	h	123	 96% . . .




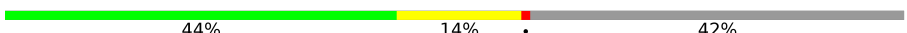





















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Mol	Chain	Length	Quality of chain
34	i	105	
35	j	97	
36	k	70	
37	l	51	
38	m	102	
39	n	25	
40	o	106	
41	p	92	
42	r	137	
43	s	318	
44	t	165	
45	2	76	
45	ii	76	
46	3	75	
47	5	3543	
48	7	120	
49	8	156	
50	9	1869	
51	AA	295	
52	BB	264	
53	CC	293	
54	DD	243	
55	EE	263	
56	FF	204	
57	GG	249	

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Mol	Chain	Length	Quality of chain
58	HH	194	 85%10%5%
59	II	208	 89%10%.
60	JJ	194	 83%10%5%
61	KK	165	 44%14%.42%
62	LL	158	 79%11%9%
63	MM	132	 77%12%11%
64	NN	151	 89%9%..
65	OO	168	 69%10%.19%
66	PP	145	 79%10%.11%
67	QQ	146	 86%12%.
68	RR	135	 86%10%..
69	SS	152	 82%13%5%
70	TT	145	 89%8%..
71	UU	119	 73%10%.16%
72	VV	83	 90%10%
73	WW	130	 82%17%..
74	XX	143	 87%10%..
75	YY	130	 84%11%.5%
76	ZZ	125	 50%8%.40%
77	aa	115	 82%6%12%
78	bb	84	 92%6%..
79	cc	69	 81%9%10%
80	dd	56	 93%5%.
81	ee	133	 41%.57%
82	ff	156	 38%5%56%

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Mol	Chain	Length	Quality of chain
83	gg	317	<div><div></div><div>96%</div><div></div><div>.</div><div>.</div></div>
84	hh	10	<div><div></div><div>90%</div><div>10%</div></div>
85	jj	462	<div><div></div><div>93%</div><div>5%</div><div>.</div></div>

## 2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 220934 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP G1TL06

- Molecule 3 is a protein called Uncharacterized protein,uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

- Molecule 4 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP G1SYJ6

- Molecule 5 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 6 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	61	ARG	GLY	conflict	UNP G1TUB1
F	93	ARG	GLY	conflict	UNP G1TUB1
F	131	MET	VAL	conflict	UNP G1TUB1
F	153	ILE	VAL	conflict	UNP G1TUB1

- Molecule 7 is a protein called eL8,Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	233	Total	C	N	O	S	0	0
			1879	1199	361	315	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 8 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 9 is a protein called Ribosomal protein L10 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 10 is a protein called Uncharacterized protein.



Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 11 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

- Molecule 12 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 13 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 14 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 15 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 16 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

- Molecule 17 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 18 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

- Molecule 19 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 20 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

- Molecule 21 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 22 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

- Molecule 23 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 24 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 25 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 26 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1	MET	GLN	conflict	UNP G1SNY0

- Molecule 27 is a protein called Uncharacterized protein,eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 28 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 29 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 30 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 31 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 32 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 33 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 34 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 35 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 36 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 37 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 38 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 39 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 40 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 41 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 42 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 43 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 44 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	153	Total	C	N	O	S	0	0
			1160	722	218	217	3		

- Molecule 45 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	2	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		
45	ii	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 46 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 47 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	5	3543	Total	C	N	O	P	0	0
			75972	33833	13910	24686	3543		

- Molecule 48 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	7	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

- Molecule 49 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	8	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 50 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	9	1697	Total	C	N	O	P	0	0
			36229	16171	6507	11855	1696		

- Molecule 51 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AA	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 52 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BB	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 53 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	CC	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 54 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	DD	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 55 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	EE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 56 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	FF	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 57 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	GG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 58 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	HH	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 59 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	II	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
II	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 60 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
60	JJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 61 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	KK	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 62 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LL	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 63 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	MM	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 64 is a protein called Uncharacterized protein.



Mol	Chain	Residues	Atoms					AltConf	Trace
64	NN	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 65 is a protein called uS11,Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	OO	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 66 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	PP	129	Total	C	N	O	S	0	0
			1058	670	201	180	7		

- Molecule 67 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	QQ	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 68 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	RR	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 69 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SS	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 70 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	TT	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
TT	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 71 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	UU	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 72 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	VV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 73 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	WW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 74 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	XX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 75 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	YY	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 76 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	ZZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 77 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	aa	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 78 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	bb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 79 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	cc	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 80 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	dd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 81 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	ee	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 82 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	ff	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 83 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	gg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 84 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	hh	10	Total	C	N	O	P	0	0
			210	94	33	73	10		

- Molecule 85 is a protein called Elongation factor 1-alpha 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	jj	441	Total	C	N	O	P	S	0	0
			3383	2148	581	636	1	17		

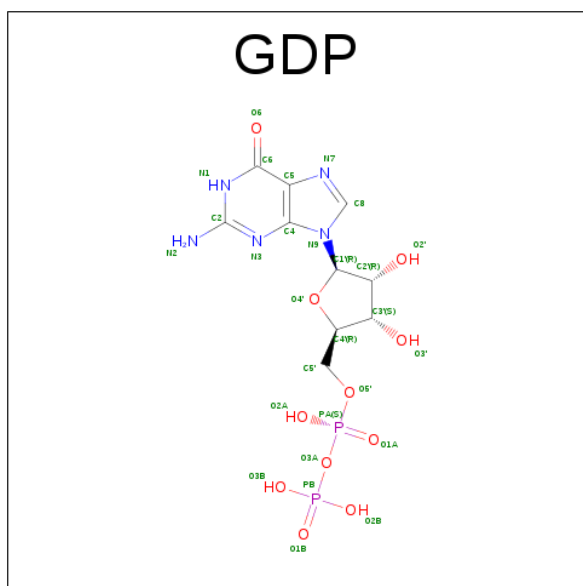
- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	P	1	Total	Mg	0
			1	1	
86	g	1	Total	Mg	0
			1	1	
86	j	1	Total	Mg	0
			1	1	
86	Q	1	Total	Mg	0
			1	1	
86	jj	1	Total	Mg	0
			1	1	
86	B	1	Total	Mg	0
			1	1	
86	I	1	Total	Mg	0
			1	1	
86	V	1	Total	Mg	0
			1	1	
86	7	6	Total	Mg	0
			6	6	
86	a	2	Total	Mg	0
			2	2	
86	5	185	Total	Mg	0
			185	185	
86	8	5	Total	Mg	0
			5	5	
86	9	70	Total	Mg	0
			70	70	

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
87	p	1	Total	Zn	0
			1	1	
87	g	1	Total	Zn	0
			1	1	
87	j	1	Total	Zn	0
			1	1	
87	dd	1	Total	Zn	0
			1	1	
87	ff	1	Total	Zn	0
			1	1	
87	aa	1	Total	Zn	0
			1	1	
87	o	1	Total	Zn	0
			1	1	
87	m	1	Total	Zn	0
			1	1	

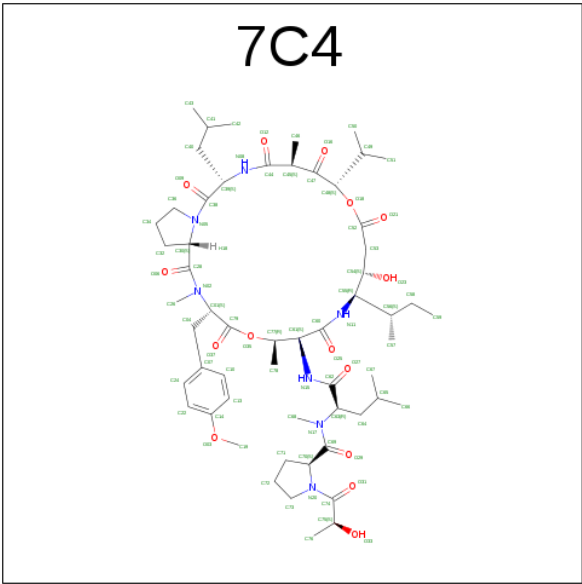
- Molecule 88 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
88	jj	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 89 is (2 {S})- {N}-[(2 {R})-1-[(3 {S},6 {S},8 {S},12 {S},13 {R},16 {S},17 {R},20 {S},23 {S})-13-[(2 {S})-butan-2-yl]-20-[(4-methoxyphenyl)methyl]-6,17,21-trimethyl-3-(2-methylpropyl)-12-oxidanyl-2,5,7,10,15,19,22-heptakis(oxidanylidene)-8-propan-2-yl-9,18-diox a-1,4,14,21-tetrazabicyclo[21.3.0]hexacosan-16-yl]amino]-4-methyl-1-oxidanylidene-pentan

-2-yl]- {N}-methyl-1-[(2 {S})-2-oxidanylpropanoyl]pyrrolidine-2-carboxamide (three-letter code: 7C4) (formula: C<sub>57</sub>H<sub>89</sub>N<sub>7</sub>O<sub>15</sub>).

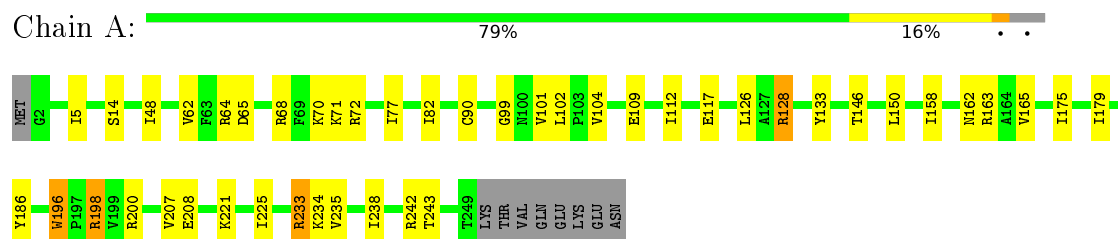


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
89	jj	1	79	57	7	15	0

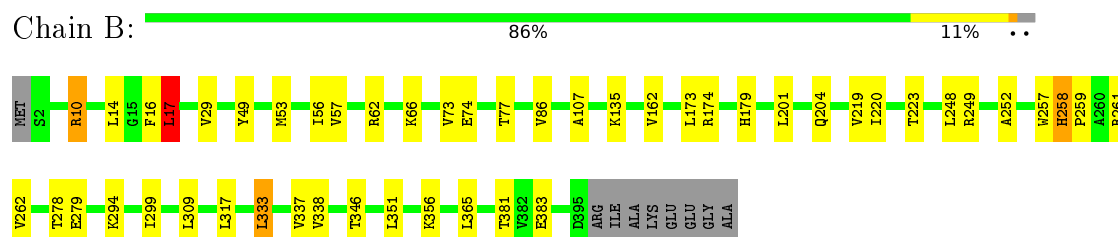
### 3 Residue-property plots [i](#)

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

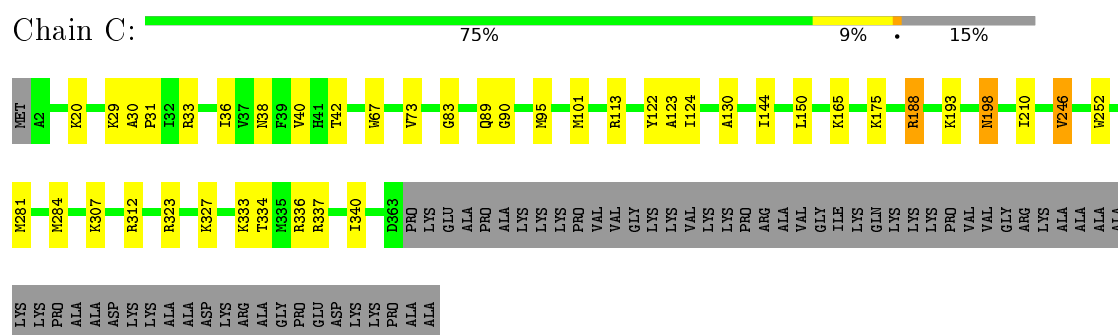
- Molecule 1: Uncharacterized protein



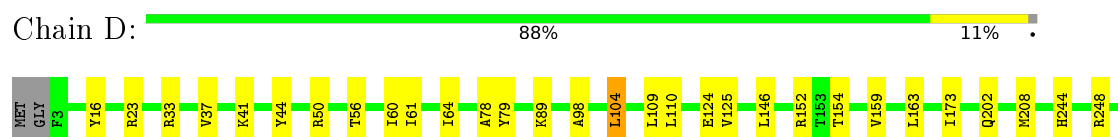
- Molecule 2: Uncharacterized protein



- Molecule 3: Uncharacterized protein,uL4



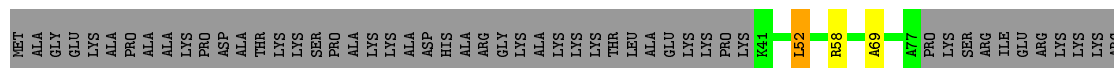
- Molecule 4: 60S ribosomal protein L5





- Molecule 5: 60S ribosomal protein L6

Chain E: 66% 7% 26%



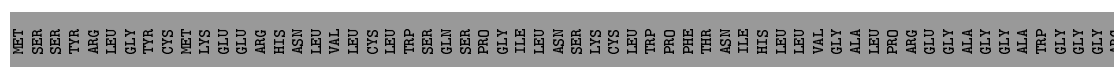
- Molecule 6: Uncharacterized protein

Chain F: 79% 11% 9%



- Molecule 7: eL8, Uncharacterized protein

Chain G: 62% 11% 27%



- Molecule 8: Uncharacterized protein

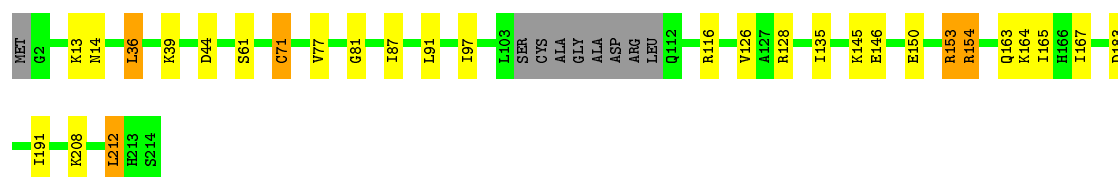
Chain H: 85% 13% 2%



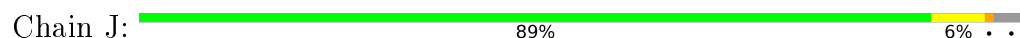
- Molecule 9: Ribosomal protein L10 (Predicted)

Chain I: 82% 11% 7%





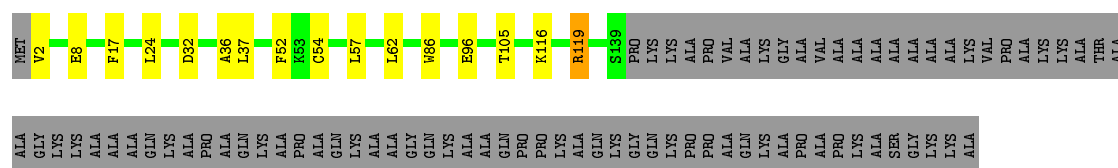
- Molecule 10: Uncharacterized protein



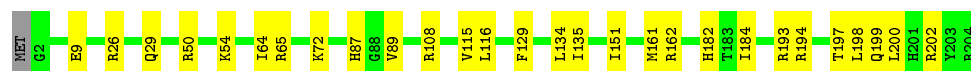
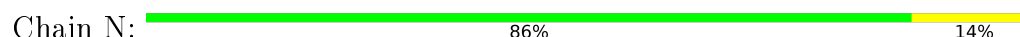
- Molecule 11: eL13



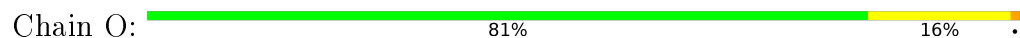
- Molecule 12: Uncharacterized protein



- Molecule 13: Ribosomal protein L15

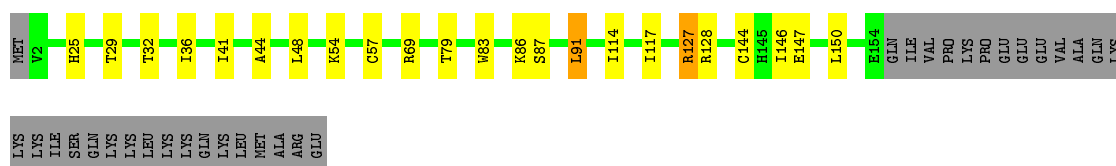


- Molecule 14: uL13



- Molecule 15: Uncharacterized protein





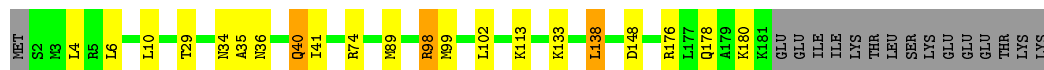
- Molecule 16: eL18

Chain Q: 88% 11% ..



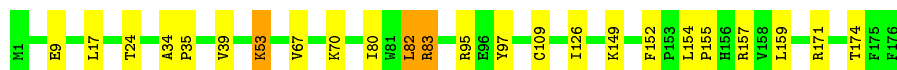
- Molecule 17: eL19

Chain R: 81% 9% 8%



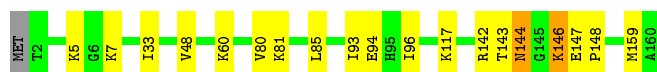
- Molecule 18: eL20

Chain S: 86% 12%



- Molecule 19: Uncharacterized protein

Chain T: 88% 11% ..



- Molecule 20: eL22

Chain U: 71% 5% 23%



- Molecule 21: Uncharacterized protein

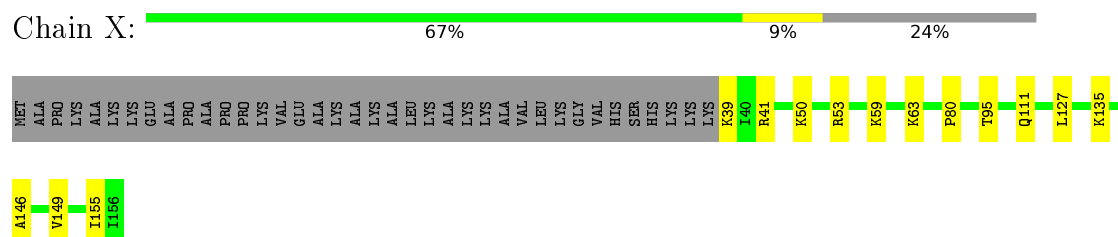
Chain V: 81% 16%



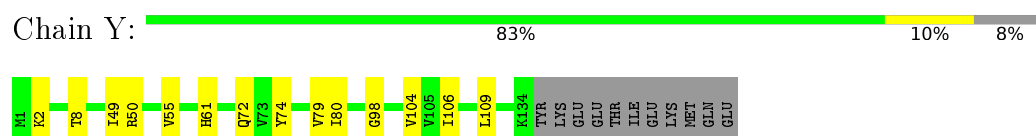
- Molecule 22: Uncharacterized protein

Chain W: 62% 32%

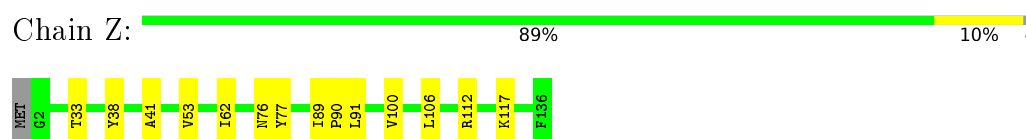
- Molecule 23: Uncharacterized protein



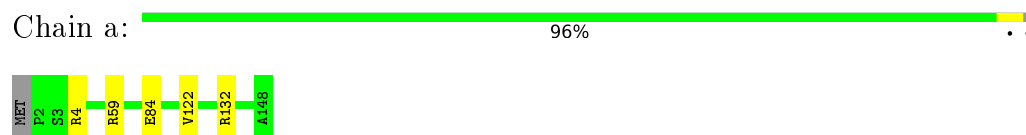
- Molecule 24: Uncharacterized protein



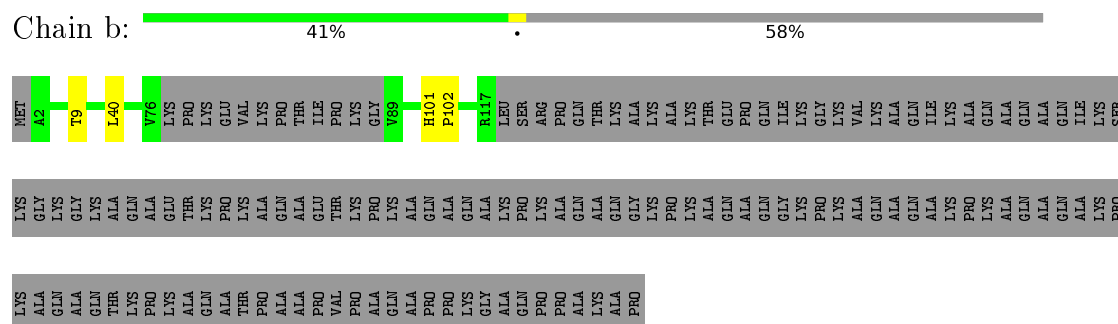
- Molecule 25: 60S ribosomal protein L27




- Molecule 26: Uncharacterized protein



- Molecule 27: Uncharacterized protein,eL29




- Molecule 28: Uncharacterized protein

Chain c:  82% 15%




- Molecule 29: Uncharacterized protein

Chain d:  77% 9% 14%




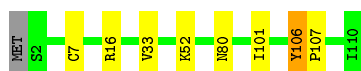
- Molecule 30: Uncharacterized protein

Chain e:  88% 7% 5%



- Molecule 31: Uncharacterized protein

Chain f:  92% 6% ..



- Molecule 32: Uncharacterized protein

Chain g:  93% 5% .



- Molecule 33: Uncharacterized protein

Chain h:  96% ..




- Molecule 34: 60S ribosomal protein L36

Chain i:  93% . .



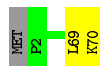
- Molecule 35: Ribosomal protein L37

Chain j:  82% 6% 11%



- Molecule 36: eL38

Chain k: 96% ..



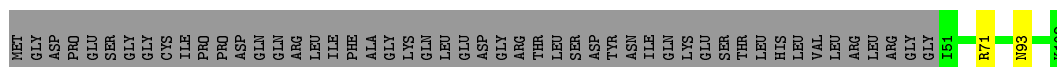
- Molecule 37: Uncharacterized protein

Chain l: 96% ..



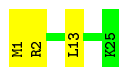
- Molecule 38: eL40

Chain m: 49% . 49%



- Molecule 39: 60s ribosomal protein l41

Chain n: 88% 12%



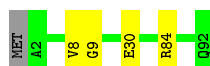
- Molecule 40: Uncharacterized protein

Chain o: 94% ..



- Molecule 41: Uncharacterized protein

Chain p: 95% ..

