



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 05:39 PM UTC

PDB ID : 5LZW / pdb_00005lzw
EMDB ID : EMD-4134
Title : Structure of the mammalian rescue complex with Pelota and Hbs1l assembled on a truncated mRNA.
Authors : Shao, S.; Murray, J.; Brown, A.; Taunton, J.; Ramakrishnan, V.; Hegde, R.S.
Deposited on : 2016-10-02
Resolution : 3.53 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

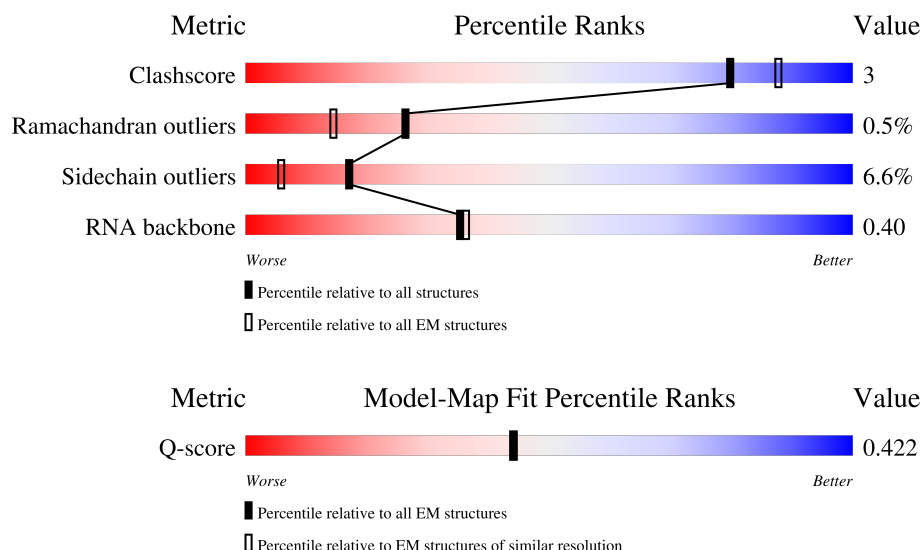
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.53 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.



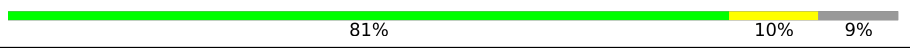
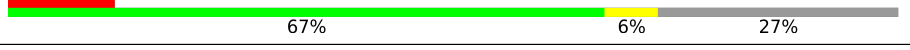
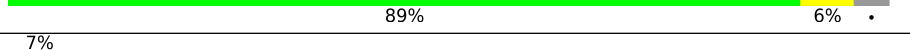
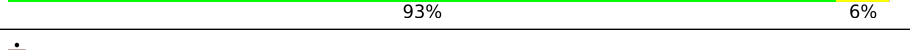
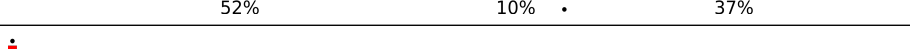
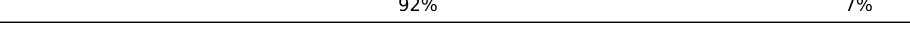
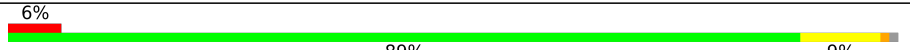
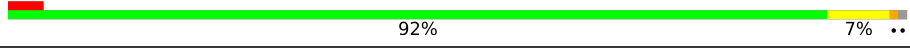
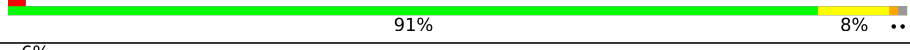
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12947 (3.03 - 4.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	
2	B	403	
3	C	425	

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Mol	Chain	Length	Quality of chain
4	D	297	
5	E	291	
6	F	247	
7	G	319	
8	H	192	
9	I	214	
10	J	178	
11	L	211	
12	M	218	
13	N	204	
14	O	203	
15	P	184	
16	Q	188	
17	R	196	
18	S	176	
19	T	160	
20	U	128	
21	V	140	
22	W	157	
23	X	156	
24	Y	145	
25	Z	136	
26	a	148	
27	b	245	
28	c	115	

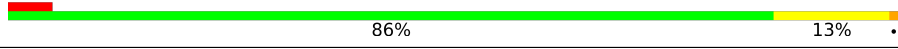
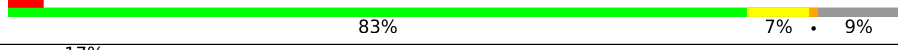
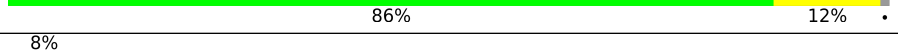
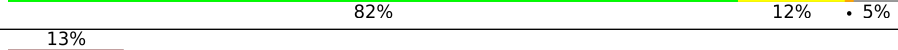
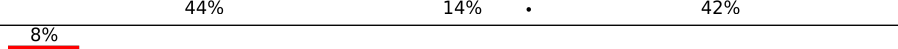
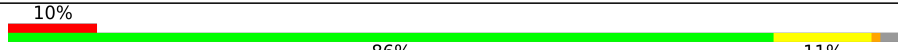
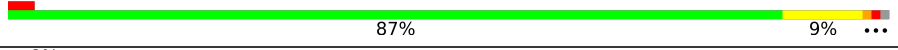
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Mol	Chain	Length	Quality of chain
29	d	125	
30	e	135	
31	f	110	
32	g	116	
33	h	123	
34	i	105	
35	j	97	
36	k	70	
37	l	51	
38	m	102	
39	n	25	
40	o	106	
41	p	92	
42	r	137	
43	s	318	
44	t	165	
45	1	15	
46	2	76	
47	3	75	
48	5	3543	
49	7	120	
50	8	156	
51	9	1869	
52	AA	295	
53	BB	264	

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Mol	Chain	Length	Quality of chain
54	CC	293	
55	DD	243	
56	EE	263	
57	FF	204	
58	GG	249	
59	HH	194	
60	II	208	
61	JJ	194	
62	KK	165	
63	LL	158	
64	MM	132	
65	NN	151	
66	OO	168	
67	PP	145	
68	QQ	146	
69	RR	135	
70	SS	152	
71	TT	145	
72	UU	119	
73	VV	83	
74	WW	130	
75	XX	143	
76	YY	130	
77	ZZ	125	
78	aa	115	

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Mol	Chain	Length	Quality of chain
79	bb	84	
80	cc	69	
81	dd	56	
82	ee	133	
83	ff	156	
84	gg	317	
85	hh	8	
86	ii	403	
87	jj	710	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
89	ZN	ff	200	-	-	X	-
89	ZN	g	201	-	-	X	-
90	GCP	9	1972	-	-	X	-

2 Entry composition [i](#)

There are 90 unique types of molecules in this entry. The entry contains 222130 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 uL2.

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 uL3.

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 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 uL18.

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	LYS	initiating methionine	UNP G1SYJ6

- Molecule 5 is a protein called eL6.

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 uL30.

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.

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 uL6.

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 uL16.

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 uL5.

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 eL14.

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 eL15.

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 uL22.

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 eL21.

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 uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 22 is a protein called eL24.

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 uL23.

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 uL24.

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 eL27.

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 uL15.

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 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 eL30.

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 eL31.

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 eL32.

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 eL33.

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 eL34.

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 uL29.

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 eL36.

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 eL37.

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 eL39.

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 eL41.

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 eL42.

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 eL43.

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 eL28.

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 uL11.

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 protein called Nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1	15	Total	C	N	O	S	0	0
			125	82	20	22	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 47 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 48 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5	3543	Total	C	N	O	P	0	0
			75972	33833	13910	24686	3543		

- Molecule 49 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 50 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	8	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 51 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	9	1698	Total	C	N	O	P	0	0
			36249	16180	6508	11864	1697		

- Molecule 52 is a protein called uS2.

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

- Molecule 53 is a protein called eS1.

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

- Molecule 54 is a protein called uS5.

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

- Molecule 55 is a protein called uS3.

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

- Molecule 56 is a protein called eS4.

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

- Molecule 57 is a protein called uS7.

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

- Molecule 58 is a protein called eS6.

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

- Molecule 59 is a protein called eS7.

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

- Molecule 60 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	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 61 is a protein called uS4.

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

- Molecule 62 is a protein called eS10.

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

- Molecule 63 is a protein called uS17.

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

- Molecule 64 is a protein called eS12.

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

- Molecule 65 is a protein called uS15.

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

- Molecule 66 is a protein called uS11.

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

- Molecule 67 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	PP	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 68 is a protein called uS9.

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

- Molecule 69 is a protein called eS17.

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

- Molecule 70 is a protein called uS13.

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

- Molecule 71 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	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 72 is a protein called uS10.

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

- Molecule 73 is a protein called eS21.

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

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called eS24.

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

- Molecule 77 is a protein called eS25.

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

- Molecule 78 is a protein called eS26.

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

- Molecule 79 is a protein called eS27.

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

- Molecule 80 is a protein called eS28.

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

- Molecule 81 is a protein called uS14.

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

- Molecule 82 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	ee	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

- Molecule 83 is a protein called eS31.

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

- Molecule 84 is a protein called RACK1.

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

- Molecule 85 is a RNA chain called mRNA (truncated).

Mol	Chain	Residues	Atoms					AltConf	Trace
85	hh	8	Total	C	N	O	P	0	0
			169	76	29	56	8		

- Molecule 86 is a protein called Pelota.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	ii	372	Total	C	N	O	S	0	0
			2947	1844	528	559	16		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ii	221	MET	LEU	conflict	UNP Q9BRX2
ii	386	GLY	-	expression tag	UNP Q9BRX2
ii	387	SER	-	expression tag	UNP Q9BRX2
ii	388	GLU	-	expression tag	UNP Q9BRX2
ii	389	ASN	-	expression tag	UNP Q9BRX2
ii	390	LEU	-	expression tag	UNP Q9BRX2
ii	391	TYR	-	expression tag	UNP Q9BRX2
ii	392	PHE	-	expression tag	UNP Q9BRX2
ii	393	GLN	-	expression tag	UNP Q9BRX2
ii	394	GLY	-	expression tag	UNP Q9BRX2
ii	395	ALA	-	expression tag	UNP Q9BRX2
ii	396	HIS	-	expression tag	UNP Q9BRX2
ii	397	HIS	-	expression tag	UNP Q9BRX2
ii	398	HIS	-	expression tag	UNP Q9BRX2
ii	399	HIS	-	expression tag	UNP Q9BRX2
ii	400	HIS	-	expression tag	UNP Q9BRX2
ii	401	HIS	-	expression tag	UNP Q9BRX2
ii	402	SER	-	expression tag	UNP Q9BRX2
ii	403	THR	-	expression tag	UNP Q9BRX2

- Molecule 87 is a protein called Hbs1l.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	jj	425	Total	C	N	O	S	0	0
			3292	2100	565	609	18		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
jj	-25	MET	-	initiating methionine	UNP Q9Y450
jj	-24	ASP	-	expression tag	UNP Q9Y450
jj	-23	TYR	-	expression tag	UNP Q9Y450
jj	-22	LYS	-	expression tag	UNP Q9Y450
jj	-21	ASP	-	expression tag	UNP Q9Y450
jj	-20	HIS	-	expression tag	UNP Q9Y450
jj	-19	ASP	-	expression tag	UNP Q9Y450
jj	-18	GLY	-	expression tag	UNP Q9Y450
jj	-17	ASP	-	expression tag	UNP Q9Y450
jj	-16	TYR	-	expression tag	UNP Q9Y450
jj	-15	LYS	-	expression tag	UNP Q9Y450
jj	-14	ASP	-	expression tag	UNP Q9Y450
jj	-13	HIS	-	expression tag	UNP Q9Y450
jj	-12	ASP	-	expression tag	UNP Q9Y450
jj	-11	ILE	-	expression tag	UNP Q9Y450
jj	-10	ASP	-	expression tag	UNP Q9Y450
jj	-9	TYR	-	expression tag	UNP Q9Y450
jj	-8	LYS	-	expression tag	UNP Q9Y450
jj	-7	ASP	-	expression tag	UNP Q9Y450
jj	-6	ASP	-	expression tag	UNP Q9Y450
jj	-5	ASP	-	expression tag	UNP Q9Y450
jj	-4	ASP	-	expression tag	UNP Q9Y450
jj	-3	LYS	-	expression tag	UNP Q9Y450
jj	-2	ALA	-	expression tag	UNP Q9Y450
jj	-1	GLY	-	expression tag	UNP Q9Y450
jj	0	SER	-	expression tag	UNP Q9Y450

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
88	B	1	Total Mg 1 1	0
88	I	1	Total Mg 1 1	0
88	P	2	Total Mg 2 2	0
88	Q	1	Total Mg 1 1	0
88	V	1	Total Mg 1 1	0
88	a	1	Total Mg 1 1	0

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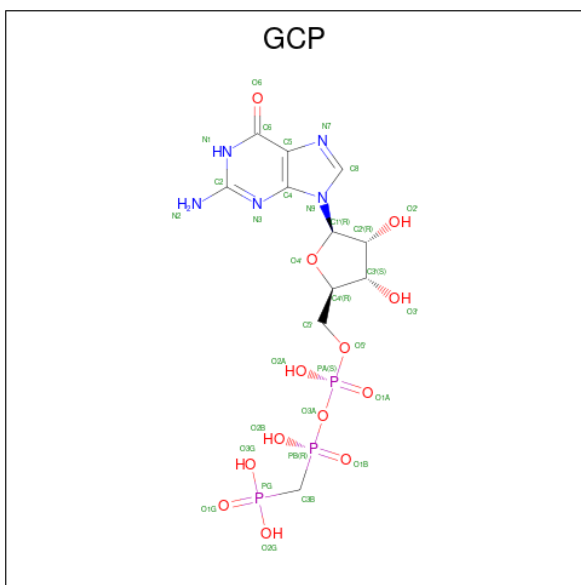
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
88	e	1	Total 1	Mg 1	0
88	g	1	Total 1	Mg 1	0
88	j	1	Total 1	Mg 1	0
88	5	188	Total 188	Mg 188	0
88	7	5	Total 5	Mg 5	0
88	8	6	Total 6	Mg 6	0
88	9	71	Total 71	Mg 71	0
88	jj	1	Total 1	Mg 1	0

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 90 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



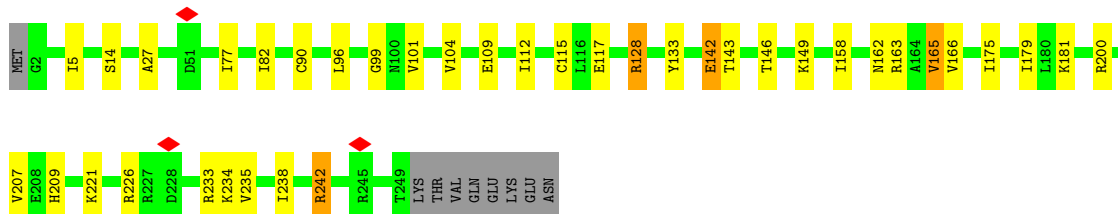
Mol	Chain	Residues	Atoms					AltConf
90	9	1	Total 32	C 11	N 5	O 13	P 3	0
90	jj	1	Total 32	C 11	N 5	O 13	P 3	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