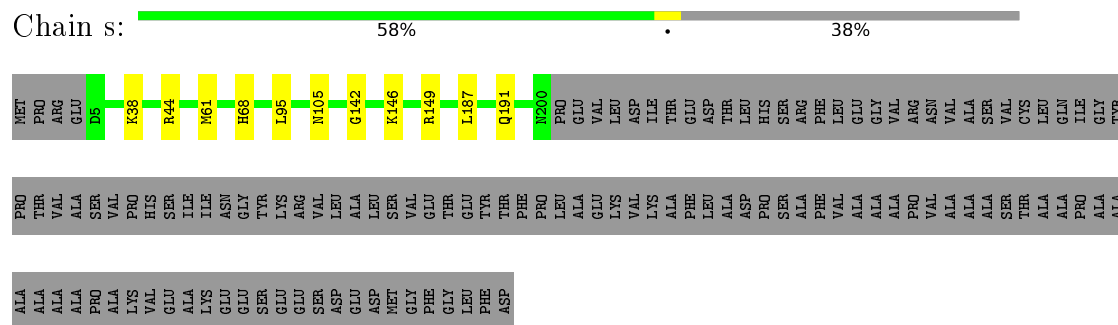


- Molecule 42: Uncharacterized protein

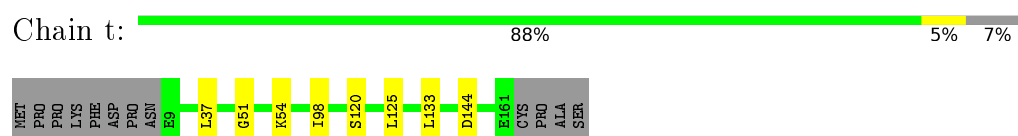
Chain r: 84% 7% 9%



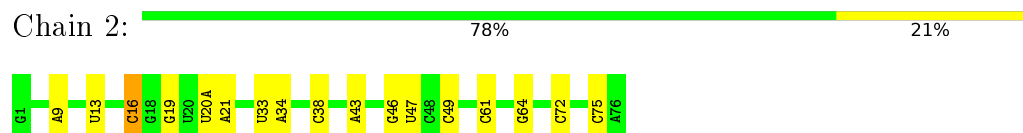
- Molecule 43: uL10



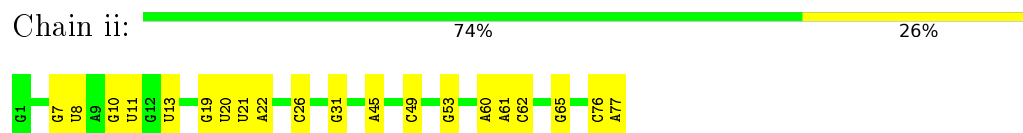
- Molecule 44: Uncharacterized protein



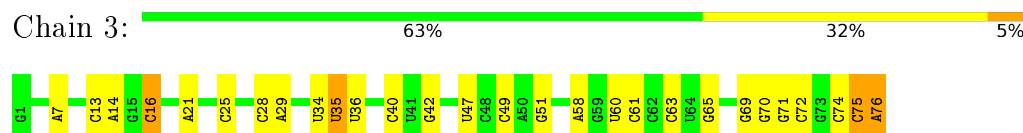
- Molecule 45: tRNA



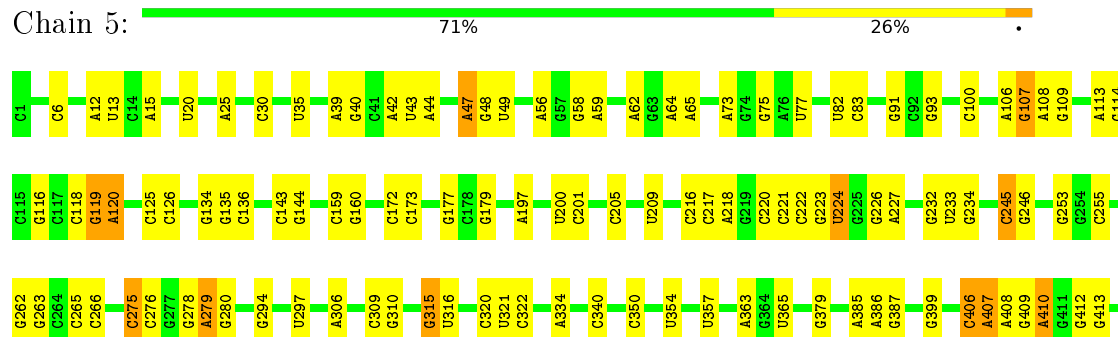
- Molecule 45: tRNA



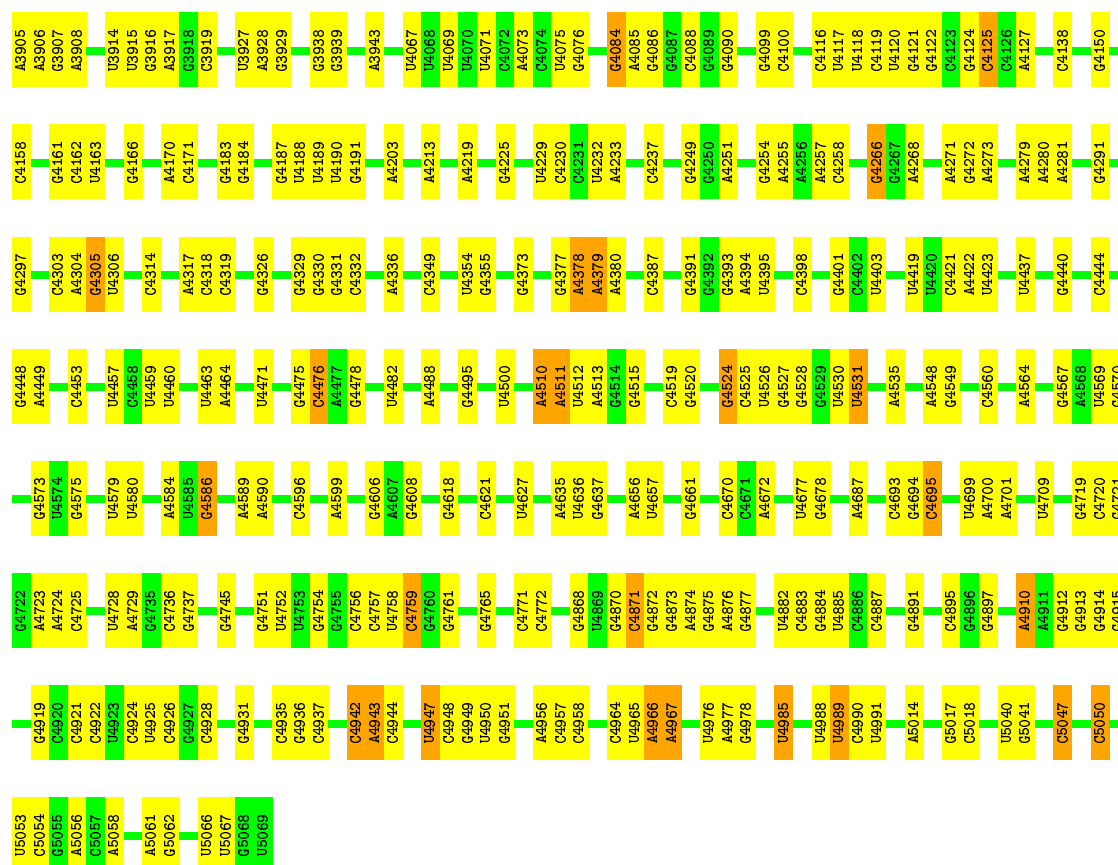
- Molecule 46: E-site tRNA



- Molecule 47: 28S ribosomal RNA



U3773	G3615	A2764	G2640	G2483	G2316	C2068	A1979	G1833	A1667	C1485	A1354	C1180	C931	G683	G417
A3774	G3617	U2769	A2647	U2485	C2325	A2069	U1980	U1834	A1676	C1486	A1354	C1183	A932	G684	G431
G3776	G3625	C2772	U2661	C2488	G2331	U2070	G1982	G1835	U1677	G1489	G1359	G1185	C933	G685	U432
G3777	G3626	A2787	G2662	C2489	A2332	G2084	A1983	G1836	C1690	A1497	U1364	G1195	A935	A686	
U3778	A3630	U2788	G2663	U2490	G2333	G2085	G1985	A1837	G1498	G1502	G1370	U1209	G935A	U687	C446
A3783	A3635	A2789	C2669	C2491	G2348	A2088	U1986	G1855	U1726	G1502	A1371	U1210	C936	G696	
A3784	G2669	U2790	C2670	C2492	G2351	G2089	G1988	A1867	A1729	A1371	A1372	C1210	U937	G697	C449
A3785	G2493	G2673	G2670	G2493	C2351	G2090	G1989	A1868	G1733	G1516	G1377	C1211	G939	U702	G450
U3786	U2494	G2673	G2670	U2495	G2364	G2092	A1990	A1869	G1734	G1517	G1378	C1212	C940	A452	
U3798	U2495	G2676	G2670	U2495	G2364	G2093	A1991	G1869	G1734	G1518	C1379	C1213	C941	G453	
A3799	A2503	A2676	G2670	U2495	G2364	C2094	U1992	G1872	C1740	A1523	C1379	C1214	A944	U454	
G3809	G2502	G2681	G2670	U2495	A2367	A2095	C1993	G1872	C1740	A1523	C1379	C1215	U945	C455	
G3810	C2504	G2681	G2670	U2495	A2367	A2096	U1997	C1879	A1741	A1534	U1381	G1234	A945	G457	
G3811	C2505	G2686	G2670	U2495	A2370	A2097	U1997	C1879	A1742	A1534	U1381	G1235	A956	U716	G464
G3812	G2506	G2687	G2670	U2495	A2370	G2098	U1997	C1879	A1742	A1534	U1381	G1236	A956	U717	
U3814	A2512	G2688	G2670	U2495	A2374	G2099	G2001	A1891	G1750	A1546	G1394	C1237	G959	G718	G465
U3817	A2513	G2689	G2670	U2495	A2374	G2100	A2002	A1897	G1753	A1547	G1394	C1238	A960	C719	A466
U3818	A2513	G2690	G2670	U2495	A2374	A2101	G2003	U1907	U1754	A1547	G1394	C1239	A961	G722	A467
G3819	A2513	G2691	G2670	U2495	A2374	A2102	U2004	A1907	C1755	A1554	G1394	C1239	A962	G729	A468
U3822	A2529	U2707	G2691	U2495	A2395	A2103	G2007	G1910	U1756	A1554	G1394	C1239	A963	G730	C480
U3831	U2530	G2695	G2691	U2495	A2396	A2104	U2008	U1918	G1761	A1563	C1401	C1272	A964	G731	G481
U3839	A2537	G2696	G2691	U2495	A2396	A2105	A2009	U1919	C1762	A1564	C1402	C1273	A966	G734	C481A
U3840	G2546	G2697	G2691	U2495	A2396	A2106	C2011	G1919	C1762	A1564	C1402	C1274	A967	G739	G482
U3851	G2547	G2698	G2691	U2495	A2396	A2107	A2012	G1921	C1763	A1566	G1416	C1275	A968	U484	
G3859	G2548	G2699	G2691	U2495	A2396	A2108	A2013	G1922	G1764	U1578	G1416	C1280	C969	C485	
A3867	G2554	G2707	G2699	U2495	A2416	G2259	C2016	A1923	C1768	U1591	A1419	G1284	G971A	C486	
G3870	G2555	G2708	G2699	U2495	A2417	C2260	C2022	C1931	C1772	G1592	A1420	U1285	C972	U492	
A3871	G2556	G2709	G2699	U2495	A2417	G2261	C2023	A1932	U1773	U1596	A1421	C1286	G973	C493	
A3872	G2558	G2710	G2699	U2495	A2417	G2262	G2024	G1933	A1776	G1602	G976	C1287	G977	C494	
A3876	G2564	G2711	G2699	U2495	A2417	G2263	A2025	A1934	U1781	C1611	G978	C1288	C979	C495	
A3877	G2565	G2712	G2699	U2495	A2417	G2264	A2026	G1935	U1781	C1612	G979	C1291	G979	G496	
A3878	G2566	G2713	G2699	U2495	A2417	G2265	A2033	C1936	U1781	G1613	G983	C1292	C983	G497	
A3879	G2567	G2714	G2699	U2495	A2417	G2266	A2040	G1937	U1781	G1614	G984	C1293	C984	G498	
G3888	G2568	G2715	G2699	U2495	A2417	G2267	A2040	G1938	U1781	G1614	G985	C1294	C985	G500	
G3889	G2569	G2716	G2699	U2495	A2417	G2268	A2040	G1939	U1781	G1614	G986	C1295	C986	G504	
G3896	G2570	G2717	G2699	U2495	A2417	G2269	A2040	G1940	U1781	G1614	G987	C1296	C987	G505	
G3897	G2571	G2718	G2699	U2495	A2417	G2270	A2040	G1941	U1781	G1614	G988	C1301	C1072	U510	
G3898	G2572	G2719	G2699	U2495	A2417	G2271	A2040	G1942	U1781	G1614	G989	C1302	G1073	U510	
A3901	G2573	G2720	G2699	U2495	A2417	G2272	A2040	G1943	U1781	G1614	G990	C1303	G1074	A649	
G3904	G2574	G2721	G2699	U2495	A2417	G2273	A2040	G1944	U1781	G1614	G991	C1304	G1075	A649	
	G2575	G2722	G2699	U2495	A2417	G2274	A2040	G1945	U1781	G1614	G992	C1305	G1076	C916	
	G2576	G2723	G2699	U2495	A2417	G2275	A2040	G1946	U1781	G1614	G993	C1306	C1077	A917	C654
	G2577	G2724	G2699	U2495	A2417	G2276	A2040	G1947	U1781	G1614	G994	C1307	A1078	G918	
	G2578	G2725	G2699	U2495	A2417	G2277	A2040	G1948	U1781	G1614	G995	C1308	C1079	C922B	
	G2579	G2726	G2699	U2495	A2417	G2278	A2040	G1949	U1781	G1614	G996	C1309	C1080	C923	A667
	G2580	G2727	G2699	U2495	A2417	G2279	A2040	G1950	U1781	G1614	G997	C1310	C1081	C924	C668
	G2581	G2728	G2699	U2495	A2417	G2280	A2040	G1951	U1781	G1614	G998	C1311	C1082	C925	C669
	G2582	G2729	G2699	U2495	A2417	G2281	A2040	G1952	U1781	G1614	G999	C1312	C1083	G926	
	G2583	G2730	G2699	U2495	A2417	G2282	A2040	G1953	U1781	G1614	G1000	C1313	C1084	A929	
	G2584	G2731	G2699	U2495	A2417	G2283	A2040	G1954	U1781	G1614	G1001	C1314	C1085	G671	
	G2585	G2732	G2699	U2495	A2417	G2284	A2040	G1955	U1781	G1614	G1002	C1315	C1086	G672	
	G2586	G2733	G2699	U2495	A2417	G2285	A2040	G1956	U1781	G1614	G1003	C1316	C1087	G673	
	G2587	G2734	G2699	U2495	A2417	G2286	A2040	G1957	U1781	G1614	G1004	C1317	C1088	G674	
	G2588	G2735	G2699	U2495	A2417	G2287	A2040	G1958	U1781	G1614	G1005	C1318	C1089	G675	
	G2589	G2736	G2699	U2495	A2417	G2288	A2040	G1959	U1781	G1614	G1006	C1319	C1090	G676	
	G2590	G2737	G2699	U2495	A2417	G2289	A2040	G1960	U1781	G1614	G1007	C1320	C1091	G677	
	G2591	G2738	G2699	U2495	A2417	G2290	A2040	G1961	U1781	G1614	G1008	C1321	C1092	G678	
	G2592	G2739	G2699	U2495	A2417	G2291	A2040	G1962	U1781	G1614	G1009	C1322	C1093	G679	
	G2593	G2740	G2699	U2495	A2417	G2292	A2040	G1963	U1781	G1614	G1010	C1323	C1094	G680	
	G2594	G2741	G2699	U2495	A2417	G2293	A2040	G1964	U1781	G1614	G1011	C1324	C1095	G681	
	G2595	G2742	G2699	U2495	A2417	G2294	A2040	G1965	U1781	G1614	G1012	C1325	C1096	G682	
	G2596	G2743	G2699	U2495	A2417	G2295	A2040	G1966	U1781	G1614	G1013	C1326	C1097	G683	
	G2597	G2744	G2699	U2495	A2417	G2296	A2040	G1967	U1781	G1614	G1014	C1327	C1098	G684	
	G2598	G2745	G2699	U2495	A2417	G2297	A2040	G1968	U1781	G1614	G1015	C1328	C1099	G685	
	G2599	G2746	G2699	U2495	A2417	G2298	A2040	G1969	U1781	G1614	G1016	C1329	C1100	G686	
	G2600	G2747	G2699	U2495	A2417	G2299	A2040	G1970	U1781	G1614	G1017	C1330	C1101	G687	
	G2601	G2748	G2699	U2495	A2417	G2300	A2040	G1971	U1781	G1614	G1018	C1331	C1102	G688	
	G2602	G2749	G2699	U2495	A2417	G2301	A2040	G1972	U1781	G1614	G1019	C1332	C1103	G689	
	G2603	G2750	G2699	U2495	A2417	G2302	A2040	G1973	U1781	G1614	G1020	C1333	C1104	G690	
	G2604	G2751	G2699	U2495	A2417	G2303	A2040	G1974	U1781	G1614	G1021	C1334	C1105	G691	
	G2605	G2752	G2699	U2495	A2417	G2304	A2040	G1975	U1781	G1614	G1022	C1335	C1106	G692	
	G2606	G2753	G2699	U2495	A2417	G2305	A2040	G1976	U1781	G1614	G1023	C1336	C1107	G693	
	G2607	G2754	G2699	U2495	A2417	G2306	A2040	G1977	U1781	G1614	G1024	C1337	C1108	G694	
	G2608	G2755	G2699	U2495	A2417	G2307	A2040	G1978	U1781	G1614	G1025	C1338	C1109	G695	
	G2609	G2756	G2699	U2495	A2417	G2308	A2040	G1979	U1781	G1614	G1026	C1339	C1110	G696	
	G2610	G2757	G2699	U2495	A2417	G2309	A2040	G1980	U1781	G1614	G1027	C1340	C1111	G697	
	G2611	G2758	G2699	U2495	A2417	G2310	A2040	G1981	U1781	G1614	G1028	C1341	C1112	G698	
	G2612	G2759	G2699	U2495	A2417	G2311	A2040	G1982	U1781	G1614	G1029	C1342	C1113	G699	
	G2613	G2760	G2699	U2495	A2417	G2312	A2040	G1983	U1781	G1614	G1030	C1343	C1114	G700	
	G2614	G2761	G2699	U2495	A2417	G2313	A2040	G1984	U1781	G1614	G1031	C1344	C1115	G701	
	G2615	G2762	G2699	U2495	A2417	G2314	A2040	G1985	U1781	G1614	G1032	C1345	C1116	G702	
	G2616	G2763	G2699	U2495	A2417	G2315	A2040	G1986	U1781	G1614	G1033	C1346	C1117	G703	



- Molecule 48: 5S ribosomal RNA

Chain 7:  86% 13%



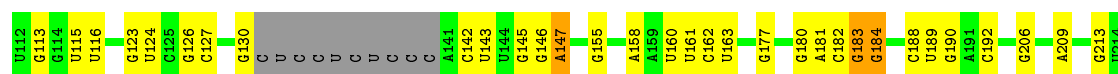
- Molecule 49: 5.8S ribosomal RNA

Chain 8:  73% 23% ..



- Molecule 50: 18S ribosomal RNA

Chain 9:  63% 25% 9%

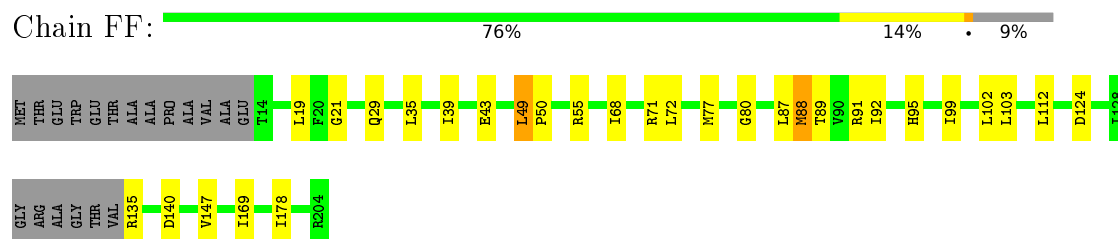




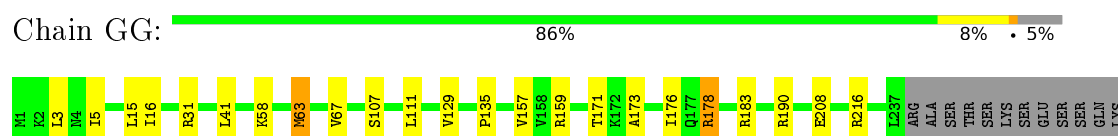




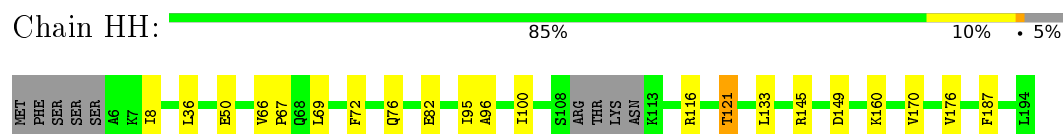
- Molecule 56: Uncharacterized protein



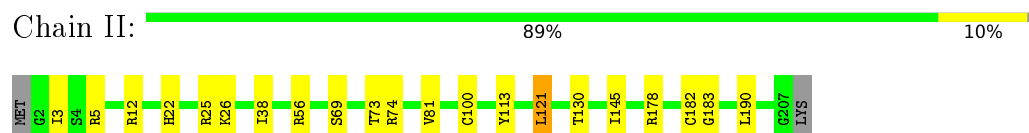
- Molecule 57: 40S ribosomal protein S6



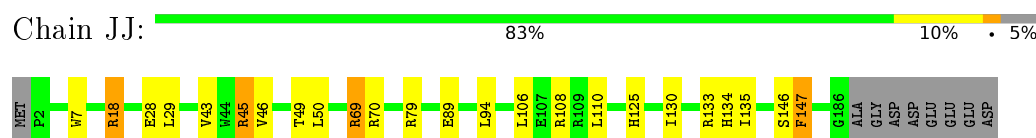
- Molecule 58: Uncharacterized protein



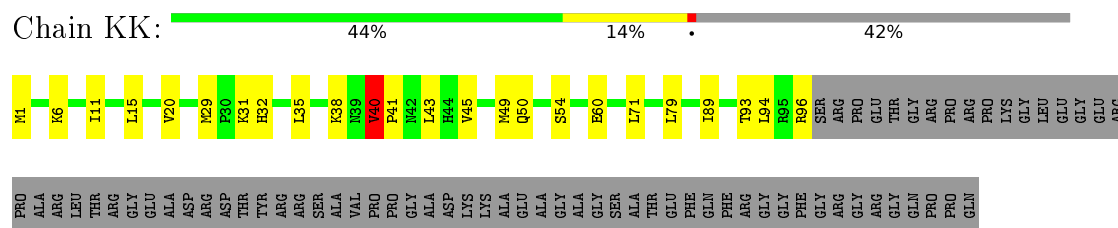
- Molecule 59: 40S ribosomal protein S8



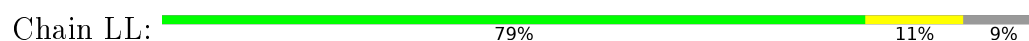
- Molecule 60: Ribosomal protein S9 (Predicted)



- Molecule 61: Uncharacterized protein



- Molecule 62: Uncharacterized protein





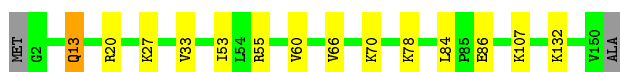
- Molecule 63: 40S ribosomal protein S12

Chain MM: 77% 12% 11%



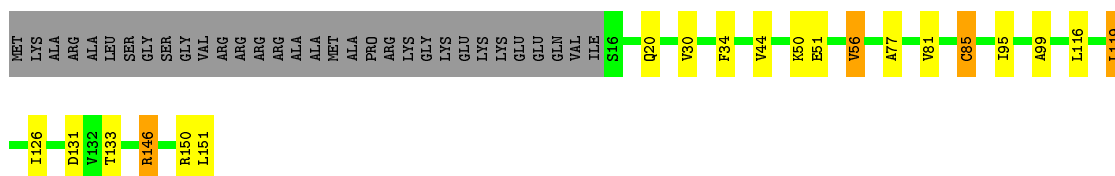
- Molecule 64: Uncharacterized protein

Chain NN: 89% 9% ..



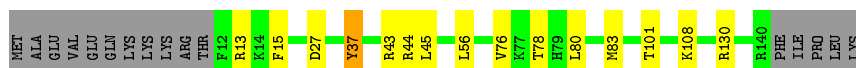
- Molecule 65: uS11, Uncharacterized protein

Chain OO: 69% 10% 19%



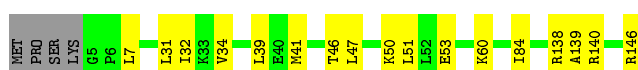
- Molecule 66: Uncharacterized protein

Chain PP: 79% 10% 11%



- Molecule 67: Uncharacterized protein

Chain QQ: 86% 12% .



- Molecule 68: Uncharacterized protein

Chain RR: 86% 10% ..



- Molecule 69: Uncharacterized protein

Chain SS: 82% 13% 5%



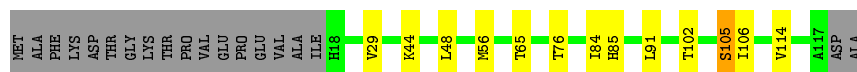
- Molecule 70: Uncharacterized protein

Chain TT: 89% 8% ..



- Molecule 71: Uncharacterized protein

Chain UU: 73% 10% 16%



- Molecule 72: eS21

Chain VV: 90% 10%



- Molecule 73: Uncharacterized protein

Chain WW: 82% 17% ..



- Molecule 74: uS12

Chain XX: 87% 10% ..