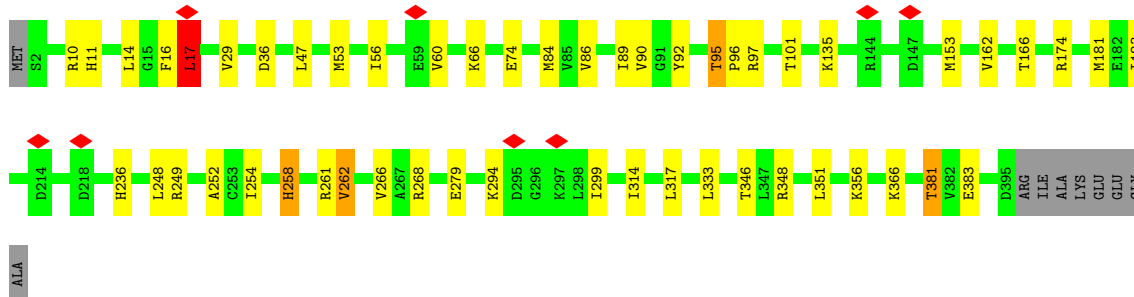
• Molecule 1: uL2

Chain A: 



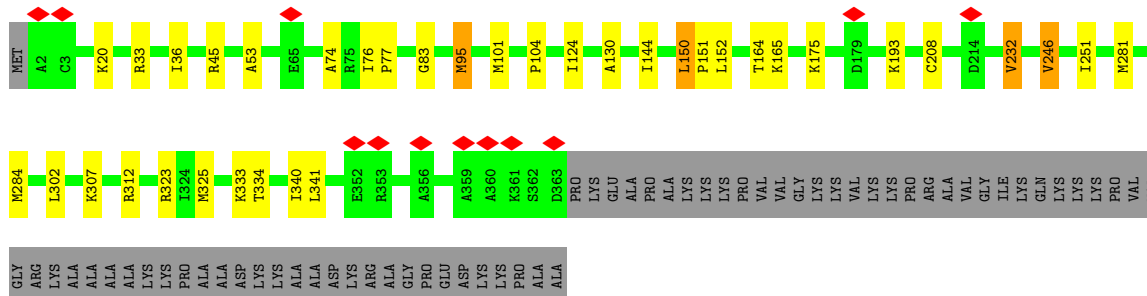
• Molecule 2: uL3

Chain B: 

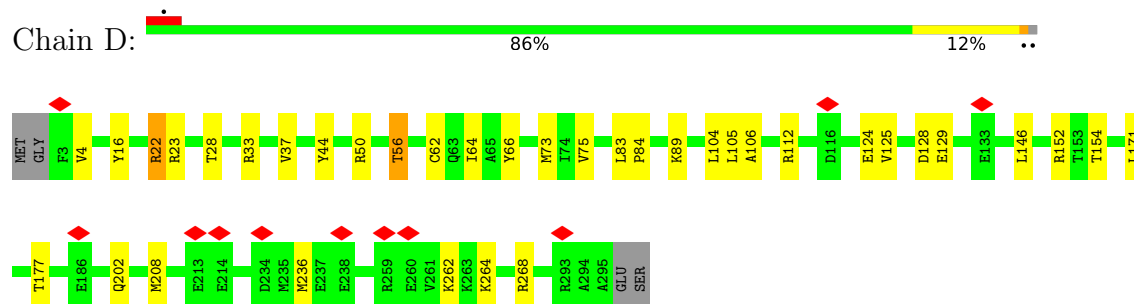


• Molecule 3: uL4

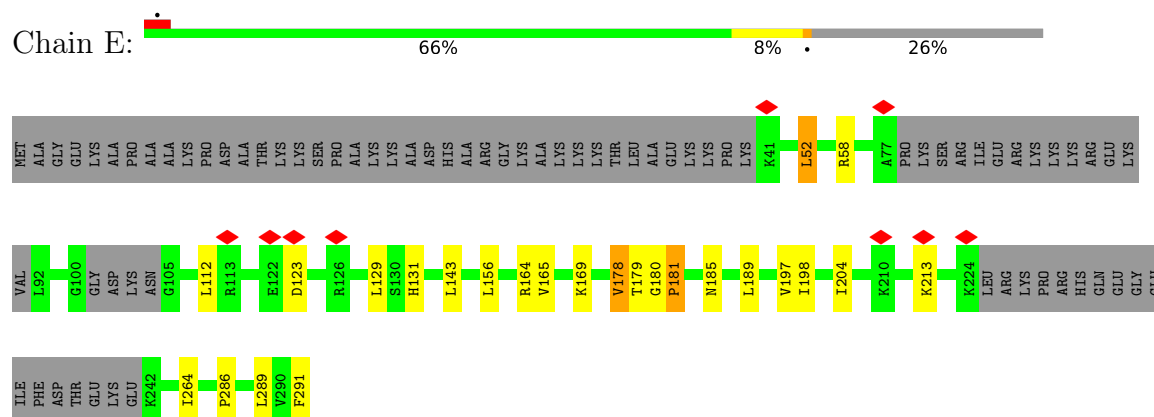
Chain C: 