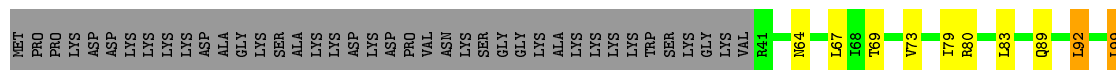
- Molecule 75: eS24

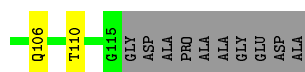
Chain YY: 84% 11% 5%



- Molecule 76: Uncharacterized protein

Chain ZZ: 50% 8% 40%





- Molecule 77: eS26

Chain aa: 82% 6% 12%



- Molecule 78: 40S ribosomal protein S27

Chain bb: 92% 6% ..



- Molecule 79: Uncharacterized protein

Chain cc: 81% 9% 10%



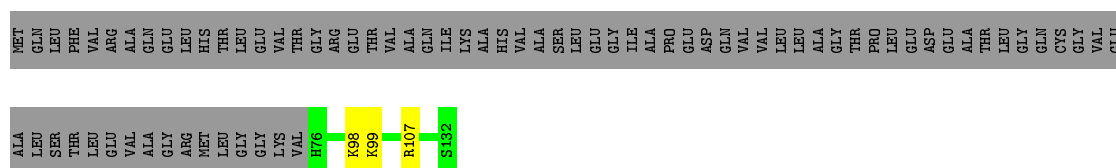
- Molecule 80: Uncharacterized protein

Chain dd: 93% 5% .



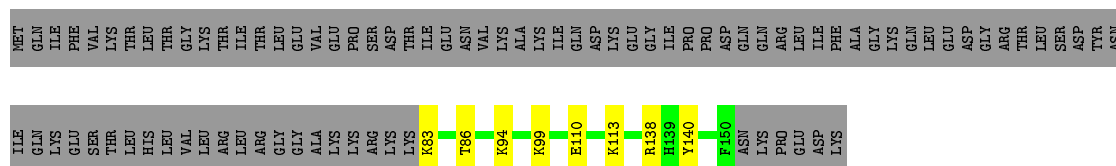
- Molecule 81: Uncharacterized protein

Chain ee: 41% . 57%



- Molecule 82: Uncharacterized protein

Chain ff: 38% 5% 56%



- Molecule 83: Uncharacterized protein

Chain gg: 

96%

..



● Molecule 84: mRNA

Chain hh: 

90%

10%



● Molecule 85: Elongation factor 1-alpha 1

Chain jj: 

93%

5%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	40347	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	134615	Depositor
Image detector	Not provided	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, SEP, ZN, 7C4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 2$	RMSZ	# $ Z  > 2$
1	A	0.38	0/1936	0.71	0/2596
10	J	0.33	0/1385	0.60	0/1852
11	L	0.43	0/1733	0.77	0/2316
12	M	0.43	0/1158	0.74	0/1547
13	N	0.43	0/1746	0.75	0/2338
14	O	0.47	0/1662	0.79	0/2222
15	P	0.41	0/1268	0.67	0/1700
16	Q	0.39	0/1539	0.77	0/2054
17	R	0.49	0/1524	0.82	0/2013
18	S	0.38	0/1501	0.69	0/2012
19	T	0.35	0/1326	0.62	0/1770
2	B	0.38	0/3240	0.68	0/4339
20	U	0.36	0/823	0.56	0/1104
21	V	0.38	0/1048	0.67	0/1402
22	W	0.36	0/873	0.61	0/1158
23	X	0.36	0/984	0.63	0/1323
24	Y	0.36	0/1132	0.65	0/1504
25	Z	0.38	0/1130	0.65	0/1507
26	a	0.39	0/1191	0.67	0/1590
27	b	0.40	0/861	0.67	0/1138
28	c	0.35	0/771	0.58	0/1034
29	d	0.38	0/903	0.68	0/1216
3	C	0.42	0/2937	0.73	0/3946
30	e	0.38	0/1071	0.68	0/1429
31	f	0.41	0/895	0.73	0/1198
32	g	0.35	0/916	0.72	0/1220
33	h	0.51	0/1021	0.78	0/1348
34	i	0.50	0/841	0.77	0/1112
35	j	0.42	0/720	0.76	0/952
36	k	0.41	0/575	0.65	0/761
37	l	0.46	0/459	0.72	0/608
38	m	0.40	0/435	0.66	0/575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	n	0.59	0/240	0.94	0/305
4	D	0.39	0/2437	0.63	0/3264
40	o	0.38	0/864	0.65	0/1140
41	p	0.44	0/718	0.72	0/953
42	r	0.44	0/1010	0.76	0/1354
43	s	0.44	0/1530	0.64	0/2064
44	t	0.47	0/1174	0.68	0/1582
45	2	0.23	0/1803	0.67	0/2801
45	ii	0.21	0/1805	0.71	0/2809
46	3	0.21	0/1777	0.65	0/2763
47	5	0.33	1/84973 (0.0%)	0.70	19/132508 (0.0%)
48	7	0.26	0/2836	0.65	0/4421
49	8	0.31	0/3581	0.68	0/5577
5	E	0.35	0/1762	0.65	0/2362
50	9	0.26	0/40502	0.70	15/63100 (0.0%)
51	AA	0.33	0/1747	0.58	0/2374
52	BB	0.33	0/1756	0.60	0/2350
53	CC	0.34	0/1753	0.62	0/2369
54	DD	0.36	0/1796	0.64	0/2417
55	EE	0.34	0/2118	0.63	0/2849
56	FF	0.34	0/1492	0.61	0/2005
57	GG	0.34	0/1946	0.66	0/2590
58	HH	0.34	0/1510	0.59	0/2022
59	II	0.34	0/1715	0.64	0/2287
6	F	0.44	0/1911	0.74	1/2549 (0.0%)
60	JJ	0.36	0/1550	0.68	0/2069
61	KK	0.34	0/834	0.65	1/1125 (0.1%)
62	LL	0.35	0/1195	0.62	0/1597
63	MM	0.35	0/918	0.58	0/1233
64	NN	0.33	0/1226	0.63	0/1649
65	OO	0.35	0/1029	0.74	2/1380 (0.1%)
66	PP	0.35	0/1079	0.63	0/1441
67	QQ	0.33	0/1146	0.60	0/1534
68	RR	0.34	0/1082	0.58	0/1452
69	SS	0.35	0/1208	0.66	0/1618
7	G	0.42	0/1910	0.72	0/2569
70	TT	0.37	0/1115	0.62	1/1493 (0.1%)
71	UU	0.34	0/805	0.64	0/1081
72	VV	0.34	0/643	0.65	0/860
73	WW	0.37	0/1051	0.71	0/1406
74	XX	0.35	0/1116	0.67	0/1490
75	YY	0.36	0/1028	0.63	0/1366
76	ZZ	0.34	0/604	0.60	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
77	aa	0.37	0/828	0.70	0/1109
78	bb	0.37	0/665	0.62	0/891
79	cc	0.35	0/490	0.68	0/656
8	H	0.34	0/1535	0.63	0/2063
80	dd	0.39	0/470	0.70	0/623
81	ee	0.35	0/462	0.68	0/607
82	ff	0.36	0/567	0.56	0/753
83	gg	0.33	0/2493	0.55	0/3394
84	hh	0.25	0/233	0.69	0/360
85	jj	0.35	0/3442	0.51	0/4656
9	I	0.36	0/1702	0.61	0/2272
All	All	0.34	1/236786 (0.0%)	0.68	39/347256 (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
2	B	0	3
21	V	0	1
31	f	0	1
74	XX	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	5	2025	A	O3'-P	-30.56	1.24	1.61

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	5	2025	A	OP1-P-O3'	-39.69	17.89	105.20
47	5	2025	A	P-O3'-C3'	-17.17	99.09	119.70
61	KK	40	VAL	C-N-CD	-10.98	96.44	120.60
50	9	581	U	N1-C1'-C2'	-10.17	100.77	114.00
50	9	582	U	N1-C1'-C2'	-9.01	102.09	112.00
50	9	1835	A	C2'-C3'-O3'	8.52	128.24	109.50
47	5	3888	G	C2'-C3'-O3'	7.63	126.28	109.50
50	9	110	U	C2'-C3'-O3'	7.30	125.57	109.50
65	OO	146	ARG	NE-CZ-NH1	7.16	123.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	585	C	N1-C1'-C2'	-6.90	104.41	112.00
47	5	3697	U	C2'-C3'-O3'	6.69	124.40	113.70
47	5	1477	C	C2'-C3'-O3'	6.65	124.34	113.70
47	5	2695	A	C2'-C3'-O3'	6.48	124.07	113.70
47	5	4947	U	C2'-C3'-O3'	6.30	123.78	113.70
47	5	406	C	C2'-C3'-O3'	6.21	123.64	113.70
47	5	1211	G	C2'-C3'-O3'	6.15	123.54	113.70
47	5	275	C	C2'-C3'-O3'	5.94	123.21	113.70
47	5	1455	G	C2'-C3'-O3'	5.91	123.16	113.70
50	9	561	A	C2'-C3'-O3'	5.86	123.07	113.70
47	5	47	A	C4'-C3'-O3'	5.75	124.50	113.00
47	5	1329	G	C2'-C3'-O3'	5.72	122.86	113.70
50	9	627	U	C2'-C3'-O3'	5.71	122.83	113.70
47	5	2046	G	C2'-C3'-O3'	5.68	122.79	113.70
47	5	1370	G	C2'-C3'-O3'	5.56	122.60	113.70
50	9	581	U	C4'-C3'-O3'	5.54	124.07	113.00
70	TT	110	LEU	CA-CB-CG	5.45	127.83	115.30
47	5	480	C	C2'-C3'-O3'	5.43	122.39	113.70
47	5	930	G	C2'-C3'-O3'	5.43	122.39	113.70
47	5	1818	G	C2'-C3'-O3'	5.41	122.35	113.70
50	9	1060	A	N9-C1'-C2'	5.40	121.02	114.00
50	9	1255	G	C2'-C3'-O3'	5.39	122.32	113.70
50	9	1137	U	C2'-C3'-O3'	5.34	122.24	113.70
6	F	88	LEU	CA-CB-CG	5.31	127.51	115.30
50	9	24	C	C2'-C3'-O3'	5.26	122.12	113.70
50	9	584	A	N9-C1'-C2'	-5.19	106.29	112.00
47	5	1329	G	C4'-C3'-O3'	5.15	123.31	113.00
50	9	553	U	C2'-C3'-O3'	5.08	121.82	113.70
65	OO	146	ARG	NE-CZ-NH2	-5.07	117.77	120.30
50	9	532	C	C2'-C3'-O3'	5.00	121.70	113.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	16	PHE	Peptide
2	B	257	TRP	Peptide
2	B	258	HIS	Peptide
21	V	6	ARG	Sidechain
74	XX	61	GLN	Peptide
31	f	106	TYR	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	A	1898	0	1993	28	0
2	B	3172	0	3310	20	0
3	C	2883	0	3053	15	0
4	D	2391	0	2424	13	0
5	E	1729	0	1887	10	0
6	F	1875	0	1995	17	0
7	G	1879	0	2027	18	0
8	H	1516	0	1597	9	0
9	I	1664	0	1712	17	0
10	J	1362	0	1399	5	0
11	L	1702	0	1820	9	0
12	M	1137	0	1211	6	0
13	N	1701	0	1749	15	0
14	O	1630	0	1778	20	0
15	P	1242	0	1274	10	0
16	Q	1515	0	1634	6	0
17	R	1508	0	1664	6	0
18	S	1462	0	1508	12	0
19	T	1298	0	1366	17	0
20	U	809	0	833	5	0
21	V	1034	0	1097	17	0
22	W	860	0	903	6	0
23	X	967	0	1040	4	0
24	Y	1115	0	1205	5	0
25	Z	1107	0	1182	6	0
26	a	1162	0	1209	0	0
27	b	848	0	920	0	0
28	c	761	0	794	0	0
29	d	888	0	930	0	0
30	e	1053	0	1147	0	0
31	f	876	0	912	0	0
32	g	906	0	1000	0	0
33	h	1013	0	1147	0	0
34	i	830	0	916	0	0
35	j	705	0	738	0	0
36	k	569	0	637	0	0
37	l	447	0	480	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	m	429	0	465	0	0
39	n	239	0	289	0	0
40	o	851	0	921	0	0
41	p	708	0	756	0	0
42	r	994	0	1051	0	0
43	s	1507	0	1564	0	0
44	t	1160	0	1218	0	0
45	2	1616	0	826	3	0
45	ii	1616	0	824	0	0
46	3	1593	0	811	4	0
47	5	75972	0	38391	191	0
48	7	2538	0	1286	5	0
49	8	3208	0	1629	2	0
50	9	36229	0	18306	102	0
51	AA	1710	0	1708	30	0
52	BB	1729	0	1803	7	0
53	CC	1716	0	1806	11	0
54	DD	1768	0	1866	10	0
55	EE	2076	0	2177	13	0
56	FF	1471	0	1522	13	0
57	GG	1923	0	2089	7	0
58	HH	1488	0	1582	7	0
59	II	1686	0	1772	7	0
60	JJ	1525	0	1640	12	0
61	KK	810	0	836	14	0
62	LL	1175	0	1249	1	0
63	MM	908	0	939	4	0
64	NN	1202	0	1289	4	0
65	OO	1016	0	1039	7	0
66	PP	1058	0	1104	3	0
67	QQ	1128	0	1195	7	0
68	RR	1068	0	1121	5	0
69	SS	1190	0	1249	4	0
70	TT	1097	0	1132	2	0
71	UU	795	0	862	6	0
72	VV	636	0	637	6	0
73	WW	1034	0	1080	9	0
74	XX	1098	0	1167	7	0
75	YY	1011	0	1083	5	0
76	ZZ	598	0	656	6	0
77	aa	814	0	864	0	0
78	bb	651	0	672	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
79	cc	488	0	514	0	0
80	dd	459	0	449	0	0
81	ee	457	0	502	0	0
82	ff	555	0	565	0	0
83	gg	2436	0	2393	0	0
84	hh	210	0	106	0	0
85	jj	3383	0	3431	0	0
86	5	185	0	0	0	0
86	7	6	0	0	0	0
86	8	5	0	0	0	0
86	9	70	0	0	0	0
86	B	1	0	0	0	0
86	I	1	0	0	0	0
86	P	1	0	0	0	0
86	Q	1	0	0	0	0
86	V	1	0	0	0	0
86	a	2	0	0	0	0
86	g	1	0	0	0	0
86	j	1	0	0	0	0
86	jj	1	0	0	0	0
87	aa	1	0	0	0	0
87	dd	1	0	0	0	0
87	ff	1	0	0	0	0
87	g	1	0	0	0	0
87	j	1	0	0	0	0
87	m	1	0	0	0	0
87	o	1	0	0	0	0
87	p	1	0	0	0	0
88	jj	28	0	12	0	0
89	jj	79	0	0	0	0
All	All	220934	0	164939	707	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 3.