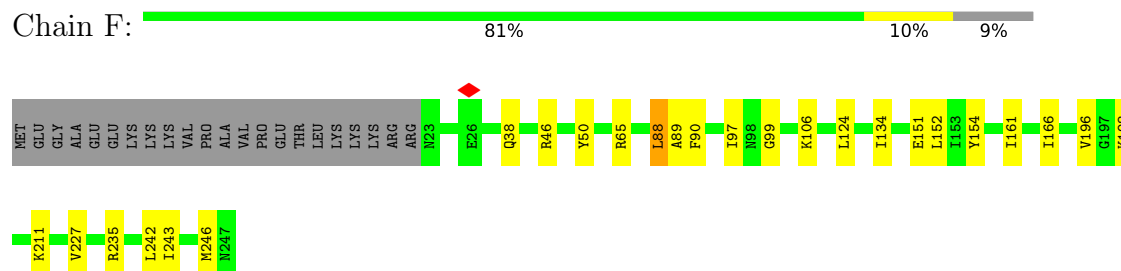
- Molecule 4: uL18



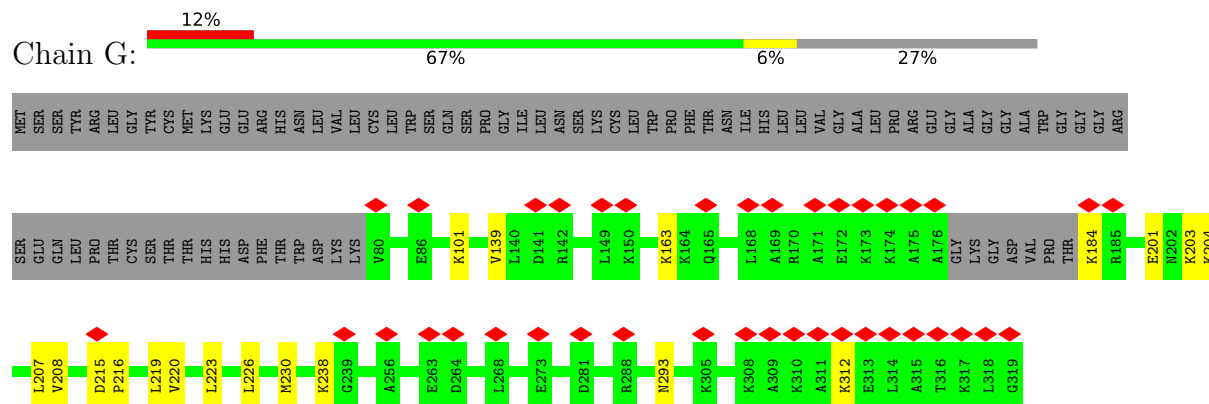
- Molecule 5: eL6



- Molecule 6: uL30



- Molecule 7: eL8



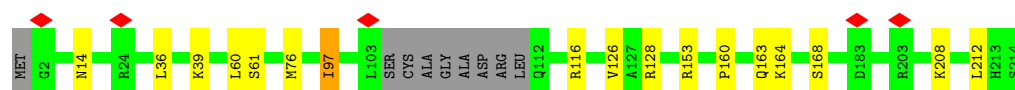
- Molecule 8: uL6

Chain H:  86% 12%

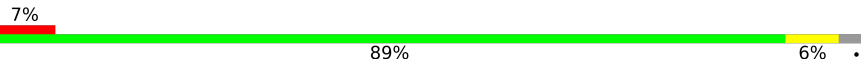


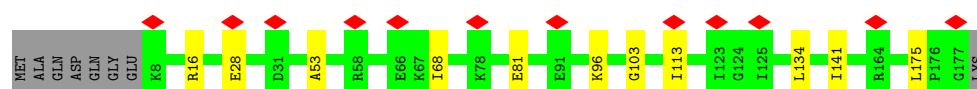
- Molecule 9: uL16

Chain I:  88% 7%

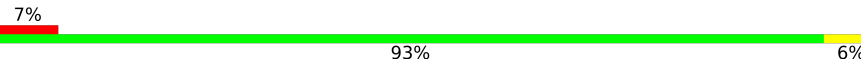


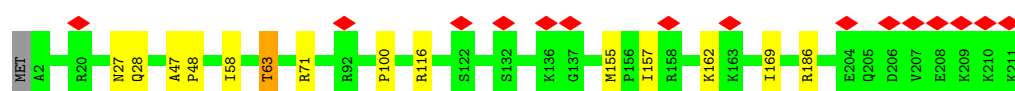
- Molecule 10: uL5

Chain J:  7% 89% 6%



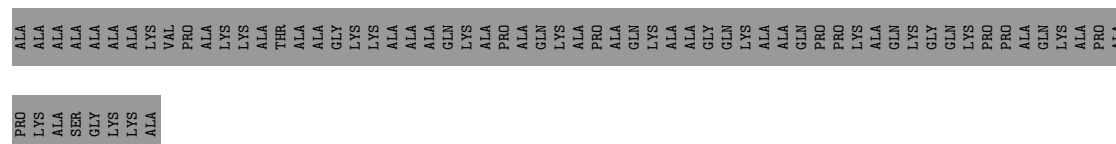
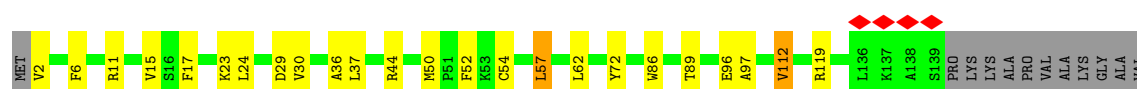
- Molecule 11: eL13

Chain L:  7% 93% 6%

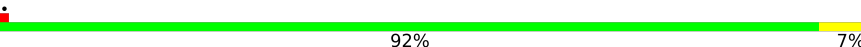


- Molecule 12: eL14

Chain M:  52% 10% 37%



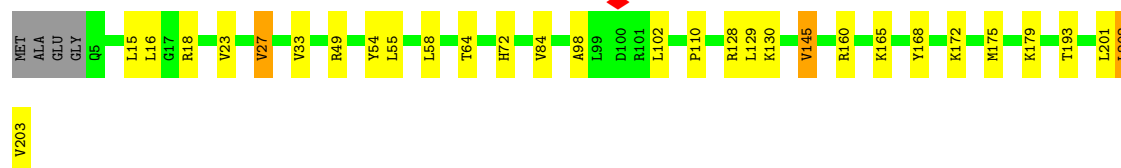
- Molecule 13: eL15

Chain N:  92% 7%



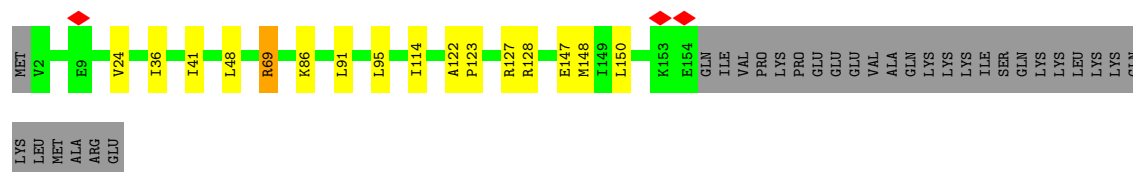
- Molecule 14: uL13

Chain O:  83% 13% ..



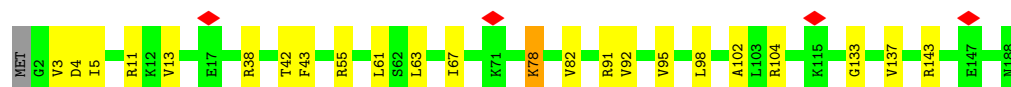
• Molecule 15: uL22

Chain P:  74% 8% 17%



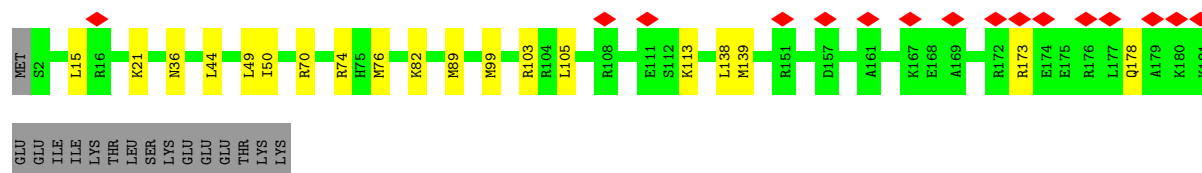
• Molecule 16: eL18

Chain Q:  87% 12% ..



• Molecule 17: eL19

Chain R:  8% 82% 10% 8%



• Molecule 18: eL20

Chain S:  88% 13%

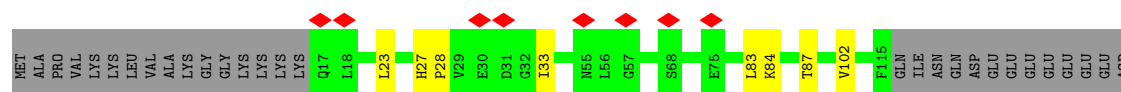


• Molecule 19: eL21

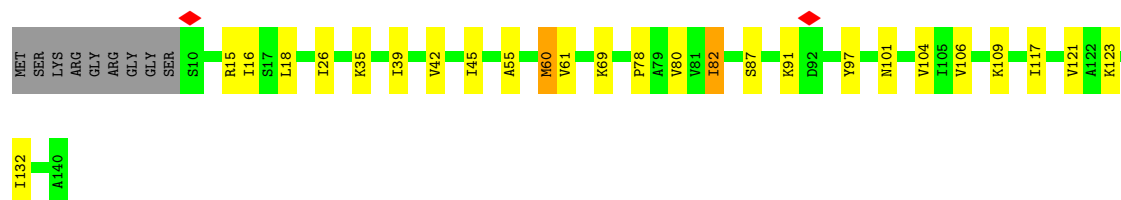
Chain T:  6% 89% 9% ..