All (707) 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)
47:5:1962:A:H2	47:5:2026:A:N3	1.15	1.38
47:5:3914:U:O4	47:5:4378:A:N1	1.62	1.32
47:5:1962:A:C2	47:5:2026:A:N3	1.97	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:1979:A:C2	47:5:1980:U:O2	1.84	1.28
47:5:1962:A:N1	47:5:2026:A:H1'	1.48	1.26
47:5:2367:A:N1	47:5:2788:U:O4	1.66	1.26
51:AA:189:ILE:HD11	51:AA:195:TRP:NE1	1.57	1.19
51:AA:189:ILE:CD1	51:AA:195:TRP:CD1	2.28	1.17
51:AA:189:ILE:HD11	51:AA:195:TRP:CD1	1.84	1.13
1:A:68:ARG:NH2	47:5:4084:G:C2	2.22	1.07
9:I:150:GLU:OE2	9:I:154:ARG:NH2	1.85	1.07
51:AA:181:GLU:O	51:AA:185:MET:HG3	1.54	1.06
55:EE:200:ARG:HA	55:EE:206:ASP:OD2	1.56	1.05
21:V:3:LYS:HG3	21:V:128:LEU:HD11	1.37	1.02
19:T:142:ARG:NH1	47:5:1090:G:OP1	1.92	1.02
51:AA:189:ILE:HD13	51:AA:195:TRP:CD1	2.01	0.96
50:9:583:A:H2'	50:9:584:A:H5'	1.49	0.94
21:V:6:ARG:HG3	21:V:6:ARG:HH21	1.32	0.94
47:5:1962:A:N1	47:5:2026:A:C1'	2.30	0.94
1:A:68:ARG:HH21	47:5:4084:G:N2	1.64	0.94
50:9:568:C:N4	50:9:582:U:O2	2.01	0.94
47:5:1979:A:C2	47:5:1980:U:C2	2.56	0.94
9:I:154:ARG:HG2	9:I:154:ARG:HH21	1.36	0.91
47:5:1979:A:N1	47:5:1980:U:O2	2.03	0.90
21:V:6:ARG:O	47:5:4596:C:OP1	1.90	0.88
21:V:3:LYS:CG	21:V:128:LEU:HD11	2.03	0.87
19:T:147:GLU:HB3	19:T:148:PRO:CD	2.06	0.84
50:9:584:A:C6	50:9:585:C:C4	2.67	0.82
47:5:1962:A:C2	47:5:2026:A:H1'	2.14	0.81
50:9:566:U:O2	50:9:584:A:N1	2.13	0.81
47:5:2395:A:O2'	47:5:2806:A:H1'	1.81	0.81
47:5:1982:G:P	47:5:1982:G:H3'	2.23	0.79
52:BB:66:VAL:HG22	52:BB:87:ILE:HG22	1.63	0.78
47:5:2367:A:N1	47:5:2788:U:C4	2.51	0.78
50:9:582:U:O2'	50:9:583:A:O4'	2.01	0.78
19:T:147:GLU:HB3	19:T:148:PRO:HD2	1.64	0.78
66:PP:56:LEU:HD13	66:PP:78:THR:HG21	1.67	0.77
47:5:1963:C:C5	47:5:1964:A:H2	2.01	0.77
50:9:584:A:N6	50:9:585:C:N4	2.33	0.77
19:T:146:LYS:O	19:T:146:LYS:HD2	1.84	0.77
50:9:583:A:C2'	50:9:584:A:H5'	2.13	0.76
19:T:80:VAL:HG21	19:T:85:LEU:HD12	1.67	0.76
56:FF:99:ILE:HG23	76:ZZ:67:LEU:HD21	1.67	0.76
47:5:1982:G:H2'	47:5:1983:A:H5''	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:6:ARG:CG	21:V:6:ARG:HH21	1.99	0.75
47:5:3914:U:C4	47:5:4378:A:N1	2.54	0.74
50:9:584:A:N6	50:9:585:C:C4	2.57	0.73
51:AA:189:ILE:CD1	51:AA:195:TRP:NE1	2.42	0.73
51:AA:185:MET:CE	72:VV:39:VAL:HG21	2.17	0.73
25:Z:53:VAL:HG21	25:Z:62:ILE:HG23	1.71	0.73
47:5:3914:U:H3	47:5:4378:A:N6	1.86	0.73
50:9:1091:C:HO2'	73:WW:2:VAL:N	1.86	0.72
75:YY:34:THR:HG23	75:YY:69:THR:HG21	1.69	0.72
51:AA:185:MET:HE2	72:VV:39:VAL:CG2	2.18	0.72
51:AA:185:MET:HE2	72:VV:39:VAL:HG21	1.68	0.72
21:V:6:ARG:HG3	21:V:6:ARG:NH2	2.05	0.72
50:9:561:A:O2'	60:JJ:134:HIS:NE2	2.24	0.71
54:DD:70:THR:HG22	54:DD:86:LEU:HD13	1.72	0.70
9:I:191:ILE:HD11	9:I:212:LEU:HD11	1.73	0.69
14:O:27:VAL:HG12	14:O:98:ALA:HB1	1.73	0.69
47:5:4579:U:H2'	47:5:4580:U:C6	2.28	0.69
47:5:1979:A:O2'	47:5:1980:U:OP1	2.11	0.68
50:9:585:C:O2'	50:9:586:G:H5'	1.92	0.68
47:5:2367:A:N6	47:5:2788:U:N3	2.42	0.68
53:CC:209:VAL:HG21	53:CC:233:LEU:HD13	1.76	0.68
47:5:1962:A:N1	47:5:2026:A:O2'	2.25	0.68
47:5:1982:G:H2'	47:5:1983:A:C5'	2.24	0.67
47:5:3914:U:O4	47:5:4378:A:C2	2.47	0.67
50:9:566:U:O2	50:9:584:A:C2	2.47	0.67
11:L:116:ARG:NH1	11:L:155:MET:O	2.27	0.67
65:OO:95:ILE:HD11	65:OO:126:ILE:HD12	1.77	0.66
50:9:980:A:H2'	50:9:981:A:C8	2.31	0.66
47:5:1963:C:C5	47:5:1964:A:C2	2.84	0.66
63:MM:22:LEU:HD11	63:MM:89:VAL:HA	1.78	0.65
51:AA:60:LEU:HD13	51:AA:159:ILE:HD11	1.78	0.65
19:T:142:ARG:HB3	19:T:142:ARG:NH1	2.12	0.65
47:5:3914:U:N3	47:5:4378:A:N6	2.42	0.65
1:A:68:ARG:NH2	47:5:4084:G:N3	2.43	0.65
47:5:5047:C:O2'	47:5:5050:C:OP2	2.15	0.64
9:I:154:ARG:HG2	9:I:154:ARG:NH2	2.12	0.64
17:R:102:LEU:HD22	17:R:138:LEU:HD12	1.78	0.64
47:5:1982:G:C8	47:5:1983:A:C8	2.85	0.64
47:5:1986:U:C4	47:5:2013:A:N6	2.66	0.64
19:T:144:ASN:ND2	19:T:144:ASN:H	1.94	0.63
9:I:97:ILE:HD13	9:I:126:VAL:HG11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:4695:C:H6	47:5:4695:C:OP2	1.82	0.63
51:AA:189:ILE:HD11	51:AA:195:TRP:HE1	1.62	0.63
15:P:114:ILE:HD11	15:P:117:ILE:HB	1.81	0.63
53:CC:195:LEU:HD23	53:CC:224:THR:HG22	1.80	0.63
47:5:747:A:O2'	47:5:748:G:H3'	1.99	0.62
47:5:2370:A:N1	47:5:2390:G:O2'	2.26	0.62
2:B:261:ARG:HB2	14:O:64:THR:HG21	1.82	0.62
18:S:95:ARG:NH2	47:5:1951:G:O2'	2.32	0.61
18:S:82:LEU:HD13	18:S:126:ILE:HD13	1.82	0.61
9:I:154:ARG:CG	9:I:154:ARG:HH21	2.12	0.61
1:A:68:ARG:CZ	47:5:4084:G:C2	2.84	0.61
18:S:34:ALA:HB1	18:S:39:VAL:HG23	1.82	0.61
14:O:54:TYR:CD1	14:O:145:VAL:HG21	2.35	0.61
47:5:4476:C:O2'	47:5:4478:G:OP2	2.18	0.61
47:5:1962:A:N1	47:5:2026:A:C2'	2.63	0.61
50:9:945:U:H2'	50:9:946:U:C6	2.36	0.61
1:A:68:ARG:NE	47:5:4084:G:N1	2.48	0.60
50:9:501:C:H2'	50:9:501:C:O2	2.02	0.60
6:F:227:VAL:HA	18:S:39:VAL:HG12	1.83	0.60
47:5:4608:G:OP1	60:JJ:69:ARG:NE	93.13	0.60
47:5:1963:C:C4	47:5:1964:A:C2	2.90	0.60
47:5:1979:A:H2'	47:5:1980:U:O4'	2.03	0.59
61:KK:31:LYS:HA	61:KK:40:VAL:O	2.02	0.59
14:O:27:VAL:CG1	14:O:98:ALA:HB1	2.31	0.59
52:BB:69:VAL:HG11	52:BB:74:LEU:HD13	1.83	0.59
50:9:1611:G:OP2	69:SS:121:ARG:NH1	2.36	0.59
5:E:165:VAL:HG11	5:E:178:VAL:HG13	1.83	0.59
12:M:24:LEU:HD11	12:M:86:TRP:CG	2.38	0.58
47:5:3896:C:O2	47:5:4564:A:N1	2.36	0.58
53:CC:251:LEU:HD23	72:VV:23:ILE:HG23	1.85	0.58
47:5:4942:C:H4'	47:5:4943:A:OP1	2.03	0.58
74:XX:51:VAL:HG13	74:XX:70:VAL:HG13	1.85	0.58
1:A:101:VAL:HB	1:A:165:VAL:HG12	1.84	0.58
61:KK:15:LEU:HD22	61:KK:49:MET:CE	2.34	0.58
47:5:1979:A:N3	47:5:1980:U:C2	2.72	0.58
47:5:1982:G:N7	47:5:1983:A:N7	2.52	0.58
50:9:1274:G:N7	61:KK:43:LEU:HD13	2.19	0.57
55:EE:31:PRO:HG2	55:EE:38:LEU:HD12	1.86	0.57
19:T:80:VAL:CG2	19:T:85:LEU:HD12	2.34	0.57
8:H:4:ILE:HD11	18:S:152:PHE:CD2	2.39	0.57
1:A:70:LYS:NZ	47:5:2503:G:N7	2.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:KK:35:LEU:HD11	61:KK:38:LYS:HD3	1.87	0.57
55:EE:139:LEU:HD11	55:EE:154:ILE:HG21	1.87	0.57
51:AA:192:GLU:OE2	51:AA:192:GLU:N	2.37	0.57
47:5:3928:A:H2'	47:5:3929:G:O4'	2.05	0.57
23:X:146:ALA:O	23:X:149:VAL:HG12	2.05	0.57
45:2:38:C:O2'	50:9:1058:A:OP1	2.22	0.57
2:B:14:LEU:HD23	2:B:17:LEU:HD23	1.85	0.57
19:T:143:THR:HG23	19:T:143:THR:O	2.04	0.57
47:5:978:G:O2'	47:5:979:C:OP2	2.20	0.56
47:5:1979:A:C4	47:5:1980:U:C2	2.92	0.56
47:5:4723:A:H2'	47:5:4724:A:C8	2.40	0.56
46:3:16:C:O2	46:3:16:C:O4'	2.24	0.56
50:9:1298:G:O2'	50:9:1299:A:O5'	2.24	0.56
50:9:1535:U:O2	50:9:1535:U:H2'	2.05	0.56
6:F:131:MET:O	6:F:134:ILE:HG22	2.05	0.56
1:A:48:ILE:HD11	1:A:82:ILE:HG22	1.86	0.56
7:G:151:LEU:HD13	7:G:271:LEU:HD12	1.88	0.56
15:P:32:THR:HG23	15:P:91:LEU:HD21	1.88	0.56
63:MM:35:ILE:HD13	63:MM:61:TYR:CE1	2.41	0.56
1:A:207:VAL:HG12	47:5:3919:C:C5'	2.36	0.55
51:AA:8:LEU:CD2	51:AA:191:ARG:NH2	2.69	0.55
56:FF:72:LEU:HD22	56:FF:112:LEU:HD11	1.87	0.55
50:9:1407:U:H2'	50:9:1408:U:C6	2.40	0.55
21:V:3:LYS:HG3	21:V:128:LEU:CD1	2.24	0.55
56:FF:102:LEU:HD22	76:ZZ:110:THR:HG21	1.89	0.55
47:5:3811:G:O2'	47:5:3814:U:OP2	2.22	0.55
55:EE:11:ARG:HH22	55:EE:24:THR:HG1	1.54	0.55
60:JJ:130:ILE:HG12	60:JJ:135:ILE:HD11	1.89	0.55
7:G:139:VAL:HG11	7:G:238:LYS:HG3	1.88	0.55
14:O:84:VAL:HG11	14:O:102:LEU:HD22	1.89	0.55
74:XX:4:CYS:SG	74:XX:9:THR:HG21	2.46	0.55
12:M:36:ALA:HB2	12:M:52:PHE:CZ	2.42	0.55
50:9:1139:C:O4'	50:9:1139:C:O2	2.25	0.55
13:N:184:ILE:HG23	13:N:194:ARG:HH12	1.72	0.55
47:5:2045:G:O6	47:5:3870:C:O2'	2.20	0.54
47:5:2505:C:O4'	47:5:2505:C:O2	2.24	0.54
19:T:142:ARG:HB3	19:T:142:ARG:CZ	2.37	0.54
14:O:72:HIS:N	47:5:4586:G:OP1	2.39	0.54
50:9:584:A:C6	50:9:585:C:N3	2.74	0.54
73:WW:52:ILE:HG22	73:WW:61:ILE:HG12	1.89	0.54
57:GG:157:VAL:HB	57:GG:176:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:23:VAL:HG13	14:O:33:VAL:HG11	1.90	0.54
19:T:147:GLU:CB	19:T:148:PRO:CD	2.80	0.54
21:V:99:GLU:HB3	22:W:24:THR:HG23	1.90	0.54
3:C:40:VAL:HG21	3:C:123:ALA:HB2	1.90	0.54
61:KK:93:THR:HG23	61:KK:94:LEU:HD12	1.90	0.54
50:9:681:U:H4'	74:XX:9:THR:HG22	1.88	0.54
47:5:2367:A:C2	47:5:2788:U:O4	2.53	0.54
15:P:41:ILE:HD12	15:P:150:LEU:HD13	1.90	0.54
14:O:194:ASP:O	14:O:198:THR:HG23	2.08	0.54
15:P:36:ILE:HD12	15:P:48:LEU:HD11	1.90	0.54
47:5:245:C:O2	47:5:245:C:O4'	2.25	0.54
6:F:89:ALA:HB2	6:F:124:LEU:HD21	1.89	0.54
21:V:5:GLY:O	21:V:6:ARG:C	2.47	0.53
24:Y:106:ILE:HG21	24:Y:109:LEU:HD23	1.89	0.53
16:Q:104:ARG:NH2	47:5:1353:G:N7	2.55	0.53
1:A:234:LYS:HG2	1:A:238:ILE:HD12	1.89	0.53
65:OO:44:VAL:HG11	65:OO:85:CYS:SG	2.48	0.53
47:5:1979:A:C6	47:5:1980:U:N3	2.77	0.53
50:9:1568:C:OP1	70:TT:96:SER:OG	2.21	0.53
55:EE:125:LYS:HA	55:EE:159:THR:HG22	1.91	0.53
7:G:210:ILE:HG12	7:G:254:THR:HG22	1.91	0.53
47:5:1483:C:O4'	47:5:1483:C:O2	2.24	0.53
54:DD:21:LEU:HD21	54:DD:48:ILE:HD11	1.90	0.53
15:P:36:ILE:HD11	15:P:44:ALA:HB1	1.91	0.53
45:2:16:C:O2	45:2:16:C:O4'	2.23	0.53
6:F:88:LEU:HD22	6:F:89:ALA:N	2.23	0.53
47:5:1962:A:C2	47:5:2026:A:C4	2.89	0.53
19:T:85:LEU:HD13	47:5:4305:G:C2	2.44	0.53
24:Y:49:ILE:HD11	24:Y:55:VAL:HG21	1.90	0.53
1:A:90:CYS:HB2	1:A:101:VAL:HG13	1.91	0.53
14:O:35:VAL:HG21	14:O:80:PHE:CE2	2.44	0.53
47:5:1325:C:O2	47:5:1325:C:O5'	2.27	0.52
50:9:1364:U:O4'	50:9:1364:U:O2	2.27	0.52
55:EE:173:ILE:HD11	55:EE:235:TRP:CE3	2.44	0.52
21:V:3:LYS:HD3	21:V:129:TRP:CH2	2.45	0.52
51:AA:122:LEU:HB3	51:AA:144:THR:HG23	1.92	0.52
47:5:1979:A:C5	47:5:1980:U:N3	2.78	0.52
50:9:1315:U:O2	50:9:1315:U:O4'	2.27	0.52
50:9:562:U:H2'	50:9:563:G:C8	2.44	0.52
1:A:82:ILE:HD11	1:A:99:GLY:CA	2.39	0.52
6:F:161:ILE:HB	6:F:166:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:9:190:G:O2'	50:9:209:A:N6	2.43	0.52
47:5:1237:C:O2	47:5:1237:C:O4'	2.27	0.52
47:5:1982:G:C3'	47:5:1982:G:P	2.97	0.52
50:9:1298:G:O2'	50:9:1299:A:O4'	2.26	0.52
50:9:183:G:O2'	50:9:184:G:O5'	2.28	0.52
20:U:23:LEU:HD11	20:U:83:LEU:HD21	1.91	0.52
1:A:82:ILE:HD11	1:A:99:GLY:HA3	1.92	0.52
58:HH:95:ILE:HD11	58:HH:133:LEU:HG	1.91	0.52
18:S:35:PRO:HD2	18:S:39:VAL:HG21	1.92	0.52
24:Y:49:ILE:HD13	24:Y:80:ILE:HD13	1.92	0.52
47:5:224:U:O2	47:5:224:U:O4'	2.28	0.51
11:L:47:ALA:HB3	11:L:48:PRO:HD3	1.91	0.51
76:ZZ:73:VAL:HG12	76:ZZ:79:ILE:HD11	1.91	0.51
1:A:62:VAL:CG1	1:A:71:LYS:HG2	2.40	0.51
47:5:4989:U:O2	47:5:4989:U:O4'	2.27	0.51
4:D:152:ARG:HG3	4:D:154:THR:HG23	1.91	0.51
21:V:26:ILE:HG22	21:V:101:ASN:HB3	1.93	0.51
73:WW:75:ILE:HD11	73:WW:93:LEU:HD11	1.92	0.51
51:AA:159:ILE:HG23	51:AA:159:ILE:O	2.10	0.51
45:2:33:U:OP2	67:QQ:146:ARG:NH2	2.44	0.51
3:C:334:THR:HG21	6:F:50:TYR:OH	2.09	0.51
50:9:1734:G:O2'	50:9:1800:A:N6	2.43	0.51
66:PP:37:TYR:OH	66:PP:45:LEU:HD11	2.10	0.51
21:V:57:VAL:HG11	21:V:122:ALA:HB3	1.92	0.51
47:5:1979:A:N1	47:5:1980:U:C2	2.76	0.51
47:5:3723:A:H2'	47:5:3724:A:C8	2.46	0.51
47:5:747:A:H4'	47:5:748:G:OP1	2.11	0.51
57:GG:63:MET:N	57:GG:63:MET:SD	2.84	0.51
15:P:29:THR:HG21	15:P:146:ILE:HD11	1.93	0.51
48:7:11:A:O2'	48:7:13:A:OP2	2.29	0.51
14:O:54:TYR:OH	14:O:73:PHE:O	2.29	0.51
2:B:219:VAL:HG21	2:B:333:LEU:HD23	1.92	0.51
4:D:23:ARG:NH2	47:5:4280:A:OP2	2.44	0.50
47:5:62:A:N3	47:5:77:U:O2'	2.42	0.50
47:5:498:C:O4'	47:5:498:C:O2	2.30	0.50
1:A:225:ILE:HD12	1:A:233:ARG:CZ	2.41	0.50
55:EE:45:ILE:HD12	55:EE:80:ILE:HD12	1.92	0.50
11:L:18:TRP:CE3	13:N:198:LEU:HD12	2.46	0.50
18:S:53:LYS:NZ	48:7:74:A:O2'	2.45	0.50
47:5:3642:A:OP1	47:5:3644:U:OP1	2.30	0.50
47:5:4966:A:H2'	47:5:4967:A:C8	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:4510:A:O2'	47:5:4511:A:O4'	2.30	0.50
50:9:1718:G:O2'	50:9:1815:A:N6	2.45	0.50
61:KK:38:LYS:HD2	61:KK:38:LYS:N	2.27	0.50
50:9:501:C:O2	50:9:501:C:C2'	2.59	0.50
50:9:584:A:C5	50:9:585:C:C5	2.99	0.50
53:CC:214:LEU:HD23	53:CC:219:ILE:HD12	1.93	0.50
64:NN:13:GLN:HE21	64:NN:13:GLN:N	2.09	0.50
4:D:64:ILE:HD13	4:D:109:LEU:HD22	1.94	0.50
56:FF:103:LEU:HD23	56:FF:178:ILE:HD13	1.93	0.50
8:H:88:PHE:CE1	8:H:151:ILE:HD12	2.47	0.50
1:A:208:GLU:HG2	47:5:1629:G:H1	1.76	0.50
5:E:165:VAL:HG13	5:E:180:GLY:N	2.27	0.50
61:KK:32:HIS:CD2	61:KK:45:VAL:HG21	2.46	0.50
47:5:3810:C:O4'	47:5:3810:C:O2	2.26	0.50
13:N:135:ILE:CD1	13:N:151:ILE:HD13	2.42	0.50
46:3:75:C:H2'	46:3:76:A:H4'	1.94	0.49
17:R:74:ARG:NH2	47:5:2891:U:OP2	2.45	0.49
55:EE:44:LEU:HD13	55:EE:72:ILE:HD11	1.94	0.49
50:9:448:A:H5''	59:II:25:ARG:HA	1.93	0.49
15:P:127:ARG:NH2	47:5:2422:C:OP1	2.44	0.49
76:ZZ:79:ILE:HB	76:ZZ:83:LEU:HD12	1.94	0.49
51:AA:66:VAL:HG21	51:AA:185:MET:HB2	1.93	0.49
4:D:41:LYS:CG	19:T:93:ILE:HD11	2.43	0.49
23:X:80:PRO:HB2	23:X:155:ILE:HD13	1.95	0.49
47:5:2088:A:O2'	47:5:2089:G:OP2	2.26	0.49
49:8:125:C:O4'	49:8:125:C:O2	2.31	0.49
50:9:526:A:O2'	60:JJ:125:HIS:HA	2.12	0.49
50:9:93:U:H2'	50:9:94:G:O4'	2.12	0.49
1:A:77:ILE:HD13	1:A:128:ARG:HB2	1.95	0.49
61:KK:15:LEU:HD22	61:KK:49:MET:HE3	1.95	0.49
56:FF:92:ILE:HD13	56:FF:169:ILE:HG21	1.94	0.49
4:D:163:LEU:HD11	4:D:173:ILE:HG21	1.94	0.49
47:5:1979:A:O2'	47:5:1980:U:H5'	2.13	0.49
47:5:2268:A:H4'	47:5:2269:C:H5'	1.94	0.49
47:5:2763:U:O2	47:5:2763:U:O4'	2.31	0.49
50:9:1395:C:H2'	50:9:1396:A:O4'	2.13	0.49
7:G:139:VAL:HG11	7:G:238:LYS:CG	2.43	0.49
10:J:141:ILE:HD11	48:7:55:A:C2	2.48	0.49
21:V:82:ILE:HG12	21:V:121:VAL:HG13	1.93	0.49
50:9:944:A:C5	50:9:945:U:C5	3.01	0.48
57:GG:5:ILE:HD12	57:GG:16:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:67:ILE:HD12	16:Q:96:PRO:HD2	1.94	0.48
73:WW:26:LEU:HD11	73:WW:60:LYS:HB3	1.94	0.48
2:B:174:ARG:NH1	47:5:4985:U:O2	2.46	0.48
50:9:1374:C:H2'	50:9:1375:G:O4'	2.13	0.48
2:B:249:ARG:NH1	47:5:2837:U:OP1	2.46	0.48
2:B:77:THR:HG21	2:B:337:VAL:HG22	1.95	0.48
9:I:191:ILE:CD1	9:I:212:LEU:HD11	2.40	0.48
59:II:113:TYR:CE1	59:II:121:LEU:HD23	2.48	0.48
47:5:4608:G:OP1	60:JJ:69:ARG:HD2	95.02	0.48
1:A:207:VAL:HG12	47:5:3919:C:H5'	1.95	0.48
51:AA:134:LEU:CD2	51:AA:144:THR:HG21	2.42	0.48
13:N:50:ARG:NH2	47:5:279:A:OP1	2.46	0.48
1:A:207:VAL:HG11	47:5:1633:G:C6	2.49	0.48
51:AA:183:LEU:HD23	51:AA:186:ARG:NH1	2.29	0.48
6:F:89:ALA:CB	6:F:124:LEU:HD21	2.43	0.48
56:FF:88:MET:HE1	56:FF:92:ILE:HD11	1.94	0.48
17:R:35:ALA:HA	17:R:40:GLN:HG2	1.95	0.48
22:W:3:VAL:HG21	22:W:12:LYS:CE	2.44	0.48
47:5:1964:A:OP1	47:5:1964:A:H4'	2.13	0.48
50:9:1624:U:O2	50:9:1624:U:O4'	2.30	0.48
55:EE:126:VAL:HG23	55:EE:156:VAL:O	2.12	0.48
12:M:119:ARG:NH1	14:O:202:LEU:HD21	2.27	0.48
47:5:4966:A:C2	47:5:5067:U:N3	2.81	0.48
2:B:49:TYR:HH	2:B:179:HIS:HD1	1.62	0.48
65:OO:99:ALA:H	65:OO:133:THR:HG22	1.79	0.48
68:RR:16:ILE:HG22	68:RR:24:LEU:HD11	1.96	0.48
68:RR:31:ASN:C	68:RR:31:ASN:HD22	2.17	0.48
1:A:186:TYR:HB2	1:A:196:TRP:CZ3	2.49	0.48
13:N:135:ILE:HD13	13:N:151:ILE:HD13	1.94	0.48
18:S:80:ILE:HG22	18:S:82:LEU:HD22	1.95	0.48
50:9:1149:A:C6	50:9:1151:G:C4	3.02	0.48
51:AA:181:GLU:O	51:AA:185:MET:CG	2.44	0.48
2:B:14:LEU:HD23	2:B:17:LEU:CD2	2.43	0.48
18:S:83:ARG:HA	47:5:2022:C:OP1	49.01	0.48
3:C:323:ARG:NH1	47:5:1279:A:O2'	2.46	0.48
47:5:2094:C:O4'	47:5:2094:C:O2	2.32	0.48
47:5:964:A:H2'	47:5:965:G:O4'	2.14	0.48
54:DD:105:LEU:HD23	54:DD:184:ILE:HG23	1.96	0.48
50:9:1589:A:N3	50:9:1653:U:O2'	2.43	0.47
2:B:252:ALA:HB1	47:5:4524:G:N3	2.28	0.47
2:B:56:ILE:HG12	2:B:365:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:247:VAL:HG21	7:G:249:ARG:NH1	2.29	0.47
21:V:39:ILE:HG23	21:V:61:VAL:CG2	2.44	0.47
47:5:1981:G:H2'	47:5:1982:G:H5'	1.96	0.47
47:5:4723:A:C2	47:5:4724:A:C6	3.02	0.47
59:II:38:ILE:HD11	59:II:81:VAL:HG23	1.97	0.47
9:I:77:VAL:O	9:I:77:VAL:HG13	3.04	0.47
64:NN:13:GLN:NE2	64:NN:13:GLN:N	2.62	0.47
17:R:98:ARG:NH2	47:5:2262:G:OP2	170.50	0.47
68:RR:53:TYR:CE2	68:RR:57:LEU:HD11	2.49	0.47
50:9:914:U:O2	50:9:914:U:O4'	2.33	0.47
1:A:65:ASP:HB2	1:A:72:ARG:HG2	1.94	0.47
52:BB:212:VAL:O	52:BB:212:VAL:HG23	2.14	0.47
3:C:33:ARG:HD2	3:C:36:ILE:HD12	1.95	0.47
5:E:185:ASN:ND2	5:E:274:LEU:O	2.47	0.47
15:P:32:THR:HG21	15:P:87:SER:HB3	1.96	0.47
47:5:1982:G:C2'	47:5:1983:A:C5'	2.92	0.47
47:5:2627:C:O4'	47:5:2627:C:O2	2.28	0.47
47:5:1872:G:O2'	47:5:4219:A:N3	2.43	0.47
50:9:1444:U:H2'	50:9:1445:U:C6	2.49	0.47
15:P:54:LYS:HA	15:P:83:TRP:CD1	2.48	0.47
10:J:113:ILE:HD12	69:SS:14:ARG:HD2	1.95	0.47
46:3:35:U:O4'	50:9:1641:A:OP1	2.31	0.47
50:9:4:C:O2'	60:JJ:18:ARG:NH1	2.47	0.47
51:AA:33:GLN:HB3	51:AA:154:LEU:HD12	1.96	0.47
3:C:334:THR:HG22	3:C:337:ARG:HH22	1.80	0.47
60:JJ:45:ARG:O	60:JJ:49:THR:HG23	2.15	0.47
23:X:127:LEU:HD11	23:X:135:LYS:HE3	1.96	0.47
24:Y:61:HIS:N	47:5:232:G:O6	2.46	0.47
47:5:1982:G:N7	47:5:1983:A:C8	2.83	0.47
47:5:4724:A:C6	47:5:4725:C:C4	3.02	0.47
22:W:4:GLU:OE1	22:W:20:ARG:NH2	2.48	0.47
1:A:126:LEU:HD13	1:A:150:LEU:HD21	1.96	0.47
1:A:158:ILE:HG23	1:A:162:ASN:HD21	1.80	0.47
4:D:146:LEU:HD11	4:D:159:VAL:HG11	1.96	0.47
4:D:61:ILE:HG23	4:D:79:TYR:CE2	2.50	0.47
66:PP:56:LEU:HD13	66:PP:78:THR:CG2	2.40	0.47
47:5:4305:G:N3	47:5:4305:G:H2'	2.30	0.47
47:5:4871:C:O4'	47:5:4871:C:O2	2.33	0.47
50:9:146:G:O2'	50:9:147:A:O5'	2.27	0.47
50:9:585:C:O2'	50:9:586:G:C5'	2.61	0.47
50:9:980:A:C2	50:9:981:A:C6	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DD:162:ASP:N	54:DD:163:PRO:CD	2.77	0.47
7:G:189:LEU:HD22	7:G:255:VAL:CG1	2.45	0.47
57:GG:3:LEU:HD22	57:GG:111:LEU:HD11	1.97	0.47
19:T:144:ASN:ND2	19:T:144:ASN:N	2.60	0.47
47:5:222:C:H2'	47:5:223:G:O4'	2.15	0.47
47:5:4305:G:N3	47:5:4305:G:C2'	2.77	0.47
50:9:1700:C:C2	50:9:1834:A:N6	2.83	0.47
14:O:36:VAL:HG11	14:O:108:ILE:HD12	1.96	0.47
51:AA:94:THR:HG23	51:AA:182:VAL:HG21	1.97	0.46
7:G:116:LEU:HD21	13:N:29:GLN:HG3	1.97	0.46
47:5:1381:U:O2	47:5:1381:U:O4'	2.31	0.46
20:U:82:TYR:CZ	20:U:86:LEU:HD11	2.50	0.46
47:5:4608:G:OP1	60:JJ:69:ARG:CD	94.51	0.46
8:H:41:ILE:HD11	8:H:69:THR:HB	1.98	0.46
9:I:154:ARG:CG	9:I:154:ARG:NH2	2.73	0.46
14:O:12:ARG:O	18:S:171:ARG:NH2	2.48	0.46
22:W:3:VAL:HG21	22:W:12:LYS:HE3	1.97	0.46
1:A:112:ILE:HG23	1:A:133:TYR:CD2	2.50	0.46
4:D:146:LEU:HD11	4:D:159:VAL:CG1	2.45	0.46
5:E:167:PHE:CE1	5:E:176:LEU:HD22	2.50	0.46
6:F:178:LEU:HD21	6:F:203:ALA:HA	1.96	0.46
58:HH:69:LEU:HD23	58:HH:96:ALA:HB2	1.98	0.46
11:L:58:ILE:HG23	11:L:70:VAL:CG1	2.46	0.46
69:SS:18:THR:HG21	69:SS:33:ILE:HA	1.96	0.46
47:5:1979:A:C6	47:5:1980:U:C2	3.04	0.46
47:5:4266:G:O2'	47:5:4279:A:N6	2.48	0.46
4:D:41:LYS:HG2	19:T:93:ILE:HD11	1.97	0.46
47:5:1667:A:N1	47:5:2281:U:OP2	2.48	0.46