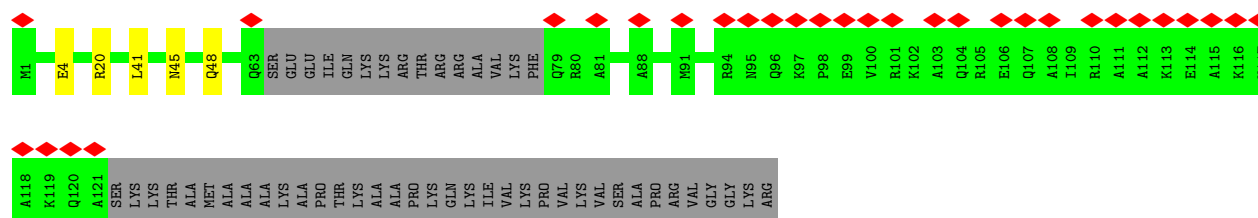
Chain U:



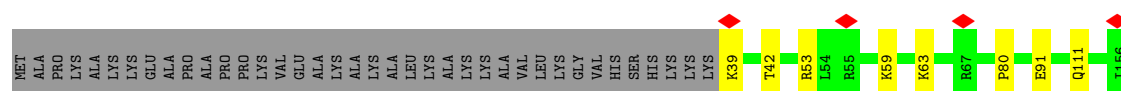
Chain V: 75% 17% 6%



Chain W:



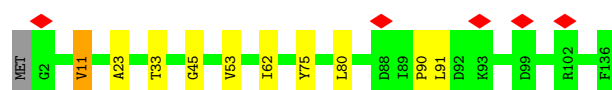
Chain X: 71% 5% 24%



Chain Y: 88% 8%

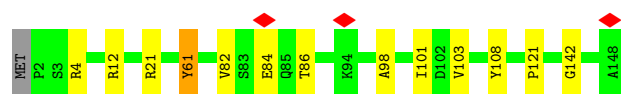


Chain Z: 92% 7%



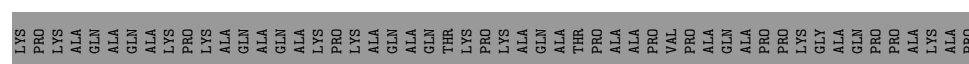
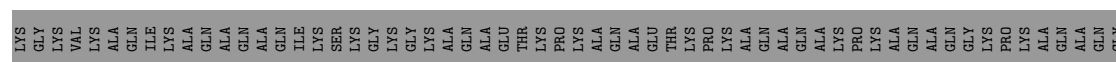
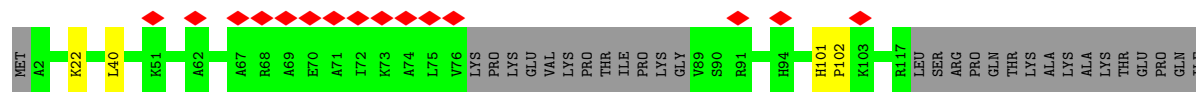
- Molecule 26: uL15

Chain a:  91% 8% ..



- Molecule 27: eL29

Chain b:  6% 41% 58%



- Molecule 28: eL30

Chain c:  5% 78% 7% 15%



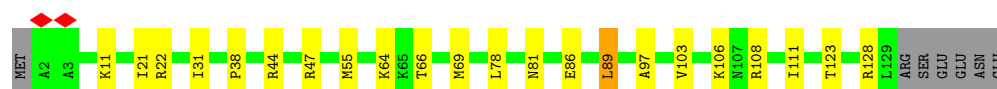
- Molecule 29: eL31

Chain d:  6% 70% 15% 14%



- Molecule 30: eL32

Chain e:  79% 16% 5%

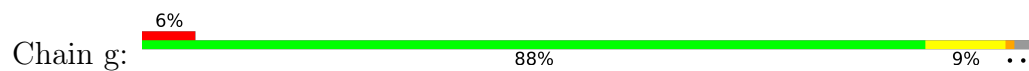


- Molecule 31: eL33

Chain f:  87% 11% ..



- Molecule 32: eL34



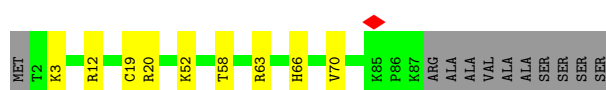
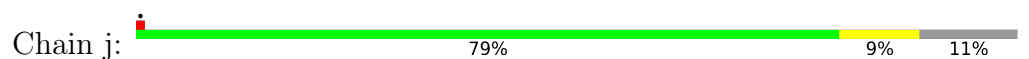
- Molecule 33: uL29



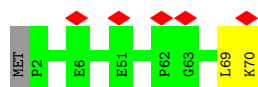
- Molecule 34: eL36



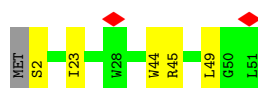
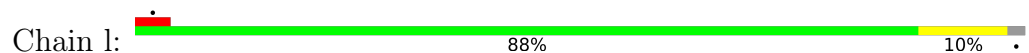
- Molecule 35: eL37



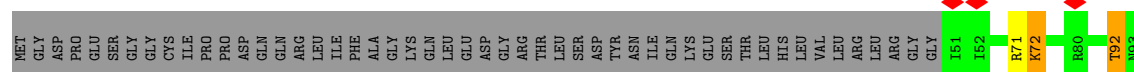
- Molecule 36: eL38



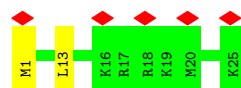
- Molecule 37: eL39



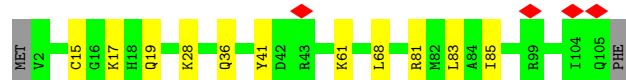
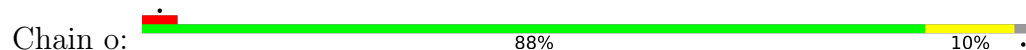
- Molecule 38: eL40



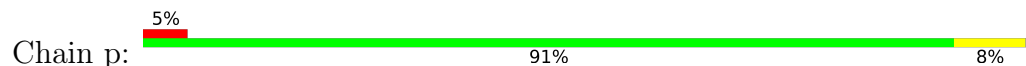
• Molecule 39: eL41



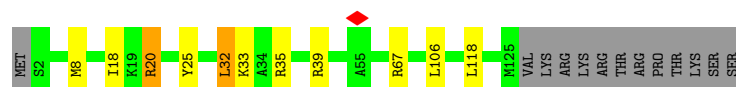
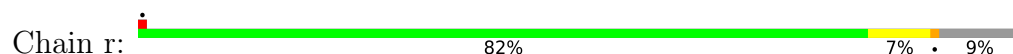
• Molecule 40: eL42