47:5:1962:A:C2	47:5:2026:A:C1'	2.90	0.46
47:5:1986:U:C4	47:5:2013:A:C6	3.03	0.46
4:D:16:TYR:O	48:7:11:A:N6	2.48	0.46
50:9:1228:A:H2'	50:9:1229:G:C8	2.50	0.46
50:9:1535:U:O2	50:9:1535:U:C2'	2.63	0.46
50:9:1336:C:H2'	50:9:1337:C:O4'	2.16	0.46
6:F:91:VAL:HG21	6:F:132:LEU:HD21	1.97	0.46
58:HH:66:VAL:HG22	58:HH:96:ALA:HB1	1.96	0.46
12:M:17:PHE:CE2	12:M:54:CYS:HA	2.51	0.46
47:5:747:A:HO2'	47:5:748:G:H3'	1.79	0.46
50:9:412:G:O2'	50:9:812:A:N6	2.47	0.46
58:HH:170:VAL:HG13	58:HH:187:PHE:HB2	1.98	0.46
11:L:18:TRP:CZ3	13:N:198:LEU:HD12	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SS:15:VAL:HG22	69:SS:68:ILE:HD11	1.96	0.46
19:T:48:VAL:HG21	19:T:94:GLU:HG2	1.96	0.46
52:BB:79:VAL:HG21	52:BB:81:PHE:CZ	2.51	0.46
9:I:61:SER:HA	9:I:126:VAL:HG23	1.96	0.46
50:9:1395:C:O2'	50:9:1396:A:OP1	2.28	0.45
71:UU:29:VAL:HG22	71:UU:85:HIS:CE1	2.51	0.45
21:V:16:ILE:HD12	21:V:16:ILE:O	2.15	0.45
56:FF:99:ILE:CG2	76:ZZ:67:LEU:HD21	2.40	0.45
9:I:91:LEU:HD12	9:I:135:ILE:HG23	1.98	0.45
50:9:566:U:C2	50:9:584:A:N1	2.84	0.45
54:DD:109:LEU:CD2	54:DD:115:VAL:HG22	2.47	0.45
50:9:380:G:OP2	59:II:56:ARG:NH2	2.49	0.45
73:WW:6:VAL:HG12	73:WW:34:ILE:HD11	1.97	0.45
74:XX:74:LEU:HD21	74:XX:81:ILE:HD12	1.97	0.45
50:9:1137:U:N3	50:9:1148:A:N6	2.63	0.45
7:G:189:LEU:HD22	7:G:255:VAL:HG12	1.99	0.45
71:UU:105:SER:OG	71:UU:105:SER:O	2.34	0.45
47:5:106:A:H2'	47:5:107:G:O4'	2.17	0.45
6:F:222:LYS:HE3	47:5:1907:A:H4'	1.98	0.45
14:O:85:ARG:HG3	14:O:99:LEU:HD11	1.99	0.45
65:OO:56:VAL:HG13	65:OO:77:ALA:HB1	1.97	0.45
19:T:142:ARG:NH1	19:T:142:ARG:CB	2.80	0.45
47:5:4378:A:O2'	47:5:4379:A:H2'	2.16	0.45
50:9:581:U:O4'	75:YY:62:THR:HG21	2.17	0.45
2:B:29:VAL:HG23	2:B:346:THR:HG21	1.98	0.45
56:FF:49:LEU:HD13	56:FF:50:PRO:HD2	1.98	0.45
60:JJ:46:VAL:HG11	60:JJ:106:LEU:CD1	2.47	0.45
47:5:4759:C:O2	47:5:4759:C:O4'	2.34	0.45
5:E:124:VAL:HG21	47:5:702:U:H5'	1.99	0.45
56:FF:39:ILE:HG23	56:FF:68:ILE:HD13	1.98	0.45
67:QQ:32:ILE:HG21	67:QQ:39:LEU:HD11	1.99	0.45
51:AA:122:LEU:HD13	51:AA:142:LEU:HD13	1.98	0.45
3:C:210:ILE:HG21	3:C:252:TRP:CZ3	2.51	0.45
53:CC:106:VAL:HG22	53:CC:128:VAL:HG22	1.99	0.45
58:HH:133:LEU:HD21	58:HH:176:VAL:HG11	1.99	0.45
74:XX:128:VAL:HG11	74:XX:133:LEU:HD21	1.99	0.45
47:5:119:G:H3'	47:5:120:A:C5'	2.47	0.45
6:F:46:ARG:NH1	47:5:976:G:O3'	2.50	0.45
51:AA:68:ILE:HG21	51:AA:74:VAL:HG23	1.98	0.45
54:DD:109:LEU:HD21	54:DD:115:VAL:HG22	1.99	0.45
63:MM:35:ILE:HD13	63:MM:61:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:XX:61:GLN:HB3	74:XX:62:PRO:CD	2.47	0.45
50:9:427:U:O5'	50:9:427:U:O2	2.35	0.44
50:9:145:G:N7	57:GG:178:ARG:NH1	2.63	0.44
13:N:116:LEU:HD22	13:N:135:ILE:HD11	1.97	0.44
47:5:2862:G:H4'	47:5:3625:G:N7	2.32	0.44
47:5:4579:U:O2	47:5:4580:U:C2	2.71	0.44
14:O:151:ALA:O	14:O:155:THR:HG23	2.17	0.44
67:QQ:51:LEU:HD22	67:QQ:84:ILE:HD11	1.99	0.44
47:5:1982:G:H3'	47:5:1982:G:OP2	2.17	0.44
50:9:572:U:OP1	75:YY:60:PHE:N	2.48	0.44
3:C:327:LYS:O	6:F:46:ARG:NH2	2.50	0.44
50:9:453:C:C2'	50:9:454:U:H5'	2.47	0.44
51:AA:124:VAL:HG13	51:AA:130:ASP:HB2	1.99	0.44
2:B:57:VAL:HG22	2:B:73:VAL:HG12	1.99	0.44
3:C:336:ARG:O	3:C:340:ILE:HG12	2.17	0.44
47:5:320:C:H2'	47:5:321:U:O4'	2.18	0.44
47:5:3724:A:N6	47:5:3725:G:C6	2.85	0.44
47:5:4423:U:O2	47:5:4423:U:O4'	2.35	0.44
56:FF:39:ILE:HG23	56:FF:68:ILE:HG21	1.99	0.44
60:JJ:28:GLU:HG2	60:JJ:43:VAL:HG11	1.99	0.44
47:5:113:A:H2'	47:5:114:G:O4'	2.18	0.44
47:5:1612:G:C2'	47:5:1612:G:N3	2.80	0.44
50:9:1616:U:H2'	50:9:1617:G:O4'	2.17	0.44
50:9:27:A:H2'	50:9:28:U:O4'	2.18	0.44
13:N:202:ARG:NH2	47:5:1372:A:OP1	2.50	0.44
16:Q:11:ARG:NH2	47:5:1690:C:OP2	2.51	0.44
8:H:64:ARG:NH2	47:5:4693:C:OP1	2.51	0.44
47:5:4977:A:H2'	47:5:4978:G:O4'	2.18	0.44
50:9:459:C:H2'	50:9:460:A:O4'	2.18	0.44
7:G:199:LEU:HD12	7:G:205:ALA:HB2	1.99	0.44
8:H:12:ILE:HG21	8:H:18:ILE:HD13	1.99	0.44
61:KK:35:LEU:O	61:KK:35:LEU:HD13	2.18	0.44
50:9:1401:A:C2	50:9:1402:A:C6	3.06	0.44
52:BB:44:ILE:HD11	52:BB:86:LEU:HD13	2.00	0.44
47:5:1381:U:O2	47:5:1381:U:H5''	2.18	0.44
47:5:4589:A:N1	47:5:4621:C:O2'	2.44	0.44
47:5:82:U:H2'	47:5:83:C:O4'	2.17	0.44
50:9:183:G:O2'	50:9:183:G:N3	2.50	0.44
51:AA:60:LEU:HD13	51:AA:159:ILE:CD1	2.47	0.44
3:C:188:ARG:NH2	47:5:2299:G:O6	2.51	0.44
8:H:92:MET:SD	8:H:161:ILE:HD11	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:HH:116:ARG:NH2	58:HH:121:THR:OG1	2.51	0.44
25:Z:89:ILE:HD11	25:Z:117:LYS:HB3	2.00	0.44
60:JJ:146:SER:O	60:JJ:147:PHE:C	2.56	0.43
47:5:4189:U:H2'	47:5:4190:U:O4'	2.18	0.43
50:9:1401:A:H2'	50:9:1402:A:C8	2.53	0.43
50:9:183:G:C2'	50:9:183:G:N3	2.80	0.43
1:A:196:TRP:O	1:A:198:ARG:N	2.51	0.43
5:E:165:VAL:CG1	5:E:178:VAL:HG13	2.47	0.43
7:G:119:GLN:HA	7:G:122:ILE:HD12	1.99	0.43
73:WW:28:ARG:CZ	73:WW:28:ARG:HB3	2.48	0.43
47:5:2439:G:C6	47:5:2440:U:C4	3.07	0.43
50:9:1303:C:O2	50:9:1303:C:O4'	2.36	0.43
50:9:1395:C:H2'	50:9:1396:A:N3	2.32	0.43
55:EE:181:CYS:SG	55:EE:225:ILE:HG23	2.59	0.43
7:G:223:LEU:CD1	7:G:254:THR:HG21	2.48	0.43
50:9:1822:A:H2'	50:9:1823:A:O4'	2.18	0.43
50:9:433:A:H5''	59:II:22:HIS:HB3	2.00	0.43
57:GG:58:LYS:HA	57:GG:107:SER:HB2	2.00	0.43
14:O:54:TYR:HD1	14:O:145:VAL:HG21	1.82	0.43
14:O:85:ARG:CG	14:O:99:LEU:HD11	2.48	0.43
47:5:407:A:O2'	47:5:410:A:OP1	2.36	0.43
6:F:75:ARG:NE	47:5:730:G:OP2	2.48	0.43
56:FF:68:ILE:HD12	56:FF:112:LEU:HD22	1.99	0.43
71:UU:48:LEU:HD11	71:UU:91:LEU:HD22	2.00	0.43
21:V:50:ASN:ND2	47:5:4457:U:OP1	2.52	0.43
51:AA:63:ARG:HE	72:VV:78:ILE:HG23	1.83	0.43
74:XX:107:ARG:HB3	74:XX:110:HIS:HB3	2.00	0.43
25:Z:41:ALA:HB2	25:Z:77:TYR:CE1	2.54	0.43
47:5:1301:C:O2	47:5:1301:C:O4'	2.33	0.43
47:5:686:A:N3	47:5:686:A:H2'	2.34	0.43
1:A:117:GLU:HB2	1:A:162:ASN:HB2	2.00	0.43
3:C:67:TRP:CE3	3:C:73:VAL:HG21	2.54	0.43
53:CC:84:PHE:HZ	53:CC:262:THR:HG23	1.82	0.43
54:DD:72:VAL:HG23	61:KK:20:VAL:HG21	1.99	0.43
2:B:56:ILE:CG1	2:B:365:LEU:HD22	2.49	0.43
54:DD:109:LEU:HD12	54:DD:184:ILE:HD11	2.01	0.43
10:J:128:LEU:HD11	10:J:130:PHE:CE1	2.53	0.43
50:9:428:U:C6	60:JJ:7:TRP:CH2	3.07	0.43
11:L:28:GLN:HB3	11:L:29:PRO:HD3	2.01	0.43
47:5:1990:A:H3'	47:5:1991:A:H5''	2.00	0.43
47:5:294:G:O6	47:5:315:G:H1'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:4525:C:H2'	47:5:4526:U:O4'	2.19	0.43
50:9:1551:U:O2	50:9:1551:U:O4'	2.36	0.43
57:GG:159:ARG:HB3	57:GG:173:ALA:HB2	2.00	0.43
47:5:2690:C:H2'	47:5:2691:U:O4'	2.19	0.43
47:5:3706:C:H2'	47:5:3707:U:O4'	2.19	0.43
50:9:1095:C:O2	50:9:1095:C:C2'	2.66	0.43
50:9:1255:G:OP1	50:9:1256:G:H1'	2.19	0.43
2:B:86:VAL:HG13	2:B:162:VAL:HG22	2.01	0.43
6:F:178:LEU:HB3	6:F:183:ILE:HB	2.01	0.43
11:L:28:GLN:HB3	11:L:29:PRO:CD	2.49	0.43
13:N:65:ARG:HG3	13:N:129:PHE:CE1	2.54	0.43
64:NN:13:GLN:H	64:NN:13:GLN:HE21	1.66	0.43
17:R:10:LEU:HB3	17:R:41:ILE:CD1	2.49	0.43
50:9:1095:C:O2	50:9:1095:C:H2'	2.19	0.43
50:9:1298:G:O2'	50:9:1299:A:C8	2.69	0.43
50:9:1438:A:H2'	50:9:1439:A:C8	2.54	0.43
5:E:180:GLY:O	5:E:181:PRO:C	2.57	0.43
6:F:100:VAL:HG23	6:F:138:TYR:CZ	2.54	0.43
8:H:41:ILE:HG12	8:H:73:ILE:HD11	2.00	0.43
59:II:182:CYS:SG	59:II:183:GLY:N	2.92	0.43
47:5:1613:A:H3'	47:5:1614:C:H5'	2.00	0.42
47:5:2367:A:N6	47:5:2788:U:C4	2.84	0.42
52:BB:143:THR:HG21	52:BB:156:ALA:HB2	2.00	0.42
7:G:207:LEU:HD23	7:G:208:VAL:N	2.34	0.42
61:KK:11:ILE:HD12	61:KK:45:VAL:HG22	2.01	0.42
25:Z:38:TYR:CD1	25:Z:76:ASN:OD1	2.72	0.42
10:J:155:HIS:HB2	48:7:55:A:H4'	2.01	0.42
50:9:853:C:O4'	50:9:853:C:O2	2.35	0.42
1:A:104:VAL:CG1	1:A:146:THR:HG21	2.48	0.42
51:AA:38:ILE:HD11	51:AA:150:THR:HG22	2.00	0.42
2:B:299:ILE:N	2:B:299:ILE:HD12	2.34	0.42
5:E:261:LEU:N	5:E:262:PRO:HD2	2.34	0.42
7:G:199:LEU:CD1	7:G:205:ALA:HB2	2.49	0.42
9:I:81:GLY:CA	47:5:1990:A:OP1	2.67	0.42
13:N:115:VAL:HG22	13:N:134:LEU:CD2	2.49	0.42
20:U:70:ILE:N	20:U:70:ILE:HD12	2.34	0.42
47:5:4586:G:H5''	47:5:4586:G:H8	1.84	0.42
50:9:1444:U:O2'	50:9:1580:A:N1	2.53	0.42
11:L:22:VAL:CG1	13:N:200:LEU:HD12	2.49	0.42
17:R:4:LEU:HD11	17:R:29:THR:HG23	2.00	0.42
73:WW:56:HIS:O	73:WW:57:ARG:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:976:G:N2	47:5:977:C:C2	2.87	0.42
50:9:933:G:H1'	50:9:1001:A:O4'	2.19	0.42
51:AA:104:THR:O	51:AA:107:THR:HG23	2.20	0.42
3:C:30:ALA:HB1	3:C:31:PRO:HD2	2.01	0.42
13:N:193:ARG:O	13:N:197:THR:HG23	2.20	0.42
7:G:210:ILE:HG23	7:G:220:VAL:HG11	2.01	0.42
63:MM:22:LEU:HD21	63:MM:89:VAL:HG23	2.01	0.42
47:5:4530:U:H2'	47:5:4531:U:C6	2.54	0.42
50:9:384:U:O4	59:II:5:ARG:NH2	2.51	0.42
12:M:116:LYS:HE3	14:O:201:LEU:HD13	2.00	0.42
65:OO:119:LEU:HD11	65:OO:126:ILE:HD11	2.01	0.42
73:WW:37:PHE:CE2	73:WW:103:VAL:HG13	2.55	0.42
47:5:3707:U:H2'	47:5:3708:C:C6	2.55	0.42
50:9:1199:A:H2'	50:9:1200:A:O4'	2.19	0.42
2:B:223:THR:HA	2:B:338:VAL:HG22	2.01	0.42
53:CC:176:LYS:O	53:CC:200:ARG:NH1	2.52	0.42
9:I:71:CYS:SG	9:I:154:ARG:HB3	2.60	0.42
47:5:1982:G:C2'	47:5:1983:A:O5'	2.67	0.42
1:A:179:ILE:O	47:5:3653:A:O3'	2.38	0.42
47:5:481(A):C:O4'	47:5:481(A):C:O2	2.36	0.42
9:I:145:LYS:HE3	9:I:167:ILE:HD13	2.02	0.42
25:Z:41:ALA:HB2	25:Z:77:TYR:HE1	1.85	0.42
50:9:92:A:O4'	55:EE:3:ARG:NH1	2.52	0.42
8:H:126:VAL:HG11	8:H:161:ILE:HG23	2.01	0.42
47:5:1867:A:N3	47:5:4403:U:O2'	2.49	0.42
47:5:1962:A:H2	47:5:2026:A:C4	2.13	0.42
50:9:1628:C:H2'	50:9:1629:C:C6	2.54	0.42
13:N:115:VAL:HA	13:N:134:LEU:HD23	2.01	0.42
75:YY:62:THR:HA	75:YY:69:THR:HG22	2.02	0.42
47:5:1982:G:O2'	47:5:1983:A:O5'	2.26	0.41
14:O:18:ARG:NH2	47:5:2057:A:OP1	2.52	0.41
2:B:107:ALA:HB2	2:B:201:LEU:HG	2.02	0.41
7:G:136:PHE:HA	7:G:236:ILE:HD13	2.01	0.41
9:I:153:ARG:HA	9:I:165:ILE:HD11	2.02	0.41
20:U:23:LEU:HD11	20:U:83:LEU:CD2	2.49	0.41
22:W:3:VAL:O	22:W:3:VAL:HG23	2.20	0.41
50:9:1141:G:H2'	50:9:1142:G:O4'	2.21	0.41
2:B:220:ILE:HG12	2:B:278:THR:HG23	2.01	0.41
5:E:153:LEU:HD13	5:E:197:VAL:HG11	2.02	0.41
3:C:340:ILE:HG21	5:E:52:LEU:HD12	2.03	0.41
67:QQ:51:LEU:HD22	67:QQ:84:ILE:CD1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:33:ILE:HD12	20:U:96:LEU:HD22	2.02	0.41
22:W:9:SER:OG	22:W:36:CYS:SG	2.76	0.41
73:WW:104:LEU:HB3	73:WW:125:ILE:HA	2.01	0.41
47:5:4187:G:H2'	47:5:4188:U:O4'	2.21	0.41
51:AA:18:PHE:CD2	51:AA:51:LEU:HD22	2.55	0.41
10:J:103:GLY:O	10:J:134:LEU:HD12	2.21	0.41
11:L:58:ILE:HG23	11:L:70:VAL:HG11	2.01	0.41
62:LL:61:PRO:HA	62:LL:66:VAL:HG13	2.03	0.41
16:Q:61:LEU:HD12	16:Q:82:VAL:HG22	2.02	0.41
68:RR:119:VAL:O	68:RR:119:VAL:HG13	2.20	0.41
47:5:1546:C:N3	47:5:1612:G:O6	2.54	0.41
50:9:1599:U:O4'	50:9:1599:U:O2	2.38	0.41
2:B:317:LEU:HD21	2:B:381:THR:HA	2.03	0.41
53:CC:108:LYS:CB	53:CC:233:LEU:HD23	2.50	0.41
56:FF:35:LEU:HD22	56:FF:147:VAL:HG23	2.02	0.41
7:G:215:ASP:HB3	7:G:216:PRO:HD3	2.02	0.41
9:I:36:LEU:HD12	9:I:87:ILE:HB	2.03	0.41
25:Z:100:VAL:HG13	25:Z:106:LEU:HB3	2.02	0.41
46:3:75:C:O2	46:3:75:C:O4'	2.34	0.41
47:5:100:C:O2	47:5:100:C:O4'	2.36	0.41
47:5:1879:C:O2'	47:5:1891:A:N3	2.47	0.41
47:5:2638:G:C2	47:5:2639:U:C4	3.08	0.41
15:P:79:THR:HG21	47:5:4569:U:O2	2.20	0.41
47:5:4758:U:O4'	47:5:4758:U:O2	2.37	0.41
55:EE:44:LEU:HD21	55:EE:70:ILE:HG21	2.02	0.41
7:G:105:THR:HG22	23:X:41:ARG:HD3	2.02	0.41
3:C:38:ASN:O	3:C:42:THR:HG23	2.20	0.41
55:EE:150:PRO:HA	55:EE:169:ILE:HD11	2.02	0.41
61:KK:15:LEU:HD22	61:KK:49:MET:HE1	2.02	0.41
14:O:156:LEU:HD22	47:5:4910:A:C8	2.55	0.41
65:OO:44:VAL:HG23	65:OO:81:VAL:HG11	2.03	0.41
65:OO:95:ILE:HD13	65:OO:116:LEU:HD21	2.02	0.41
7:G:98:ILE:HG21	47:5:4125:C:H4'	2.01	0.41
47:5:716:C:H2'	47:5:717:U:O4'	2.21	0.41
50:9:1566:G:N7	70:TT:101:ARG:NH2	2.69	0.41
51:AA:134:LEU:HD23	51:AA:144:THR:HG21	2.02	0.41
4:D:244:HIS:O	4:D:248:ARG:HG2	2.20	0.41
12:M:36:ALA:HB2	12:M:52:PHE:CE1	2.55	0.41
47:5:4729:A:O4'	47:5:4966:A:C8	2.74	0.41
50:9:556:U:H2'	50:9:557:U:O4'	2.21	0.41
53:CC:130:ILE:HG22	53:CC:158:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:CC:177:PRO:HD3	72:VV:9:VAL:HG21	2.02	0.41
54:DD:115:VAL:HG21	54:DD:142:LEU:HD23	2.03	0.41
58:HH:66:VAL:N	58:HH:67:PRO:CD	2.83	0.41
16:Q:85:THR:HG22	16:Q:104:ARG:HB2	2.03	0.41
24:Y:79:VAL:HG21	24:Y:98:GLY:HA3	2.03	0.41
50:9:441:C:H2'	50:9:442:C:C6	2.56	0.41
2:B:10:ARG:C	2:B:10:ARG:CD	2.89	0.41
3:C:198:ASN:N	3:C:198:ASN:OD1	2.53	0.41
53:CC:196:ILE:HB	53:CC:223:TYR:HB2	2.02	0.41
56:FF:87:LEU:CD2	67:QQ:47:LEU:HD13	2.51	0.41
61:KK:71:LEU:HD21	61:KK:79:LEU:HD12	2.03	0.41
47:5:1074:G:C2	47:5:1238:A:C2	3.09	0.41
49:8:15:G:C6	49:8:16:G:N1	2.89	0.41
50:9:1256:G:O6	71:UU:65:THR:HG22	2.21	0.41
3:C:130:ALA:HB3	3:C:246:VAL:HG12	2.03	0.41
6:F:115:GLN:CG	16:Q:3:VAL:HG22	2.50	0.41
13:N:108:ARG:NH2	13:N:161:MET:HE1	2.36	0.41
47:5:2267:U:O4'	47:5:2267:U:O2	2.37	0.40
47:5:2396:A:N6	47:5:2814:C:O2	2.54	0.40
47:5:3871:A:H2'	47:5:3872:A:O4'	2.21	0.40
50:9:92:A:H2'	50:9:446:G:N2	2.36	0.40
50:9:584:A:H62	50:9:585:C:N4	2.17	0.40
50:9:1650:A:H5''	67:QQ:139:ALA:HB2	2.02	0.40
76:ZZ:92:LEU:HD11	76:ZZ:99:LEU:HD12	2.02	0.40
47:5:4303:C:O2	47:5:4303:C:O4'	2.37	0.40
47:5:4579:U:H2'	47:5:4580:U:O4'	2.21	0.40
6:F:131:MET:HA	6:F:134:ILE:HG22	2.03	0.40
47:5:2750:G:H2'	47:5:2751:G:O4'	2.22	0.40
50:9:919:A:C2	50:9:1020:A:C4	3.10	0.40
52:BB:103:MET:SD	52:BB:188:LEU:HD22	2.61	0.40
61:KK:43:LEU:HD12	61:KK:43:LEU:C	2.42	0.40
68:RR:24:LEU:HD22	68:RR:54:VAL:HG11	2.02	0.40
54:DD:11:PHE:CZ	71:UU:84:ILE:HD11	2.57	0.40
75:YY:27:VAL:HG21	75:YY:40:ILE:HD11	2.03	0.40
47:5:2367:A:C6	47:5:2788:U:C4	3.10	0.40
4:D:60:ILE:HD13	4:D:98:ALA:HB2	2.04	0.40
4:D:78:ALA:HB1	4:D:104:LEU:HD13	2.03	0.40
8:H:105:ILE:HG22	8:H:112:VAL:HG22	2.03	0.40
9:I:14:ASN:O	9:I:128:ARG:NH2	2.53	0.40
67:QQ:34:VAL:HG21	67:QQ:84:ILE:HD12	2.04	0.40
18:S:97:TYR:CZ	18:S:109:CYS:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:4459:U:H2'	47:5:4460:U:C6	2.56	0.40
50:9:823:U:O5'	50:9:823:U:O2	2.40	0.40
50:9:964:A:N3	50:9:1054:G:O2'	2.41	0.40
64:NN:33:VAL:HG21	64:NN:66:VAL:HG11	2.03	0.40
18:S:154:LEU:HD13	18:S:157:ARG:NH1	2.37	0.40
71:UU:102:THR:HG21	71:UU:114:VAL:HG21	2.04	0.40
21:V:3:LYS:HD2	21:V:3:LYS:O	2.21	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	A	246/257 (96%)	225 (92%)	19 (8%)	2 (1%)	24	63
2	B	392/403 (97%)	364 (93%)	25 (6%)	3 (1%)	24	63
3	C	360/425 (85%)	337 (94%)	21 (6%)	2 (1%)	30	69
4	D	291/297 (98%)	275 (94%)	14 (5%)	2 (1%)	26	66
5	E	208/291 (72%)	189 (91%)	18 (9%)	1 (0%)	34	72
6	F	223/247 (90%)	211 (95%)	11 (5%)	1 (0%)	39	76
7	G	229/319 (72%)	217 (95%)	12 (5%)	0	100	100
8	H	188/192 (98%)	173 (92%)	15 (8%)	0	100	100
9	I	201/214 (94%)	185 (92%)	16 (8%)	0	100	100
10	J	168/178 (94%)	158 (94%)	10 (6%)	0	100	100
11	L	208/211 (99%)	198 (95%)	10 (5%)	0	100	100
12	M	136/218 (62%)	126 (93%)	10 (7%)	0	100	100
13	N	201/204 (98%)	190 (94%)	11 (6%)	0	100	100
14	O	197/203 (97%)	189 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	P	151/184 (82%)	145 (96%)	6 (4%)	0	100	100
16	Q	185/188 (98%)	175 (95%)	9 (5%)	1 (0%)	34	72
17	R	178/196 (91%)	172 (97%)	6 (3%)	0	100	100
18	S	174/176 (99%)	160 (92%)	12 (7%)	2 (1%)	17	57
19	T	157/160 (98%)	146 (93%)	10 (6%)	1 (1%)	30	69
20	U	97/128 (76%)	86 (89%)	11 (11%)	0	100	100
21	V	137/140 (98%)	125 (91%)	12 (9%)	0	100	100
22	W	102/157 (65%)	98 (96%)	3 (3%)	1 (1%)	19	59
23	X	116/156 (74%)	113 (97%)	3 (3%)	0	100	100
24	Y	132/145 (91%)	125 (95%)	7 (5%)	0	100	100
25	Z	133/136 (98%)	126 (95%)	5 (4%)	2 (2%)	13	49
26	a	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
27	b	100/245 (41%)	93 (93%)	6 (6%)	1 (1%)	19	59
28	c	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
29	d	105/125 (84%)	94 (90%)	10 (10%)	1 (1%)	19	59
30	e	126/135 (93%)	118 (94%)	8 (6%)	0	100	100
31	f	107/110 (97%)	101 (94%)	4 (4%)	2 (2%)	10	45
32	g	112/116 (97%)	106 (95%)	6 (5%)	0	100	100
33	h	120/123 (98%)	118 (98%)	1 (1%)	1 (1%)	24	63
34	i	100/105 (95%)	95 (95%)	5 (5%)	0	100	100
35	j	84/97 (87%)	78 (93%)	6 (7%)	0	100	100
36	k	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
37	l	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
38	m	50/102 (49%)	47 (94%)	3 (6%)	0	100	100
39	n	23/25 (92%)	23 (100%)	0	0	100	100
40	o	102/106 (96%)	99 (97%)	3 (3%)	0	100	100
41	p	89/92 (97%)	80 (90%)	8 (9%)	1 (1%)	17	57
42	r	122/137 (89%)	110 (90%)	11 (9%)	1 (1%)	24	63
43	s	194/318 (61%)	171 (88%)	22 (11%)	1 (0%)	34	72
44	t	151/165 (92%)	134 (89%)	13 (9%)	4 (3%)	7	37
51	AA	215/295 (73%)	204 (95%)	10 (5%)	1 (0%)	34	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	BB	211/264 (80%)	199 (94%)	11 (5%)	1 (0%)	34	72
53	CC	219/293 (75%)	205 (94%)	13 (6%)	1 (0%)	34	72
54	DD	226/243 (93%)	214 (95%)	9 (4%)	3 (1%)	15	53
55	EE	260/263 (99%)	246 (95%)	14 (5%)	0	100	100
56	FF	181/204 (89%)	166 (92%)	11 (6%)	4 (2%)	8	41
57	GG	235/249 (94%)	224 (95%)	10 (4%)	1 (0%)	39	76
58	HH	181/194 (93%)	171 (94%)	10 (6%)	0	100	100
59	II	204/208 (98%)	192 (94%)	11 (5%)	1 (0%)	34	72
60	JJ	183/194 (94%)	177 (97%)	5 (3%)	1 (0%)	34	72
61	KK	94/165 (57%)	88 (94%)	5 (5%)	1 (1%)	17	57
62	LL	139/158 (88%)	129 (93%)	10 (7%)	0	100	100
63	MM	115/132 (87%)	103 (90%)	12 (10%)	0	100	100
64	NN	147/151 (97%)	141 (96%)	6 (4%)	0	100	100
65	OO	134/168 (80%)	122 (91%)	10 (8%)	2 (2%)	13	49
66	PP	127/145 (88%)	117 (92%)	9 (7%)	1 (1%)	24	63
67	QQ	140/146 (96%)	130 (93%)	10 (7%)	0	100	100
68	RR	130/135 (96%)	118 (91%)	11 (8%)	1 (1%)	24	63
69	SS	142/152 (93%)	134 (94%)	8 (6%)	0	100	100
70	TT	139/145 (96%)	132 (95%)	7 (5%)	0	100	100
71	UU	98/119 (82%)	89 (91%)	9 (9%)	0	100	100
72	VV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
73	WW	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
74	XX	139/143 (97%)	129 (93%)	8 (6%)	2 (1%)	14	50
75	YY	122/130 (94%)	116 (95%)	5 (4%)	1 (1%)	24	63
76	ZZ	73/125 (58%)	71 (97%)	2 (3%)	0	100	100
77	aa	99/115 (86%)	90 (91%)	8 (8%)	1 (1%)	19	59
78	bb	81/84 (96%)	75 (93%)	5 (6%)	1 (1%)	16	54
79	cc	60/69 (87%)	59 (98%)	1 (2%)	0	100	100
80	dd	53/56 (95%)	49 (92%)	3 (6%)	1 (2%)	10	45
81	ee	55/133 (41%)	52 (94%)	3 (6%)	0	100	100
82	ff	66/156 (42%)	61 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
83	gg	311/317 (98%)	282 (91%)	28 (9%)	1 (0%)	46	81
85	jj	438/462 (95%)	419 (96%)	18 (4%)	1 (0%)	52	85
All	All	11976/13836 (87%)	11207 (94%)	713 (6%)	56 (0%)	38	72

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
44	t	120	SER
44	t	125	LEU
74	XX	62	PRO
74	XX	86	PRO
3	C	83	GLY
16	Q	14	ARG
33	h	89	ARG
43	s	142	GLY
56	FF	77	MET
60	JJ	147	PHE
66	PP	80	LEU
2	B	17	LEU
5	E	69	ALA
25	Z	91	LEU
29	d	58	GLY
31	f	107	PRO
51	AA	159	ILE
56	FF	43	GLU
56	FF	80	GLY
75	YY	126	GLY
1	A	196	TRP
2	B	259	PRO
4	D	44	TYR
18	S	53	LYS
18	S	155	PRO
27	b	102	PRO
44	t	54	LYS
54	DD	93	THR
61	KK	41	PRO
65	OO	20	GLN
85	jj	259	ILE
1	A	14	SER
2	B	258	HIS
6	F	236	GLU

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Mol	Chain	Res	Type
25	Z	90	PRO
31	f	106	TYR
42	r	33	LYS
54	DD	44	THR
57	GG	135	PRO
77	aa	47	ALA
80	dd	7	TYR
19	T	81	LYS
56	FF	21	GLY
78	bb	81	ARG
44	t	51	GLY
53	CC	171	GLY
65	OO	30	VAL
68	RR	119	VAL
83	gg	224	GLY
41	p	9	GLY
59	II	3	ILE
3	C	90	GLY
4	D	125	VAL
22	W	3	VAL
52	BB	93	GLY
54	DD	48	ILE

### 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	A	190/199 (96%)	176 (93%)	14 (7%)	17	52
2	B	342/348 (98%)	324 (95%)	18 (5%)	28	66
3	C	302/347 (87%)	281 (93%)	21 (7%)	19	56
4	D	247/250 (99%)	234 (95%)	13 (5%)	28	66
5	E	190/251 (76%)	180 (95%)	10 (5%)	28	66
6	F	196/215 (91%)	184 (94%)	12 (6%)	23	61
7	G	200/272 (74%)	189 (94%)	11 (6%)	27	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	169/171 (99%)	156 (92%)	13 (8%)	16	51
9	I	175/181 (97%)	161 (92%)	14 (8%)	15	49
10	J	143/149 (96%)	137 (96%)	6 (4%)	36	73
11	L	175/176 (99%)	166 (95%)	9 (5%)	29	67
12	M	117/161 (73%)	108 (92%)	9 (8%)	16	51
13	N	171/172 (99%)	161 (94%)	10 (6%)	25	63
14	O	171/173 (99%)	159 (93%)	12 (7%)	19	56
15	P	134/163 (82%)	125 (93%)	9 (7%)	20	58
16	Q	164/165 (99%)	151 (92%)	13 (8%)	15	49
17	R	159/175 (91%)	145 (91%)	14 (9%)	12	43
18	S	157/157 (100%)	147 (94%)	10 (6%)	22	59
19	T	139/140 (99%)	130 (94%)	9 (6%)	21	59
20	U	89/114 (78%)	87 (98%)	2 (2%)	60	84
21	V	106/107 (99%)	92 (87%)	14 (13%)	5	22
22	W	86/126 (68%)	85 (99%)	1 (1%)	78	90
23	X	106/134 (79%)	99 (93%)	7 (7%)	21	58
24	Y	124/135 (92%)	118 (95%)	6 (5%)	31	69
25	Z	117/118 (99%)	115 (98%)	2 (2%)	68	86
26	a	119/120 (99%)	114 (96%)	5 (4%)	36	73
27	b	84/184 (46%)	81 (96%)	3 (4%)	42	76
28	c	84/98 (86%)	80 (95%)	4 (5%)	31	69
29	d	98/110 (89%)	88 (90%)	10 (10%)	9	35
30	e	114/121 (94%)	105 (92%)	9 (8%)	15	49
31	f	88/89 (99%)	82 (93%)	6 (7%)	20	57
32	g	98/99 (99%)	92 (94%)	6 (6%)	23	61
33	h	109/110 (99%)	105 (96%)	4 (4%)	41	75
34	i	86/89 (97%)	82 (95%)	4 (5%)	32	70
35	j	73/80 (91%)	67 (92%)	6 (8%)	14	48
36	k	64/65 (98%)	62 (97%)	2 (3%)	47	79
37	l	47/48 (98%)	46 (98%)	1 (2%)	61	84
38	m	48/90 (53%)	46 (96%)	2 (4%)	36	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	n	24/24 (100%)	21 (88%)	3 (12%)	6	24
40	o	92/94 (98%)	88 (96%)	4 (4%)	35	72
41	p	74/75 (99%)	71 (96%)	3 (4%)	37	73
42	r	108/121 (89%)	100 (93%)	8 (7%)	17	52
43	s	164/258 (64%)	154 (94%)	10 (6%)	23	61
44	t	126/137 (92%)	122 (97%)	4 (3%)	46	79
51	AA	180/245 (74%)	167 (93%)	13 (7%)	18	54
52	BB	194/231 (84%)	173 (89%)	21 (11%)	8	32
53	CC	187/225 (83%)	175 (94%)	12 (6%)	22	59
54	DD	190/202 (94%)	175 (92%)	15 (8%)	15	49
55	EE	224/225 (100%)	205 (92%)	19 (8%)	13	46
56	FF	158/170 (93%)	146 (92%)	12 (8%)	16	51
57	GG	207/218 (95%)	195 (94%)	12 (6%)	25	63
58	HH	165/174 (95%)	154 (93%)	11 (7%)	20	58
59	II	178/180 (99%)	167 (94%)	11 (6%)	23	60
60	JJ	161/168 (96%)	149 (92%)	12 (8%)	17	52
61	KK	87/136 (64%)	78 (90%)	9 (10%)	9	34
62	LL	130/142 (92%)	114 (88%)	16 (12%)	6	25
63	MM	99/108 (92%)	87 (88%)	12 (12%)	6	26
64	NN	130/131 (99%)	118 (91%)	12 (9%)	11	40
65	OO	106/130 (82%)	96 (91%)	10 (9%)	11	39
66	PP	115/130 (88%)	104 (90%)	11 (10%)	10	38
67	QQ	117/121 (97%)	108 (92%)	9 (8%)	16	51
68	RR	119/121 (98%)	109 (92%)	10 (8%)	14	46
69	SS	125/132 (95%)	112 (90%)	13 (10%)	9	33
70	TT	111/115 (96%)	101 (91%)	10 (9%)	12	42
71	UU	92/107 (86%)	87 (95%)	5 (5%)	27	66
72	VV	67/67 (100%)	63 (94%)	4 (6%)	24	62
73	WW	112/113 (99%)	104 (93%)	8 (7%)	18	55
74	XX	113/115 (98%)	110 (97%)	3 (3%)	52	81
75	YY	107/112 (96%)	98 (92%)	9 (8%)	14	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
76	ZZ	66/103 (64%)	59 (89%)	7 (11%)	8	32
77	aa	88/98 (90%)	82 (93%)	6 (7%)	20	57
78	bb	75/76 (99%)	69 (92%)	6 (8%)	15	49
79	cc	55/62 (89%)	49 (89%)	6 (11%)	8	31
80	dd	48/49 (98%)	46 (96%)	2 (4%)	36	73
81	ee	47/106 (44%)	44 (94%)	3 (6%)	22	59
82	ff	61/140 (44%)	53 (87%)	8 (13%)	5	22
83	gg	272/275 (99%)	264 (97%)	8 (3%)	50	80
85	jj	365/378 (97%)	353 (97%)	12 (3%)	45	78
All	All	10420/11716 (89%)	9730 (93%)	690 (7%)	25	58

All (690) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	64	ARG
1	A	102	LEU
1	A	109	GLU
1	A	128	ARG
1	A	163	ARG
1	A	175	ILE
1	A	198	ARG
1	A	200	ARG
1	A	221	LYS
1	A	233	ARG
1	A	235	VAL
1	A	242	ARG
1	A	243	THR
2	B	10	ARG
2	B	17	LEU
2	B	53	MET
2	B	62	ARG
2	B	66	LYS
2	B	74	GLU
2	B	135	LYS
2	B	173	LEU
2	B	204	GLN
2	B	248	LEU
2	B	262	VAL

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Mol	Chain	Res	Type
2	B	279	GLU
2	B	294	LYS
2	B	309	LEU
2	B	333	LEU
2	B	351	LEU
2	B	356	LYS
2	B	383	GLU
3	C	20	LYS
3	C	29	LYS
3	C	89	GLN
3	C	95	MET
3	C	101	MET
3	C	113	ARG
3	C	122	TYR
3	C	124	ILE
3	C	144	ILE
3	C	150	LEU
3	C	165	LYS
3	C	175	LYS
3	C	188	ARG
3	C	193	LYS
3	C	198	ASN
3	C	246	VAL
3	C	281	MET
3	C	284	MET
3	C	307	LYS
3	C	312	ARG
3	C	333	LYS
4	D	33	ARG
4	D	37	VAL
4	D	50	ARG
4	D	56	THR
4	D	89	LYS
4	D	104	LEU
4	D	110	LEU
4	D	124	GLU
4	D	202	GLN
4	D	208	MET
4	D	264	LYS
4	D	268	ARG
4	D	279	ARG
5	E	52	LEU

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Mol	Chain	Res	Type
5	E	58	ARG
5	E	112	LEU
5	E	141	ARG
5	E	144	ARG
5	E	169	LYS
5	E	178	VAL
5	E	213	LYS
5	E	289	LEU
5	E	291	PHE
6	F	30	LYS
6	F	46	ARG
6	F	65	ARG
6	F	67	GLU
6	F	88	LEU
6	F	134	ILE
6	F	151	GLU
6	F	187	GLU
6	F	198	LYS
6	F	211	LYS
6	F	231	ASP
6	F	245	ARG
7	G	126	ARG
7	G	148	LEU
7	G	184	LYS
7	G	203	LYS
7	G	204	LYS
7	G	223	LEU
7	G	226	LEU
7	G	230	MET
7	G	242	ARG
7	G	273	GLU
7	G	293	ASN
8	H	1	MET
8	H	20	LEU
8	H	23	ARG
8	H	52	LYS
8	H	54	ARG
8	H	59	LYS
8	H	66	GLU
8	H	74	CYS
8	H	105	ILE
8	H	106	GLN

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Mol	Chain	Res	Type
8	H	128	MET
8	H	173	ARG
8	H	177	ASP
9	I	13	LYS
9	I	36	LEU
9	I	39	LYS
9	I	44	ASP
9	I	71	CYS
9	I	116	ARG
9	I	146	GLU
9	I	153	ARG
9	I	154	ARG
9	I	163	GLN
9	I	164	LYS
9	I	183	ASP
9	I	208	LYS
9	I	212	LEU
10	J	16	ARG
10	J	28	GLU
10	J	33	LEU
10	J	81	GLU
10	J	113	ILE
10	J	175	LEU
11	L	10	LEU
11	L	35	ARG
11	L	63	THR
11	L	67	HIS
11	L	74	ARG
11	L	121	ARG
11	L	162	LYS
11	L	186	ARG
11	L	195	ARG
12	M	2	VAL
12	M	8	GLU
12	M	32	ASP
12	M	37	LEU
12	M	57	LEU
12	M	62	LEU
12	M	96	GLU
12	M	105	THR
12	M	119	ARG
13	N	9	GLU

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Mol	Chain	Res	Type
13	N	26	ARG
13	N	54	LYS
13	N	64	ILE
13	N	72	LYS
13	N	87	HIS
13	N	89	VAL
13	N	162	ARG
13	N	182	HIS
13	N	199	GLN
14	O	36	VAL
14	O	37	ARG
14	O	67	SER
14	O	74	ARG
14	O	82	ARG
14	O	128	ARG
14	O	130	LYS
14	O	140	ARG
14	O	145	VAL
14	O	175	MET
14	O	179	LYS
14	O	202	LEU
15	P	25	HIS
15	P	57	CYS
15	P	69	ARG
15	P	86	LYS
15	P	91	LEU
15	P	127	ARG
15	P	128	ARG
15	P	144	CYS
15	P	147	GLU
16	Q	22	ASP
16	Q	31	LEU
16	Q	38	ARG
16	Q	61	LEU
16	Q	63	LEU
16	Q	75	ARG
16	Q	91	ARG
16	Q	97	LYS
16	Q	115	LYS
16	Q	140	SER
16	Q	143	ARG
16	Q	172	ARG

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Mol	Chain	Res	Type
16	Q	180	ARG
17	R	6	LEU
17	R	34	ASN
17	R	36	ASN
17	R	40	GLN
17	R	89	MET
17	R	98	ARG
17	R	99	MET
17	R	113	LYS
17	R	133	LYS
17	R	138	LEU
17	R	148	ASP
17	R	176	ARG
17	R	178	GLN
17	R	180	LYS
18	S	9	GLU
18	S	17	LEU
18	S	24	THR
18	S	67	VAL
18	S	70	LYS
18	S	82	LEU
18	S	83	ARG
18	S	149	LYS
18	S	159	LEU
18	S	174	THR
19	T	5	LYS
19	T	7	LYS
19	T	33	ILE
19	T	60	LYS
19	T	96	ILE
19	T	117	LYS
19	T	144	ASN
19	T	146	LYS
19	T	159	MET
20	U	33	ILE
20	U	80	LYS
21	V	2	SER
21	V	3	LYS
21	V	6	ARG
21	V	15	ARG
21	V	18	LEU
21	V	35	LYS

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Mol	Chain	Res	Type
21	V	46	LYS
21	V	59	ASP
21	V	60	MET
21	V	82	ILE
21	V	91	LYS
21	V	99	GLU
21	V	109	LYS
21	V	123	LYS
22	W	91	MET
23	X	39	LYS
23	X	50	LYS
23	X	53	ARG
23	X	59	LYS
23	X	63	LYS
23	X	95	THR
23	X	111	GLN
24	Y	2	LYS
24	Y	8	THR
24	Y	50	ARG
24	Y	72	GLN
24	Y	74	TYR
24	Y	104	VAL
25	Z	33	THR
25	Z	112	ARG
26	a	4	ARG
26	a	59	ARG
26	a	84	GLU
26	a	122	VAL
26	a	132	ARG
27	b	9	THR
27	b	40	LEU
27	b	101	HIS
28	c	37	MET
28	c	50	ASN
28	c	65	MET
28	c	78	ASN
29	d	23	ARG
29	d	26	THR
29	d	31	LYS
29	d	44	ARG
29	d	48	GLU
29	d	78	ARG

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Mol	Chain	Res	Type
29	d	79	ASN
29	d	83	ARG
29	d	85	ARG
29	d	98	SER
30	e	21	ILE
30	e	22	ARG
30	e	48	ARG
30	e	64	LYS
30	e	78	LEU
30	e	86	GLU
30	e	106	LYS
30	e	113	GLU
30	e	128	ARG
31	f	7	CYS
31	f	16	ARG
31	f	33	VAL
31	f	52	LYS
31	f	80	ASN
31	f	101	ILE
32	g	53	LEU
32	g	54	ARG
32	g	60	ARG
32	g	66	ARG
32	g	73	HIS
32	g	114	GLN
33	h	28	LEU
33	h	67	GLU
33	h	77	LYS
33	h	89	ARG
34	i	33	LEU
34	i	34	THR
34	i	77	VAL
34	i	86	LYS
35	j	3	LYS
35	j	11	ARG
35	j	20	ARG
35	j	37	CYS
35	j	58	THR
35	j	63	ARG
36	k	69	LEU
36	k	70	LYS
37	l	11	ARG

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Mol	Chain	Res	Type
38	m	71	ARG
38	m	93	ASN
39	n	1	MET
39	n	2	ARG
39	n	13	LEU
40	o	17	LYS
40	o	36	GLN
40	o	61	LYS
40	o	82	MET
41	p	8	VAL
41	p	30	GLU
41	p	84	ARG
42	r	8	MET
42	r	18	ILE
42	r	32	LEU
42	r	39	ARG
42	r	67	ARG
42	r	80	THR
42	r	103	HIS
42	r	118	LEU
43	s	38	LYS
43	s	44	ARG
43	s	61	MET
43	s	68	HIS
43	s	95	LEU
43	s	105	ASN
43	s	146	LYS
43	s	149	ARG
43	s	187	LEU
43	s	191	GLN
44	t	37	LEU
44	t	98	ILE
44	t	133	LEU
44	t	144	ASP
51	AA	12	GLU
51	AA	32	PHE
51	AA	50	ASN
51	AA	58	LEU
51	AA	59	LEU
51	AA	60	LEU
51	AA	109	THR
51	AA	111	GLN

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Mol	Chain	Res	Type
51	AA	132	GLN
51	AA	136	GLU
51	AA	178	LEU
51	AA	192	GLU
51	AA	200	ASP
52	BB	29	ASP
52	BB	50	THR
52	BB	71	LEU
52	BB	73	ASP
52	BB	82	ARG
52	BB	88	THR
52	BB	92	GLN
52	BB	105	LEU
52	BB	107	ARG
52	BB	125	VAL
52	BB	126	ASP
52	BB	129	THR
52	BB	157	GLN
52	BB	175	GLU
52	BB	181	LEU
52	BB	205	TYR
52	BB	207	LEU
52	BB	209	ASP
52	BB	213	ARG
52	BB	225	LEU
52	BB	231	LEU
53	CC	78	LEU
53	CC	114	LYS
53	CC	117	ARG
53	CC	121	ARG
53	CC	137	VAL
53	CC	146	GLU
53	CC	167	ARG
53	CC	192	LEU
53	CC	196	ILE
53	CC	247	THR
53	CC	248	TYR
53	CC	252	THR
54	DD	28	GLU
54	DD	45	ARG
54	DD	65	ARG
54	DD	76	ARG