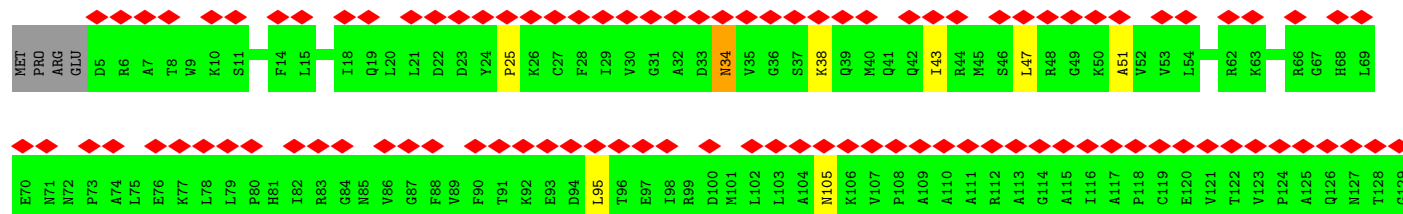
• Molecule 41: eL43

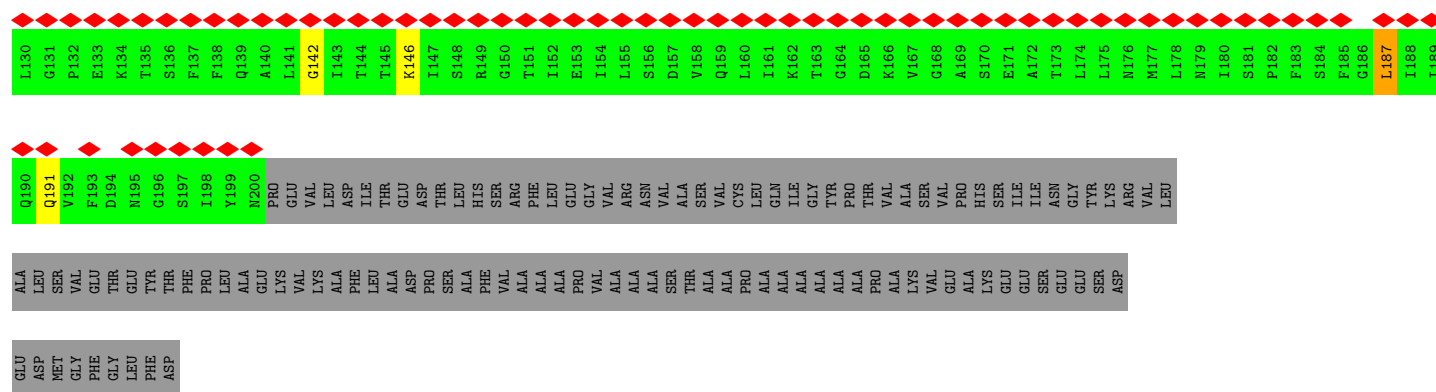


• Molecule 42: eL28

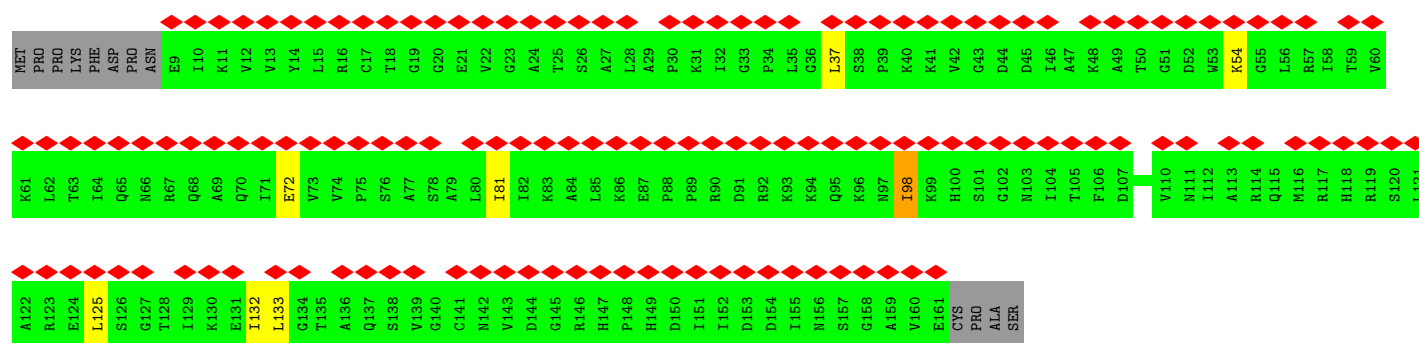
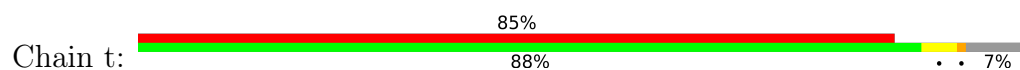


• Molecule 43: uL10

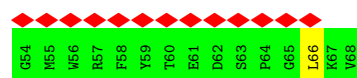
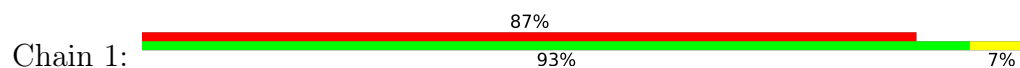




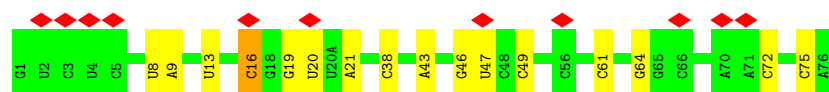
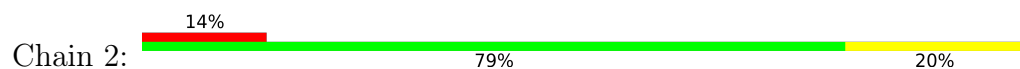
• Molecule 44: uL11



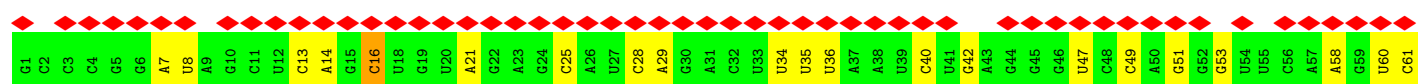
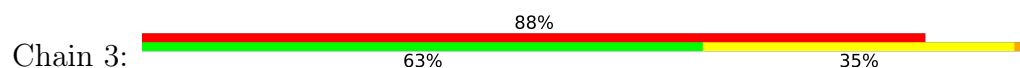
• Molecule 45: Nascent chain