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Mol	Chain	Res	Type
54	DD	106	ARG
54	DD	123	LEU
54	DD	127	MET
54	DD	142	LEU
54	DD	167	TYR
54	DD	168	VAL
54	DD	179	GLN
54	DD	216	GLU
54	DD	218	LEU
54	DD	223	ILE
54	DD	227	LYS
55	EE	21	ASP
55	EE	42	LEU
55	EE	49	ARG
55	EE	50	ASN
55	EE	51	ARG
55	EE	65	CYS
55	EE	67	GLN
55	EE	77	ARG
55	EE	81	THR
55	EE	133	THR
55	EE	196	THR
55	EE	200	ARG
55	EE	205	PHE
55	EE	206	ASP
55	EE	222	LEU
55	EE	232	ASN
55	EE	238	LEU
55	EE	246	LEU
55	EE	260	GLN
56	FF	19	LEU
56	FF	29	GLN
56	FF	49	LEU
56	FF	55	ARG
56	FF	71	ARG
56	FF	88	MET
56	FF	89	THR
56	FF	91	ARG
56	FF	95	HIS
56	FF	124	ASP
56	FF	135	ARG
56	FF	140	ASP

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Mol	Chain	Res	Type
57	GG	15	LEU
57	GG	31	ARG
57	GG	41	LEU
57	GG	63	MET
57	GG	67	VAL
57	GG	129	VAL
57	GG	171	THR
57	GG	178	ARG
57	GG	183	ARG
57	GG	190	ARG
57	GG	208	GLU
57	GG	216	ARG
58	HH	8	ILE
58	HH	36	LEU
58	HH	50	GLU
58	HH	72	PHE
58	HH	76	GLN
58	HH	82	GLU
58	HH	100	ILE
58	HH	121	THR
58	HH	145	ARG
58	HH	149	ASP
58	HH	160	LYS
59	II	12	ARG
59	II	26	LYS
59	II	69	SER
59	II	73	THR
59	II	74	ARG
59	II	100	CYS
59	II	121	LEU
59	II	130	THR
59	II	145	ILE
59	II	178	ARG
59	II	190	LEU
60	JJ	18	ARG
60	JJ	29	LEU
60	JJ	45	ARG
60	JJ	50	LEU
60	JJ	69	ARG
60	JJ	70	ARG
60	JJ	79	ARG
60	JJ	89	GLU

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Mol	Chain	Res	Type
60	JJ	94	LEU
60	JJ	108	ARG
60	JJ	110	LEU
60	JJ	133	ARG
61	KK	1	MET
61	KK	6	LYS
61	KK	29	MET
61	KK	40	VAL
61	KK	50	GLN
61	KK	54	SER
61	KK	60	GLU
61	KK	89	ILE
61	KK	96	ARG
62	LL	16	ILE
62	LL	20	LYS
62	LL	23	VAL
62	LL	39	ASN
62	LL	40	ILE
62	LL	42	LEU
62	LL	49	GLU
62	LL	56	ILE
62	LL	69	ARG
62	LL	78	THR
62	LL	85	THR
62	LL	91	ASP
62	LL	121	GLN
62	LL	126	VAL
62	LL	132	ARG
62	LL	134	LEU
63	MM	19	GLN
63	MM	24	THR
63	MM	31	LEU
63	MM	33	ARG
63	MM	36	ARG
63	MM	40	LYS
63	MM	42	LEU
63	MM	55	ASN
63	MM	85	LEU
63	MM	96	ARG
63	MM	99	LYS
63	MM	101	ARG
64	NN	13	GLN

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Mol	Chain	Res	Type
64	NN	20	ARG
64	NN	27	LYS
64	NN	53	ILE
64	NN	55	ARG
64	NN	60	VAL
64	NN	70	LYS
64	NN	78	LYS
64	NN	84	LEU
64	NN	86	GLU
64	NN	107	LYS
64	NN	132	LYS
65	OO	34	PHE
65	OO	50	LYS
65	OO	51	GLU
65	OO	56	VAL
65	OO	85	CYS
65	OO	119	LEU
65	OO	131	ASP
65	OO	146	ARG
65	OO	150	ARG
65	OO	151	LEU
66	PP	13	ARG
66	PP	15	PHE
66	PP	27	ASP
66	PP	37	TYR
66	PP	43	ARG
66	PP	44	ARG
66	PP	76	VAL
66	PP	83	MET
66	PP	101	THR
66	PP	108	LYS
66	PP	130	ARG
67	QQ	7	LEU
67	QQ	31	LEU
67	QQ	41	MET
67	QQ	46	THR
67	QQ	50	LYS
67	QQ	53	GLU
67	QQ	60	LYS
67	QQ	138	ARG
67	QQ	140	ARG
68	RR	5	ARG

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Mol	Chain	Res	Type
68	RR	31	ASN
68	RR	33	ARG
68	RR	62	GLN
68	RR	78	ARG
68	RR	82	ASP
68	RR	93	GLN
68	RR	99	ASP
68	RR	105	MET
68	RR	132	ARG
69	SS	8	LYS
69	SS	23	ARG
69	SS	46	ARG
69	SS	59	LEU
69	SS	60	THR
69	SS	63	GLU
69	SS	83	PHE
69	SS	86	ARG
69	SS	101	ASN
69	SS	108	ARG
69	SS	110	ASP
69	SS	132	ARG
69	SS	145	THR
70	TT	5	THR
70	TT	28	LEU
70	TT	62	ARG
70	TT	102	ARG
70	TT	108	GLU
70	TT	110	LEU
70	TT	121	ARG
70	TT	123	LEU
70	TT	124	THR
70	TT	142	LYS
71	UU	44	LYS
71	UU	56	MET
71	UU	76	THR
71	UU	105	SER
71	UU	106	ILE
72	VV	12	TYR
72	VV	20	SER
72	VV	51	LYS
72	VV	66	ASP
73	WW	23	ARG

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Mol	Chain	Res	Type
73	WW	36	ARG
73	WW	51	GLU
73	WW	83	LEU
73	WW	85	ASP
73	WW	90	GLN
73	WW	104	LEU
73	WW	106	THR
74	XX	67	ARG
74	XX	105	PHE
74	XX	115	ILE
75	YY	16	ARG
75	YY	17	LEU
75	YY	32	LYS
75	YY	40	ILE
75	YY	47	MET
75	YY	61	ARG
75	YY	74	MET
75	YY	80	ASP
75	YY	88	LYS
76	ZZ	64	ASN
76	ZZ	69	THR
76	ZZ	80	ARG
76	ZZ	89	GLN
76	ZZ	92	LEU
76	ZZ	99	LEU
76	ZZ	106	GLN
77	aa	21	ILE
77	aa	41	ILE
77	aa	55	GLU
77	aa	67	LEU
77	aa	95	ARG
77	aa	100	ARG
78	bb	29	ASN
78	bb	42	LYS
78	bb	64	CYS
78	bb	72	ARG
78	bb	80	ARG
78	bb	81	ARG
79	cc	27	CYS
79	cc	31	ARG
79	cc	40	ARG
79	cc	44	ARG

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Mol	Chain	Res	Type
79	cc	60	GLU
79	cc	68	LEU
80	dd	32	ARG
80	dd	38	MET
81	ee	98	LYS
81	ee	99	LYS
81	ee	107	ARG
82	ff	83	LYS
82	ff	86	THR
82	ff	94	LYS
82	ff	99	LYS
82	ff	110	GLU
82	ff	113	LYS
82	ff	138	ARG
82	ff	140	TYR
83	gg	11	LEU
83	gg	17	TRP
83	gg	20	GLN
83	gg	38	LYS
83	gg	119	GLN
83	gg	207	CYS
83	gg	273	GLU
83	gg	289	LEU
85	jj	30	LYS
85	jj	34	ILE
85	jj	75	ILE
85	jj	78	TRP
85	jj	85	TYR
85	jj	102	MET
85	jj	313	LYS
85	jj	321	ARG
85	jj	357	TYR
85	jj	362	ASP
85	jj	389	ASP
85	jj	392	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
19	T	144	ASN
83	gg	14	HIS
85	jj	343	GLN

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Mol	Chain	Res	Type
85	jj	367	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
45	2	73/76 (96%)	14 (19%)	1 (1%)
45	ii	74/76 (97%)	20 (27%)	0
46	3	72/75 (96%)	28 (38%)	2 (2%)
47	5	3514/3543 (99%)	869 (24%)	171 (4%)
48	7	118/120 (98%)	12 (10%)	1 (0%)
49	8	150/156 (96%)	34 (22%)	7 (4%)
50	9	1678/1869 (89%)	420 (25%)	65 (3%)
84	hh	9/10 (90%)	1 (11%)	0
All	All	5688/5925 (96%)	1398 (24%)	247 (4%)

All (1398) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
45	2	9	A
45	2	13	U
45	2	16	C
45	2	19	G
45	2	21	A
45	2	34	A
45	2	43	A
45	2	46	G
45	2	47	U
45	2	49	C
45	2	61	C
45	2	64	G
45	2	72	C
45	2	75	C
46	3	7	A
46	3	13	C
46	3	14	A
46	3	16	C
46	3	21	A
46	3	25	C
46	3	28	C
46	3	29	A
46	3	34	U

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Mol	Chain	Res	Type
46	3	35	U
46	3	36	U
46	3	40	C
46	3	42	G
46	3	47	U
46	3	49	C
46	3	51	G
46	3	58	A
46	3	60	U
46	3	61	C
46	3	63	C
46	3	65	G
46	3	69	G
46	3	70	G
46	3	71	G
46	3	72	C
46	3	74	C
46	3	75	C
46	3	76	A
47	5	6	C
47	5	12	A
47	5	13	U
47	5	15	A
47	5	25	A
47	5	30	C
47	5	35	U
47	5	39	A
47	5	40	G
47	5	42	A
47	5	43	U
47	5	44	A
47	5	48	G
47	5	49	U
47	5	56	A
47	5	58	G
47	5	59	A
47	5	64	A
47	5	65	A
47	5	73	A
47	5	75	G
47	5	91	G
47	5	93	G

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Mol	Chain	Res	Type
47	5	107	G
47	5	108	A
47	5	109	G
47	5	116	G
47	5	118	C
47	5	119	G
47	5	120	A
47	5	126	C
47	5	134	G
47	5	135	G
47	5	136	C
47	5	143	C
47	5	144	G
47	5	159	C
47	5	160	G
47	5	172	C
47	5	173	C
47	5	177	G
47	5	179	G
47	5	197	A
47	5	200	U
47	5	201	C
47	5	205	C
47	5	209	U
47	5	216	C
47	5	217	C
47	5	218	A
47	5	220	C
47	5	221	C
47	5	224	U
47	5	226	G
47	5	227	A
47	5	233	U
47	5	234	G
47	5	246	G
47	5	253	G
47	5	255	C
47	5	262	G
47	5	263	G
47	5	265	C
47	5	266	C
47	5	276	C

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Mol	Chain	Res	Type
47	5	278	G
47	5	279	A
47	5	280	G
47	5	297	U
47	5	306	A
47	5	309	C
47	5	310	G
47	5	315	G
47	5	316	U
47	5	322	C
47	5	334	A
47	5	340	C
47	5	350	C
47	5	354	U
47	5	357	U
47	5	363	A
47	5	365	U
47	5	379	G
47	5	386	A
47	5	387	G
47	5	399	G
47	5	407	A
47	5	408	A
47	5	409	G
47	5	410	A
47	5	412	G
47	5	413	G
47	5	431	G
47	5	432	U
47	5	446	C
47	5	449	C
47	5	450	G
47	5	452	A
47	5	453	G
47	5	454	U
47	5	455	C
47	5	457	G
47	5	464	G
47	5	466	A
47	5	467	U
47	5	468	U
47	5	469	C

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Mol	Chain	Res	Type
47	5	481	G
47	5	481(A)	C
47	5	482	G
47	5	483	G
47	5	484	U
47	5	485	C
47	5	486	C
47	5	492	U
47	5	493	G
47	5	495	C
47	5	497	G
47	5	498	C
47	5	499	G
47	5	505	G
47	5	510	U
47	5	649	A
47	5	654	C
47	5	658	C
47	5	667	A
47	5	668	C
47	5	669	C
47	5	670	G
47	5	672	C
47	5	683	C
47	5	684	G
47	5	685	C
47	5	687	U
47	5	696	C
47	5	697	G
47	5	704	C
47	5	705	G
47	5	708	G
47	5	719	C
47	5	722	G
47	5	729	G
47	5	730	G
47	5	731	G
47	5	734	G
47	5	738	C
47	5	738(A)	C
47	5	739	G
47	5	744	G

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Mol	Chain	Res	Type
47	5	747	A
47	5	748	G
47	5	749	G
47	5	756	G
47	5	758	G
47	5	911	U
47	5	913	U
47	5	914	U
47	5	917	A
47	5	918	G
47	5	922(B)	C
47	5	923	C
47	5	924	C
47	5	925	C
47	5	926	G
47	5	929	A
47	5	931	C
47	5	932	A
47	5	933	G
47	5	934	C
47	5	935	A
47	5	935(A)	G
47	5	936	C
47	5	937	U
47	5	939	G
47	5	941	C
47	5	944	A
47	5	945	U
47	5	956	A
47	5	959	G
47	5	960	A
47	5	961	G
47	5	962	C
47	5	963	G
47	5	964	A
47	5	965	G
47	5	966	A
47	5	967	C
47	5	968	C
47	5	969	C
47	5	972	C
47	5	973	G

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Mol	Chain	Res	Type
47	5	979	C
47	5	983	C
47	5	990	C
47	5	1072	C
47	5	1073	G
47	5	1075	G
47	5	1076	C
47	5	1078	A
47	5	1079	C
47	5	1082	C
47	5	1177	U
47	5	1179	U
47	5	1180	C
47	5	1184	A
47	5	1185	G
47	5	1195	G
47	5	1211	G
47	5	1212	G
47	5	1214	C
47	5	1215	C
47	5	1234	G
47	5	1235	G
47	5	1236	C
47	5	1237	C
47	5	1238	A
47	5	1239	C
47	5	1272	C
47	5	1273	G
47	5	1274	A
47	5	1275	G
47	5	1276	C
47	5	1280	C
47	5	1284	G
47	5	1285	U
47	5	1287	G
47	5	1288	G
47	5	1291	G
47	5	1292	C
47	5	1293	G
47	5	1295	U
47	5	1296	G
47	5	1301	C

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Mol	Chain	Res	Type
47	5	1303	A
47	5	1304	C
47	5	1326	A
47	5	1328	G
47	5	1329	G
47	5	1330	A
47	5	1337	A
47	5	1354	A
47	5	1359	G
47	5	1364	U
47	5	1370	G
47	5	1371	A
47	5	1377	G
47	5	1378	C
47	5	1379	C
47	5	1380	G
47	5	1381	U
47	5	1387	A
47	5	1394	G
47	5	1397	A
47	5	1398	A
47	5	1401	C
47	5	1403	G
47	5	1416	G
47	5	1419	G
47	5	1420	A
47	5	1421	G
47	5	1436	C
47	5	1437	C
47	5	1438	U
47	5	1441	C
47	5	1442	C
47	5	1445	U
47	5	1446	C
47	5	1453	G
47	5	1455	G
47	5	1456	C
47	5	1457	G
47	5	1458	C
47	5	1475	G
47	5	1477	C
47	5	1478	C

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Mol	Chain	Res	Type
47	5	1481	C
47	5	1482	G
47	5	1483	C
47	5	1484	G
47	5	1485	C
47	5	1486	C
47	5	1489	G
47	5	1497	A
47	5	1498	G
47	5	1502	G
47	5	1516	G
47	5	1518	A
47	5	1523	A
47	5	1534	A
47	5	1535	C
47	5	1547	A
47	5	1554	A
47	5	1563	A
47	5	1564	A
47	5	1566	C
47	5	1578	U
47	5	1591	U
47	5	1592	G
47	5	1596	U
47	5	1602	U
47	5	1612	G
47	5	1613	A
47	5	1624	G
47	5	1625	G
47	5	1626	G
47	5	1631	A
47	5	1633	G
47	5	1634	A
47	5	1640	C
47	5	1654	G
47	5	1661	C
47	5	1676	C
47	5	1677	U
47	5	1726	U
47	5	1729	A
47	5	1733	G
47	5	1734	G

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Mol	Chain	Res	Type
47	5	1741	G
47	5	1742	A
47	5	1750	G
47	5	1753	G
47	5	1755	C
47	5	1756	U
47	5	1757	U
47	5	1761	G
47	5	1763	C
47	5	1764	G
47	5	1768	C
47	5	1772	C
47	5	1773	U
47	5	1776	A
47	5	1781	U
47	5	1787	A
47	5	1797	G
47	5	1799	G
47	5	1803	G
47	5	1804	A
47	5	1805	A
47	5	1819	G
47	5	1821	G
47	5	1822	U
47	5	1828	C
47	5	1833	G
47	5	1834	U
47	5	1835	G
47	5	1836	G
47	5	1837	A
47	5	1842	G
47	5	1855	G
47	5	1867	A
47	5	1869	G
47	5	1897	A
47	5	1910	G
47	5	1918	U
47	5	1919	G
47	5	1920	C
47	5	1921	C
47	5	1922	G
47	5	1923	A

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Mol	Chain	Res	Type
47	5	1931	C
47	5	1933	G
47	5	1941	A
47	5	1948	G
47	5	1951	G
47	5	1952	G
47	5	1957	U
47	5	1959	U
47	5	1961	G
47	5	1962	A
47	5	1964	A
47	5	1965	G
47	5	1976	G
47	5	1977	C
47	5	1979	A
47	5	1980	U
47	5	1982	G
47	5	1983	A
47	5	1984	A
47	5	1986	U
47	5	1987	C
47	5	1988	G
47	5	1991	A
47	5	1993	C
47	5	1997	U
47	5	2001	G
47	5	2002	A
47	5	2003	G
47	5	2004	U
47	5	2007	G
47	5	2008	U
47	5	2009	A
47	5	2010	A
47	5	2011	C
47	5	2016	C
47	5	2024	G
47	5	2025	A
47	5	2026	A
47	5	2033	A
47	5	2040	A
47	5	2047	A
47	5	2048	U

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Mol	Chain	Res	Type
47	5	2052	G
47	5	2055	G
47	5	2056	G
47	5	2058	G
47	5	2062	C
47	5	2064	G
47	5	2069	A
47	5	2070	U
47	5	2084	U
47	5	2085	G
47	5	2089	G
47	5	2090	U
47	5	2092	G
47	5	2093	G
47	5	2094	C
47	5	2095	A
47	5	2097	A
47	5	2098	G
47	5	2100	G
47	5	2101	A
47	5	2102	G
47	5	2104	A
47	5	2105	A
47	5	2106	G
47	5	2107	A
47	5	2108	G
47	5	2110	G
47	5	2259	G
47	5	2260	C
47	5	2262	G
47	5	2266	C
47	5	2267	U
47	5	2268	A
47	5	2269	C
47	5	2270	G
47	5	2274	C
47	5	2275	G
47	5	2279	A
47	5	2289	C
47	5	2299	G
47	5	2300	A
47	5	2301	G

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Mol	Chain	Res	Type
47	5	2313	A
47	5	2314	G
47	5	2316	G
47	5	2325	C
47	5	2331	G
47	5	2332	A
47	5	2333	G
47	5	2348	G
47	5	2351	C
47	5	2364	G
47	5	2374	A
47	5	2395	A
47	5	2396	A
47	5	2399	G
47	5	2402	G
47	5	2416	G
47	5	2417	A
47	5	2422	C
47	5	2424	G
47	5	2425	U
47	5	2428	A
47	5	2433	G
47	5	2441	C
47	5	2447	U
47	5	2450	G
47	5	2469	C
47	5	2470	C
47	5	2471	G
47	5	2475	G
47	5	2479	G
47	5	2483	G
47	5	2485	U
47	5	2488	C
47	5	2489	C
47	5	2490	U
47	5	2491	C
47	5	2493	G
47	5	2495	U
47	5	2503	G
47	5	2504	C
47	5	2505	C
47	5	2506	G

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Mol	Chain	Res	Type
47	5	2512	A
47	5	2513	A
47	5	2530	U
47	5	2537	A
47	5	2546	G
47	5	2547	G
47	5	2553	A
47	5	2554	U
47	5	2555	G
47	5	2558	C
47	5	2564	G
47	5	2566	G
47	5	2571	C
47	5	2572	C
47	5	2575	U
47	5	2583	C
47	5	2586	G
47	5	2587	A
47	5	2588	C
47	5	2601	A
47	5	2620	G
47	5	2627	C
47	5	2638	G
47	5	2640	G
47	5	2647	A
47	5	2661	U
47	5	2662	G
47	5	2663	G
47	5	2669	C
47	5	2670	C
47	5	2673	G
47	5	2676	A
47	5	2681	G
47	5	2686	G
47	5	2687	U
47	5	2688	G
47	5	2689	C
47	5	2695	A
47	5	2696	A
47	5	2707	U
47	5	2708	U
47	5	2709	C

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Mol	Chain	Res	Type
47	5	2710	C
47	5	2711	G
47	5	2712	G
47	5	2714	G
47	5	2716	C
47	5	2719	C
47	5	2721	G
47	5	2725	A
47	5	2726	G
47	5	2740	U
47	5	2743	A
47	5	2744	A
47	5	2754	G
47	5	2760	G
47	5	2761	U
47	5	2763	U
47	5	2764	A
47	5	2769	U
47	5	2772	C
47	5	2787	A
47	5	2788	U
47	5	2789	A
47	5	2790	U
47	5	2795	A
47	5	2796	G
47	5	2798	A
47	5	2806	A
47	5	2807	A
47	5	2808	G
47	5	2814	C
47	5	2826	U
47	5	2827	G
47	5	2828	U
47	5	2829	U
47	5	2835	A
47	5	2838	G
47	5	2842	G
47	5	2845	A
47	5	2855	G
47	5	2857	A
47	5	2875	C
47	5	2884	G

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Mol	Chain	Res	Type
47	5	2896	G
47	5	2897	G
47	5	3598	C
47	5	3599	A
47	5	3604	A
47	5	3605	C
47	5	3615	G
47	5	3617	G
47	5	3625	G
47	5	3626	G
47	5	3630	A
47	5	3635	A
47	5	3644	U
47	5	3653	A
47	5	3662	A
47	5	3673	C
47	5	3674	G
47	5	3682	A
47	5	3692	A
47	5	3696	C
47	5	3698	G
47	5	3711	A
47	5	3712	A
47	5	3722	G
47	5	3729	U
47	5	3740	G
47	5	3748	A
47	5	3750	G
47	5	3753	G
47	5	3756	A
47	5	3759	A
47	5	3760	A
47	5	3765	G
47	5	3766	A
47	5	3773	U
47	5	3774	A
47	5	3776	G
47	5	3777	G
47	5	3778	U
47	5	3783	A
47	5	3784	A
47	5	3785	A

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Mol	Chain	Res	Type
47	5	3786	U
47	5	3798	U
47	5	3799	A
47	5	3810	C
47	5	3811	G
47	5	3812	C
47	5	3814	U
47	5	3817	A
47	5	3819	G
47	5	3822	U
47	5	3831	U
47	5	3838	U
47	5	3839	G
47	5	3840	U
47	5	3851	U
47	5	3859	G
47	5	3867	A
47	5	3871	A
47	5	3876	A
47	5	3877	A
47	5	3878	C
47	5	3879	G
47	5	3889	G
47	5	3897	G
47	5	3898	G
47	5	3901	A
47	5	3905	A
47	5	3906	A
47	5	3907	G
47	5	3908	A
47	5	3915	U
47	5	3916	G
47	5	3917	A
47	5	3927	U
47	5	3938	G
47	5	3939	G
47	5	3943	A
47	5	4067	U
47	5	4069	U
47	5	4071	U
47	5	4073	A
47	5	4076	G

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Mol	Chain	Res	Type
47	5	4084	G
47	5	4085	A
47	5	4086	G
47	5	4088	C
47	5	4090	G
47	5	4099	G
47	5	4100	C
47	5	4116	C
47	5	4117	U
47	5	4118	U
47	5	4119	C
47	5	4120	U
47	5	4121	G
47	5	4122	G
47	5	4125	C
47	5	4127	A
47	5	4138	C
47	5	4150	G
47	5	4158	C
47	5	4161	G
47	5	4162	C
47	5	4163	U
47	5	4166	G
47	5	4171	C
47	5	4183	G
47	5	4184	G
47	5	4191	G
47	5	4203	A
47	5	4213	A
47	5	4225	G
47	5	4229	U
47	5	4230	C
47	5	4232	U
47	5	4233	A
47	5	4237	C
47	5	4249	G
47	5	4251	A
47	5	4255	A
47	5	4257	A
47	5	4258	C
47	5	4268	A
47	5	4271	A