• Molecule 46: P-site tRNA



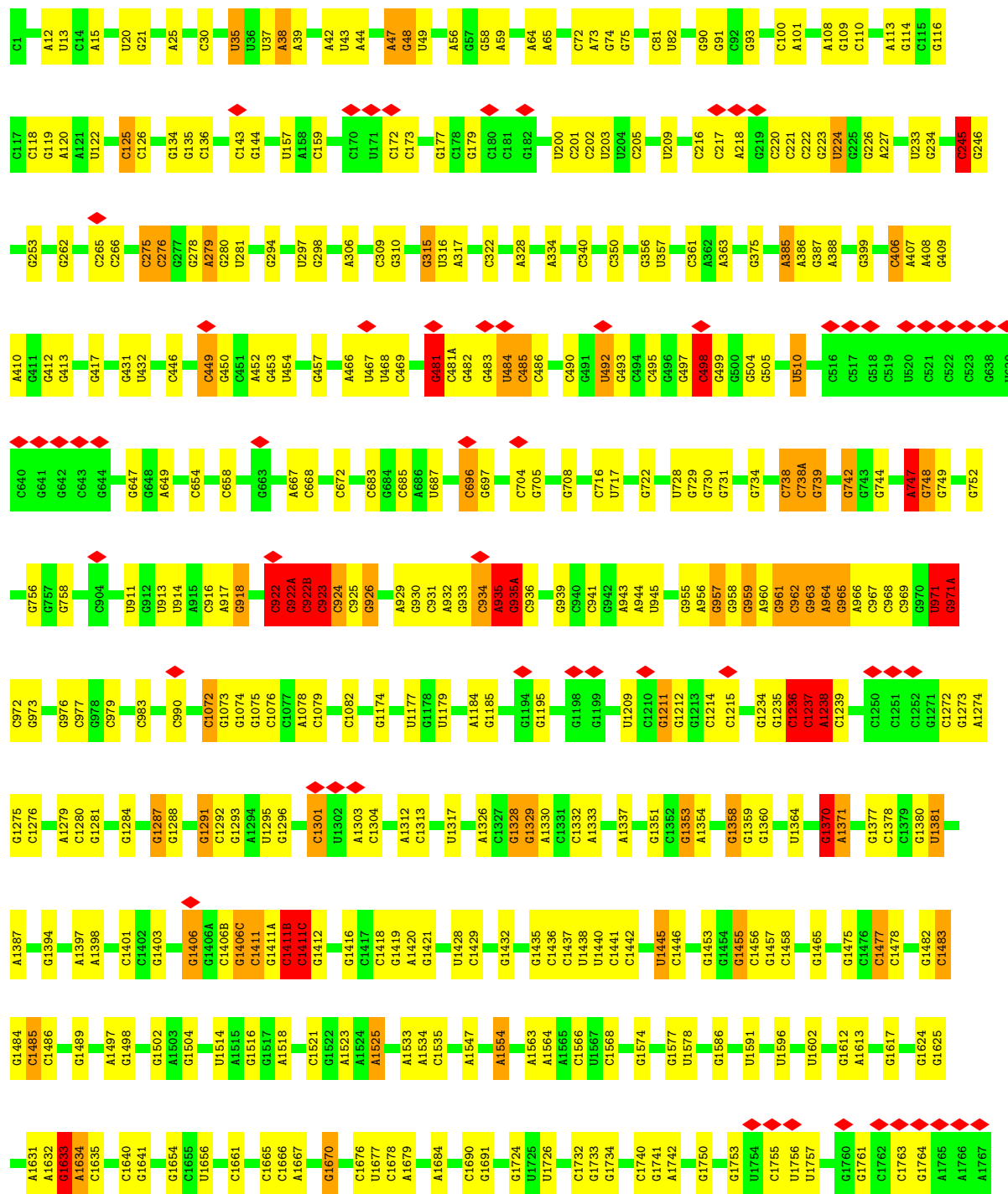
• Molecule 47: E-site tRNA

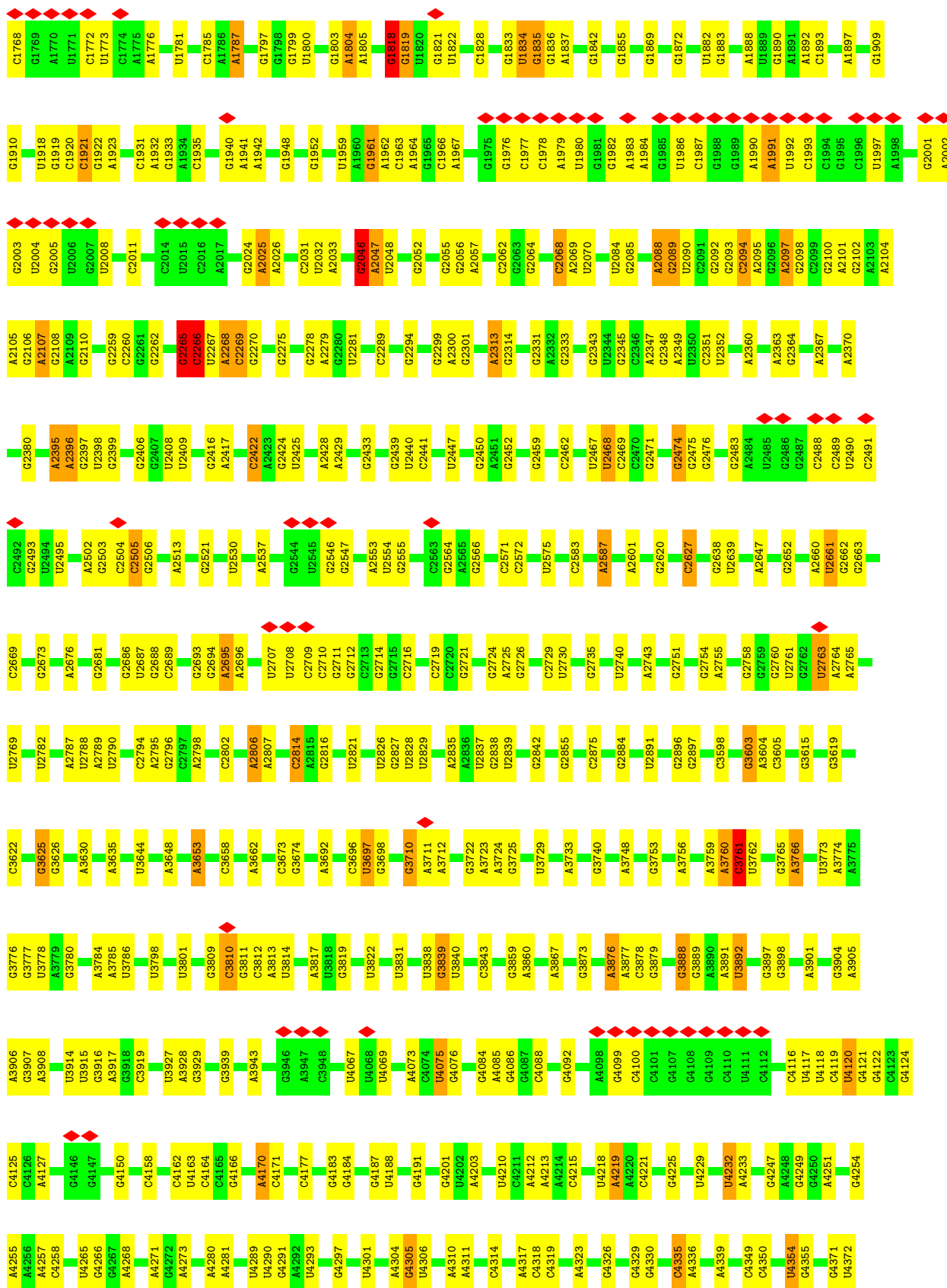


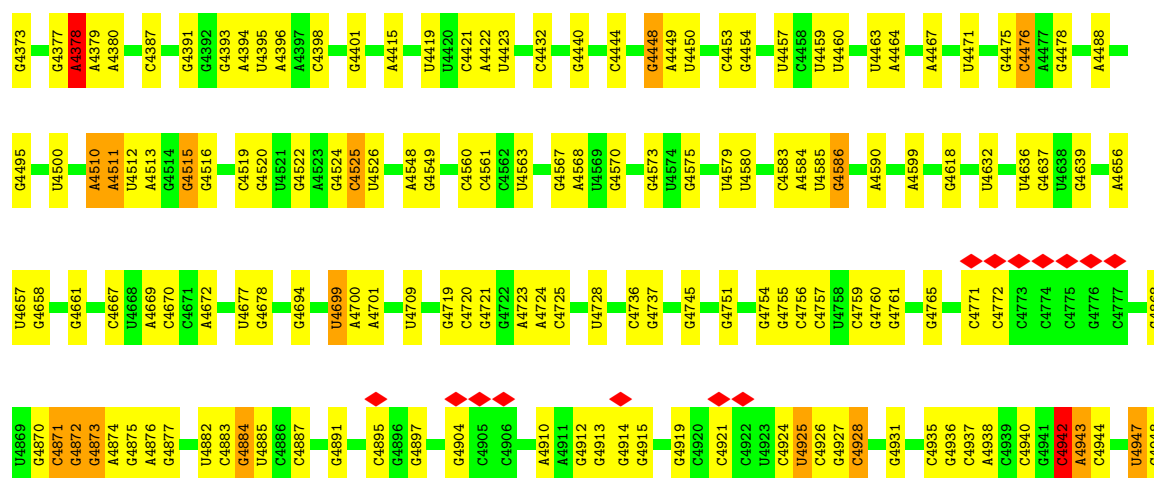


• Molecule 48: 28S ribosomal RNA

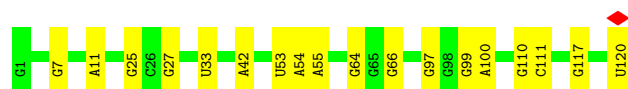
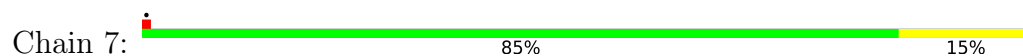
Chain 5: 69% 26%