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Mol	Chain	Res	Type
47	5	4273	A
47	5	4281	A
47	5	4291	G
47	5	4297	G
47	5	4304	A
47	5	4305	G
47	5	4306	U
47	5	4314	C
47	5	4317	A
47	5	4318	C
47	5	4319	C
47	5	4326	G
47	5	4329	G
47	5	4330	G
47	5	4331	G
47	5	4332	C
47	5	4336	A
47	5	4349	C
47	5	4354	U
47	5	4355	G
47	5	4373	G
47	5	4377	G
47	5	4378	A
47	5	4379	A
47	5	4380	A
47	5	4387	C
47	5	4391	G
47	5	4393	G
47	5	4394	A
47	5	4395	U
47	5	4398	C
47	5	4401	G
47	5	4419	U
47	5	4421	C
47	5	4422	A
47	5	4437	U
47	5	4440	G
47	5	4444	C
47	5	4448	G
47	5	4449	A
47	5	4453	C
47	5	4464	A

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Mol	Chain	Res	Type
47	5	4471	U
47	5	4475	G
47	5	4476	C
47	5	4482	U
47	5	4488	A
47	5	4495	G
47	5	4500	U
47	5	4510	A
47	5	4511	A
47	5	4512	U
47	5	4513	A
47	5	4515	G
47	5	4519	C
47	5	4520	G
47	5	4524	G
47	5	4527	G
47	5	4528	G
47	5	4531	U
47	5	4535	A
47	5	4548	A
47	5	4549	G
47	5	4560	C
47	5	4567	G
47	5	4570	G
47	5	4573	G
47	5	4575	G
47	5	4584	A
47	5	4586	G
47	5	4590	A
47	5	4599	A
47	5	4606	G
47	5	4618	G
47	5	4627	U
47	5	4635	A
47	5	4636	U
47	5	4637	G
47	5	4656	A
47	5	4657	U
47	5	4661	G
47	5	4670	C
47	5	4672	A
47	5	4677	U

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Mol	Chain	Res	Type
47	5	4678	G
47	5	4687	A
47	5	4694	G
47	5	4695	C
47	5	4700	A
47	5	4701	A
47	5	4709	U
47	5	4719	G
47	5	4720	C
47	5	4721	G
47	5	4728	U
47	5	4736	C
47	5	4737	G
47	5	4745	G
47	5	4751	G
47	5	4752	U
47	5	4754	G
47	5	4756	C
47	5	4757	C
47	5	4759	C
47	5	4761	G
47	5	4765	G
47	5	4771	C
47	5	4772	C
47	5	4868	G
47	5	4870	G
47	5	4871	C
47	5	4872	G
47	5	4873	G
47	5	4874	A
47	5	4875	G
47	5	4876	A
47	5	4877	G
47	5	4882	U
47	5	4883	C
47	5	4885	U
47	5	4887	C
47	5	4891	G
47	5	4895	C
47	5	4897	G
47	5	4910	A
47	5	4912	G

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Mol	Chain	Res	Type
47	5	4913	G
47	5	4914	G
47	5	4915	G
47	5	4919	G
47	5	4921	C
47	5	4922	C
47	5	4924	C
47	5	4925	U
47	5	4926	C
47	5	4928	C
47	5	4931	G
47	5	4935	C
47	5	4937	C
47	5	4942	C
47	5	4943	A
47	5	4944	C
47	5	4947	U
47	5	4948	C
47	5	4949	G
47	5	4950	U
47	5	4951	G
47	5	4956	A
47	5	4957	C
47	5	4958	C
47	5	4964	C
47	5	4965	U
47	5	4966	A
47	5	4967	A
47	5	4976	U
47	5	4985	U
47	5	4988	U
47	5	4989	U
47	5	4990	C
47	5	4991	U
47	5	5014	A
47	5	5017	G
47	5	5018	C
47	5	5040	U
47	5	5041	G
47	5	5047	C
47	5	5050	C
47	5	5053	U

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Mol	Chain	Res	Type
47	5	5054	C
47	5	5056	A
47	5	5058	A
47	5	5061	A
47	5	5062	G
47	5	5066	U
48	7	7	G
48	7	25	G
48	7	33	U
48	7	42	A
48	7	53	U
48	7	54	A
48	7	64	G
48	7	97	G
48	7	100	A
48	7	109	U
48	7	110	G
48	7	111	C
49	8	2	G
49	8	3	A
49	8	32	C
49	8	34	U
49	8	35	C
49	8	49	G
49	8	51	U
49	8	52	A
49	8	59	A
49	8	62	A
49	8	63	U
49	8	75	G
49	8	79	G
49	8	86	U
49	8	87	G
49	8	94	G
49	8	95	A
49	8	103	A
49	8	104	A
49	8	105	C
49	8	107	C
49	8	109	C
49	8	110	U
49	8	111	U

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Mol	Chain	Res	Type
49	8	112	G
49	8	114	G
49	8	121	G
49	8	123	U
49	8	124	U
49	8	125	C
49	8	126	C
49	8	127	U
49	8	137	A
49	8	143	G
50	9	2	A
50	9	3	C
50	9	4	C
50	9	14	C
50	9	17	C
50	9	23	G
50	9	25	A
50	9	33	G
50	9	41	G
50	9	44	U
50	9	46	A
50	9	56	G
50	9	58	C
50	9	64	A
50	9	65	C
50	9	67	C
50	9	68	A
50	9	69	C
50	9	71	G
50	9	72	C
50	9	73	C
50	9	74	G
50	9	75	G
50	9	77	A
50	9	79	A
50	9	81	U
50	9	98	C
50	9	99	A
50	9	100	U
50	9	103	A
50	9	111	A
50	9	113	G

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Mol	Chain	Res	Type
50	9	115	U
50	9	116	U
50	9	123	G
50	9	124	U
50	9	126	G
50	9	127	C
50	9	130	G
50	9	142	C
50	9	143	U
50	9	147	A
50	9	155	G
50	9	158	A
50	9	161	U
50	9	162	C
50	9	163	U
50	9	177	G
50	9	180	G
50	9	181	A
50	9	182	C
50	9	183	G
50	9	184	G
50	9	188	C
50	9	189	U
50	9	192	C
50	9	206	G
50	9	213	G
50	9	215	G
50	9	292	A
50	9	293	C
50	9	294	U
50	9	302	A
50	9	307	G
50	9	308	G
50	9	309	G
50	9	312	G
50	9	314	U
50	9	317	C
50	9	318	A
50	9	319	C
50	9	322	C
50	9	330	G
50	9	335	G

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Mol	Chain	Res	Type
50	9	347	G
50	9	351	G
50	9	362	C
50	9	364	A
50	9	368	U
50	9	369	C
50	9	370	G
50	9	372	U
50	9	377	G
50	9	381	C
50	9	382	C
50	9	383	G
50	9	384	U
50	9	385	G
50	9	386	C
50	9	388	U
50	9	400	C
50	9	408	A
50	9	409	C
50	9	416	U
50	9	417	C
50	9	418	A
50	9	419	G
50	9	441	C
50	9	448	A
50	9	449	A
50	9	450	C
50	9	451	G
50	9	452	G
50	9	454	U
50	9	460	A
50	9	462	C
50	9	464	A
50	9	465	A
50	9	466	G
50	9	469	A
50	9	471	G
50	9	472	C
50	9	473	A
50	9	474	G
50	9	476	A
50	9	482	G

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Mol	Chain	Res	Type
50	9	487	U
50	9	492	C
50	9	493	A
50	9	496	C
50	9	500	A
50	9	507	G
50	9	509	G
50	9	512	A
50	9	516	A
50	9	526	A
50	9	530	U
50	9	531	A
50	9	532	C
50	9	533	A
50	9	544	G
50	9	546	G
50	9	548	C
50	9	549	C
50	9	550	C
50	9	551	U
50	9	554	A
50	9	555	A
50	9	556	U
50	9	557	U
50	9	559	G
50	9	562	U
50	9	563	G
50	9	568	C
50	9	571	U
50	9	572	U
50	9	574	A
50	9	576	A
50	9	583	A
50	9	585	C
50	9	587	A
50	9	588	G
50	9	590	A
50	9	591	U
50	9	597	G
50	9	604	A
50	9	606	G
50	9	607	U

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Mol	Chain	Res	Type
50	9	608	C
50	9	609	U
50	9	614	C
50	9	617	G
50	9	620	G
50	9	621	C
50	9	627	U
50	9	628	A
50	9	629	A
50	9	632	C
50	9	637	U
50	9	643	A
50	9	644	G
50	9	646	G
50	9	655	A
50	9	659	G
50	9	660	C
50	9	664	A
50	9	668	A
50	9	669	A
50	9	670	A
50	9	671	A
50	9	672	A
50	9	673	G
50	9	684	G
50	9	687	C
50	9	688	U
50	9	689	U
50	9	696	G
50	9	733	C
50	9	752	G
50	9	753	C
50	9	754	G
50	9	810	A
50	9	811	A
50	9	812	A
50	9	821	G
50	9	822	U
50	9	830	A
50	9	834	C
50	9	844	U
50	9	847	A

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Mol	Chain	Res	Type
50	9	859	G
50	9	861	A
50	9	868	G
50	9	869	A
50	9	870	A
50	9	871	U
50	9	872	A
50	9	873	G
50	9	874	G
50	9	875	A
50	9	878	G
50	9	885	U
50	9	888	U
50	9	889	U
50	9	890	U
50	9	907	G
50	9	909	G
50	9	913	A
50	9	914	U
50	9	920	A
50	9	921	G
50	9	922	A
50	9	930	C
50	9	933	G
50	9	934	G
50	9	943	U
50	9	971	G
50	9	985	G
50	9	990	A
50	9	992	A
50	9	999	G
50	9	1017	U
50	9	1023	A
50	9	1041	G
50	9	1053	C
50	9	1055	A
50	9	1060	A
50	9	1061	U
50	9	1062	A
50	9	1083	A
50	9	1085	C
50	9	1089	G

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Mol	Chain	Res	Type
50	9	1100	A
50	9	1115	U
50	9	1116	C
50	9	1117	C
50	9	1118	C
50	9	1119	A
50	9	1121	G
50	9	1133	A
50	9	1138	C
50	9	1139	C
50	9	1140	G
50	9	1144	A
50	9	1148	A
50	9	1149	A
50	9	1153	C
50	9	1154	U
50	9	1165	G
50	9	1166	G
50	9	1168	G
50	9	1170	A
50	9	1195	A
50	9	1203	G
50	9	1207	G
50	9	1208	A
50	9	1215	C
50	9	1221	G
50	9	1224	G
50	9	1227	G
50	9	1235	G
50	9	1240	A
50	9	1242	U
50	9	1248	U
50	9	1250	A
50	9	1251	A
50	9	1253	A
50	9	1254	C
50	9	1256	G
50	9	1257	G
50	9	1259	A
50	9	1260	A
50	9	1269	G
50	9	1274	G

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Mol	Chain	Res	Type
50	9	1275	G
50	9	1281	G
50	9	1284	A
50	9	1285	G
50	9	1286	G
50	9	1289	U
50	9	1293	A
50	9	1294	G
50	9	1299	A
50	9	1300	U
50	9	1301	A
50	9	1302	G
50	9	1303	C
50	9	1304	U
50	9	1308	U
50	9	1309	C
50	9	1313	A
50	9	1314	U
50	9	1322	G
50	9	1324	G
50	9	1330	G
50	9	1331	C
50	9	1337	C
50	9	1342	U
50	9	1369	A
50	9	1371	U
50	9	1372	U
50	9	1375	G
50	9	1376	A
50	9	1378	A
50	9	1396	A
50	9	1397	U
50	9	1402	A
50	9	1406	G
50	9	1424	G
50	9	1428	G
50	9	1429	G
50	9	1439	A
50	9	1449	G
50	9	1454	A
50	9	1455	A
50	9	1458	G

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Mol	Chain	Res	Type
50	9	1459	G
50	9	1462	U
50	9	1463	U
50	9	1466	G
50	9	1473	G
50	9	1475	G
50	9	1476	A
50	9	1477	U
50	9	1478	U
50	9	1489	A
50	9	1490	G
50	9	1498	A
50	9	1509	U
50	9	1519	U
50	9	1520	G
50	9	1521	C
50	9	1522	A
50	9	1525	C
50	9	1531	A
50	9	1533	A
50	9	1535	U
50	9	1536	G
50	9	1544	C
50	9	1548	G
50	9	1552	G
50	9	1553	C
50	9	1555	U
50	9	1556	A
50	9	1557	C
50	9	1558	C
50	9	1560	U
50	9	1570	G
50	9	1574	C
50	9	1575	G
50	9	1580	A
50	9	1581	C
50	9	1587	G
50	9	1588	A
50	9	1601	A
50	9	1602	U
50	9	1604	G
50	9	1612	G

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Mol	Chain	Res	Type
50	9	1621	U
50	9	1622	U
50	9	1623	A
50	9	1637	A
50	9	1638	G
50	9	1639	G
50	9	1648	G
50	9	1661	A
50	9	1664	A
50	9	1665	G
50	9	1671	G
50	9	1680	G
50	9	1683	C
50	9	1686	G
50	9	1689	C
50	9	1698	C
50	9	1699	A
50	9	1703	C
50	9	1715	A
50	9	1721	U
50	9	1722	G
50	9	1726	G
50	9	1730	U
50	9	1740	C
50	9	1747	C
50	9	1748	G
50	9	1750	C
50	9	1753	C
50	9	1757	G
50	9	1758	G
50	9	1760	G
50	9	1783	C
50	9	1785	C
50	9	1800	A
50	9	1819	A
50	9	1823	A
50	9	1824	A
50	9	1829	G
50	9	1835	A
50	9	1836	G
50	9	1838	U
50	9	1839	U

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Mol	Chain	Res	Type
50	9	1849	G
50	9	1851	A
50	9	1852	C
50	9	1861	G
50	9	1862	G
50	9	1863	A
50	9	1865	C
50	9	1866	A
50	9	1867	U
50	9	1869	A
84	hh	22	G
45	ii	7	G
45	ii	8	U
45	ii	10	G
45	ii	11	U
45	ii	13	U
45	ii	19	G
45	ii	20	U
45	ii	21	U
45	ii	22	A
45	ii	26	C
45	ii	31	G
45	ii	45	A
45	ii	49	C
45	ii	53	G
45	ii	60	A
45	ii	61	A
45	ii	62	C
45	ii	65	G
45	ii	76	C
45	ii	77	A

All (247) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
45	2	20(A)	U
46	3	7	A
46	3	74	C
47	5	12	A
47	5	20	U
47	5	47	A
47	5	48	G

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Mol	Chain	Res	Type
47	5	64	A
47	5	119	G
47	5	125	C
47	5	134	G
47	5	143	C
47	5	159	C
47	5	200	U
47	5	217	C
47	5	226	G
47	5	234	G
47	5	245	C
47	5	265	C
47	5	275	C
47	5	278	G
47	5	315	G
47	5	354	U
47	5	385	A
47	5	406	C
47	5	408	A
47	5	409	G
47	5	417	G
47	5	449	C
47	5	480	C
47	5	484	U
47	5	485	C
47	5	492	U
47	5	497	G
47	5	498	C
47	5	504	G
47	5	669	C
47	5	696	C
47	5	729	G
47	5	738(A)	C
47	5	747	A
47	5	915	A
47	5	916	C
47	5	930	G
47	5	933	G
47	5	935(A)	G
47	5	936	C
47	5	955	G
47	5	959	G

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Mol	Chain	Res	Type
47	5	963	G
47	5	966	A
47	5	968	C
47	5	969	C
47	5	971(A)	G
47	5	1072	C
47	5	1209	U
47	5	1211	G
47	5	1214	C
47	5	1236	C
47	5	1238	A
47	5	1287	G
47	5	1291	G
47	5	1295	U
47	5	1324	A
47	5	1329	G
47	5	1358	G
47	5	1359	G
47	5	1370	G
47	5	1378	C
47	5	1380	G
47	5	1420	A
47	5	1440	U
47	5	1445	U
47	5	1455	G
47	5	1477	C
47	5	1481	C
47	5	1484	G
47	5	1485	C
47	5	1611	C
47	5	1633	G
47	5	1654	G
47	5	1676	C
47	5	1733	G
47	5	1740	C
47	5	1804	A
47	5	1815	G
47	5	1818	G
47	5	1833	G
47	5	1834	U
47	5	1835	G
47	5	1919	G

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Mol	Chain	Res	Type
47	5	1921	C
47	5	1935	C
47	5	1947	U
47	5	1979	A
47	5	1983	A
47	5	1984	A
47	5	1986	U
47	5	2001	G
47	5	2025	A
47	5	2046	G
47	5	2054	U
47	5	2068	C
47	5	2088	A
47	5	2089	G
47	5	2094	C
47	5	2100	G
47	5	2265	G
47	5	2266	C
47	5	2278	G
47	5	2313	A
47	5	2370	A
47	5	2396	A
47	5	2398	U
47	5	2428	A
47	5	2467	U
47	5	2468	U
47	5	2474	G
47	5	2475	G
47	5	2490	U
47	5	2502	A
47	5	2529	A
47	5	2530	U
47	5	2546	G
47	5	2553	A
47	5	2587	A
47	5	2661	U
47	5	2695	A
47	5	2724	G
47	5	2754	G
47	5	2794	C
47	5	2806	A
47	5	2834	C

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Mol	Chain	Res	Type
47	5	3603	G
47	5	3625	G
47	5	3673	C
47	5	3697	U
47	5	3710	G
47	5	3809	G
47	5	3876	A
47	5	3878	C
47	5	3888	G
47	5	3904	G
47	5	4075	U
47	5	4076	G
47	5	4084	G
47	5	4116	C
47	5	4119	C
47	5	4120	U
47	5	4121	G
47	5	4124	G
47	5	4162	C
47	5	4170	A
47	5	4232	U
47	5	4254	G
47	5	4266	G
47	5	4272	G
47	5	4331	G
47	5	4378	A
47	5	4379	A
47	5	4395	U
47	5	4448	G
47	5	4463	U
47	5	4510	A
47	5	4527	G
47	5	4699	U
47	5	4719	G
47	5	4871	C
47	5	4884	G
47	5	4925	U
47	5	4936	G
47	5	4942	C
47	5	4947	U
47	5	4965	U
48	7	109	U

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Mol	Chain	Res	Type
49	8	2	G
49	8	51	U
49	8	85	U
49	8	86	U
49	8	94	G
49	8	110	U
49	8	124	U
50	9	2	A
50	9	3	C
50	9	24	C
50	9	25	A
50	9	43	U
50	9	72	C
50	9	98	C
50	9	110	U
50	9	126	G
50	9	142	C
50	9	160	U
50	9	182	C
50	9	293	C
50	9	369	C
50	9	370	G
50	9	448	A
50	9	464	A
50	9	465	A
50	9	500	A
50	9	516	A
50	9	532	C
50	9	550	C
50	9	553	U
50	9	555	A
50	9	561	A
50	9	563	G
50	9	584	A
50	9	620	G
50	9	627	U
50	9	655	A
50	9	670	A
50	9	688	U
50	9	752	G
50	9	861	A
50	9	869	A

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Mol	Chain	Res	Type
50	9	870	A
50	9	872	A
50	9	912	C
50	9	1016	U
50	9	1137	U
50	9	1138	C
50	9	1165	G
50	9	1253	A
50	9	1255	G
50	9	1284	A
50	9	1286	G
50	9	1313	A
50	9	1330	G
50	9	1395	C
50	9	1396	A
50	9	1441	U
50	9	1476	A
50	9	1489	A
50	9	1494	U
50	9	1534	C
50	9	1621	U
50	9	1636	G
50	9	1637	A
50	9	1647	A
50	9	1664	A
50	9	1679	A
50	9	1721	U
50	9	1835	A
50	9	1862	G
50	9	1868	U

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
85	SEP	jj	163	85	7,9,10	0.69	0	8,12,14	1.54	1 (12%)

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
85	SEP	jj	163	85	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	jj	163	SEP	OG-CB-CA	2.63	110.55	108.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 286 ligands modelled in this entry, 284 are monoatomic - leaving 2 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	$\# Z  > 2$
88	GDP	jj	501	86	24,30,30	1.22	2 (8%)	26,47,47	1.90	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
89	7C4	jj	503	-	80,82,82	1.02	5 (6%)	109,117,117	1.21	14 (12%)

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
88	GDP	jj	501	86	-	0/12/32/32	0/3/3/3
89	7C4	jj	503	-	-	0/120/140/140	0/3/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	jj	503	7C4	C72-C71	-4.47	1.32	1.51
89	jj	503	7C4	C54-C55	-2.95	1.50	1.53
89	jj	503	7C4	C45-C47	2.12	1.55	1.53
89	jj	503	7C4	C53-C54	2.18	1.56	1.53
89	jj	503	7C4	C48-C47	2.44	1.54	1.52
88	jj	501	GDP	C5-C4	3.16	1.47	1.40
88	jj	501	GDP	C6-C5	3.92	1.49	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	jj	501	GDP	C5-C6-N1	-3.93	118.39	123.52
88	jj	501	GDP	N3-C2-N1	-3.71	122.51	127.56
88	jj	501	GDP	C6-C5-C4	-3.54	116.81	120.86
89	jj	503	7C4	C36-N05-C30	-3.19	107.19	112.00
89	jj	503	7C4	C73-N20-C70	-2.83	107.73	112.00
89	jj	503	7C4	O12-C44-C45	-2.53	118.84	121.13
89	jj	503	7C4	O37-C79-C01	-2.35	119.36	124.58
89	jj	503	7C4	O29-C69-C70	-2.26	115.53	120.12
88	jj	501	GDP	C1'-N9-C4	-2.19	124.36	126.81
89	jj	503	7C4	C32-C30-C28	-2.08	106.55	110.72
89	jj	503	7C4	C28-C30-N05	-2.01	106.37	110.98
89	jj	503	7C4	C53-C54-C55	-2.00	110.19	112.86
89	jj	503	7C4	C39-C38-N05	2.06	121.97	118.68
89	jj	503	7C4	C77-O35-C79	2.17	120.93	117.47
89	jj	503	7C4	C71-C70-C69	2.22	115.19	110.72
89	jj	503	7C4	C30-C28-N02	2.71	123.90	119.03
89	jj	503	7C4	C70-C69-N17	3.29	124.95	119.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	jj	503	7C4	O35-C79-C01	3.46	118.35	110.75
88	jj	501	GDP	C6-N1-C2	5.35	122.15	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	5	31
50	9	7
45	2	3
46	3	2
45	ii	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	41.26
1	5	1252:C	O3'	1271:G	P	36.28
1	5	1219:G	O3'	1233:G	P	22.71
1	5	3948:C	O3'	4065:G	P	19.70
1	5	1406(C):G	O3'	1411:C	P	18.70
1	5	990:C	O3'	1064:G	P	18.38
1	5	523:C	O3'	638:G	P	18.03
1	5	4138:C	O3'	4146:G	P	18.01
1	5	4101:C	O3'	4107:G	P	17.45
1	5	4777:C	O3'	4859:C	P	16.68
1	5	760:G	O3'	904:C	P	15.18
1	5	5022:U	O3'	5028:G	P	14.74
1	5	182:G	O3'	189:G	P	14.42

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	1364:U	O3'	1368:A	P	14.31
1	5	1696:C	O3'	1720:C	P	14.19
1	5	2901:G	O3'	3597:G	P	13.49
1	5	4729:A	O3'	4735:G	P	9.67
1	5	512:U	O3'	515:C	P	9.60
1	5	1180:C	O3'	1183:C	P	8.81
1	5	500:G	O3'	504:G	P	6.82
1	5	1100:U	O3'	1168:G	P	5.92
1	2	20:U	O3'	20(A):U	P	5.90
1	3	19:G	O3'	20:U	P	5.80
1	9	689:U	O3'	690:G	P	5.56
1	ii	16:C	O3'	18:G	P	5.55
1	3	16:C	O3'	18:U	P	5.33
1	5	1239:C	O3'	1244:G	P	5.32
1	9	322:C	O3'	323:C	P	5.23
1	5	4740:G	O3'	4743:G	P	4.91
1	2	19:G	O3'	20:U	P	4.72
1	9	798:G	O3'	799:U	P	4.67
1	2	16:C	O3'	18:G	P	4.42
1	9	304:C	O3'	305:U	P	4.35
1	5	170:C	O3'	171:U	P	3.94
1	5	1957:U	O3'	1958:A	P	3.81
1	9	902:G	O3'	903:A	P	3.38
1	5	1438:U	O3'	1440:U	P	3.34
1	5	4899:G	O3'	4902:C	P	3.34
1	9	886:A	O3'	887:U	P	3.33
1	5	5020:G	O3'	5021:C	P	3.30
1	9	903:A	O3'	904:A	P	3.30
1	5	267:G	O3'	268:G	P	3.19
1	5	751:G	O3'	752:G	P	3.03
1	5	2025:A	O3'	2026:A	P	1.24