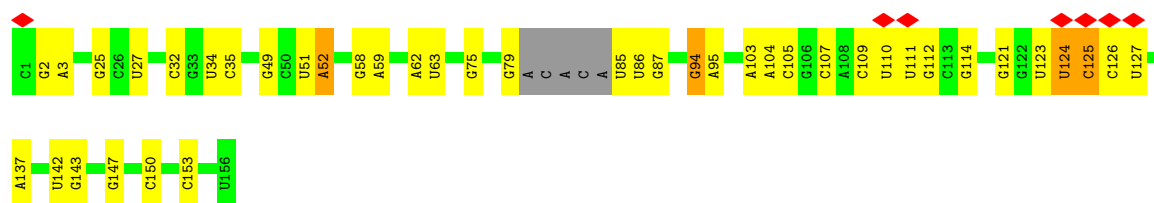




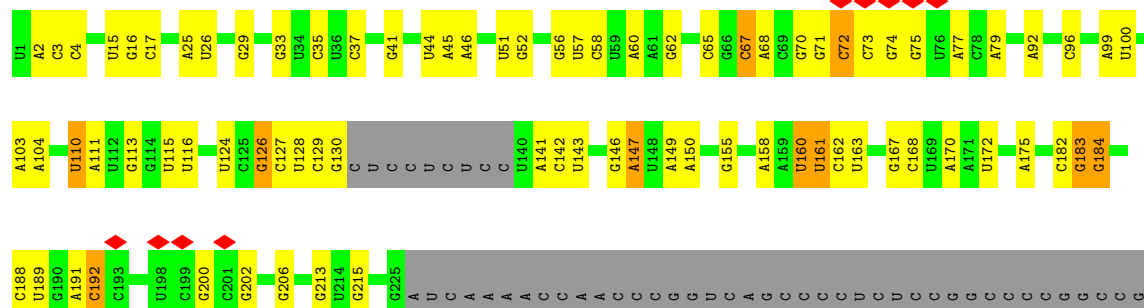
• Molecule 49: 5S ribosomal RNA



• Molecule 50: 5.8S ribosomal RNA

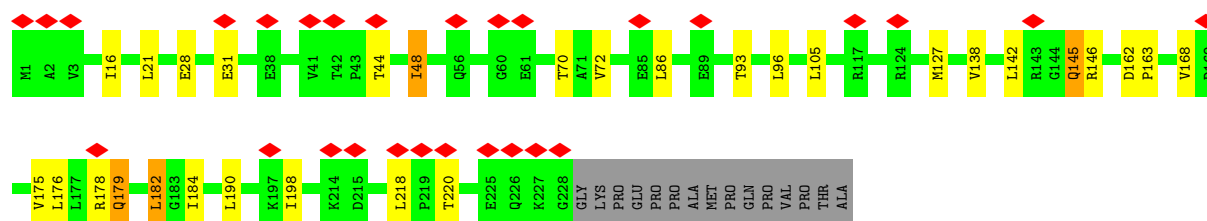
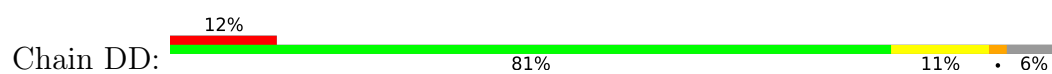


• Molecule 51: 18S ribosomal RNA

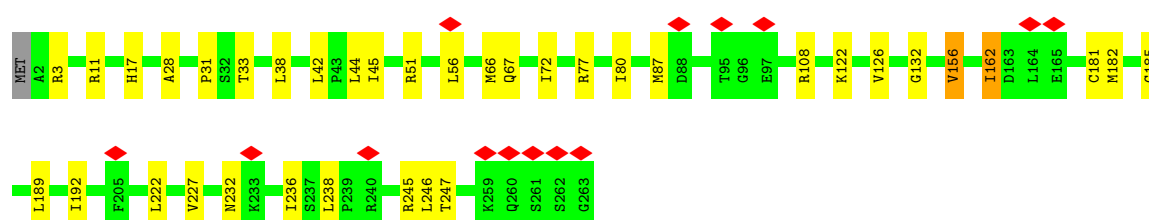
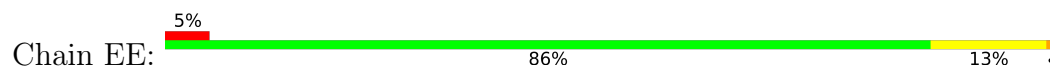




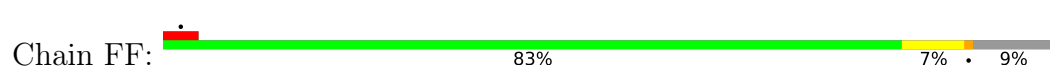




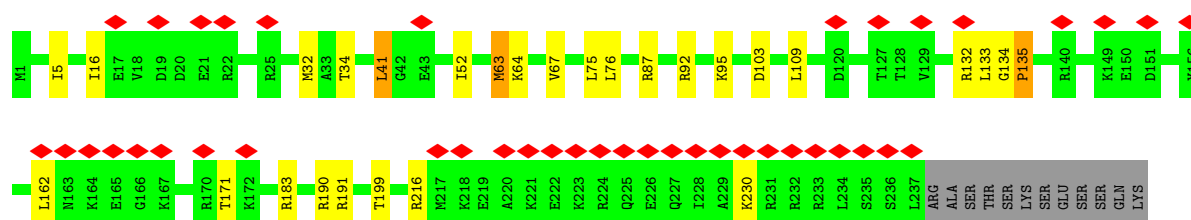
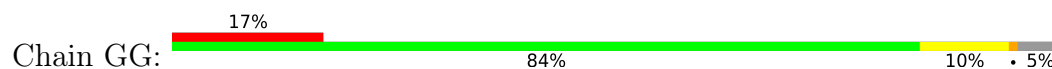
• Molecule 56: eS4



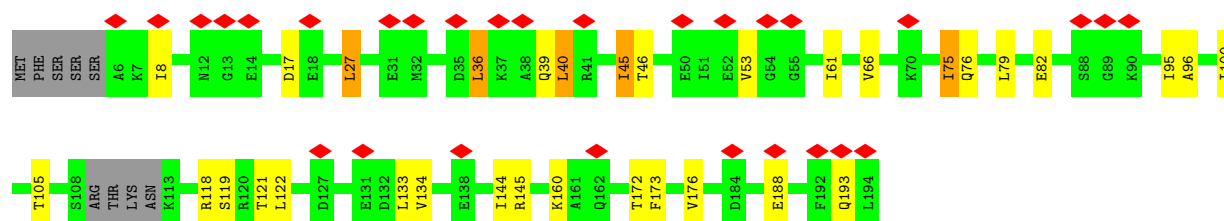
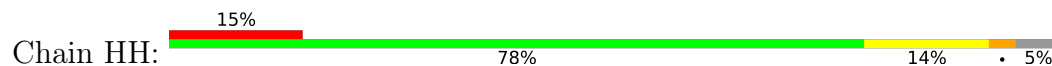
• Molecule 57: uS7



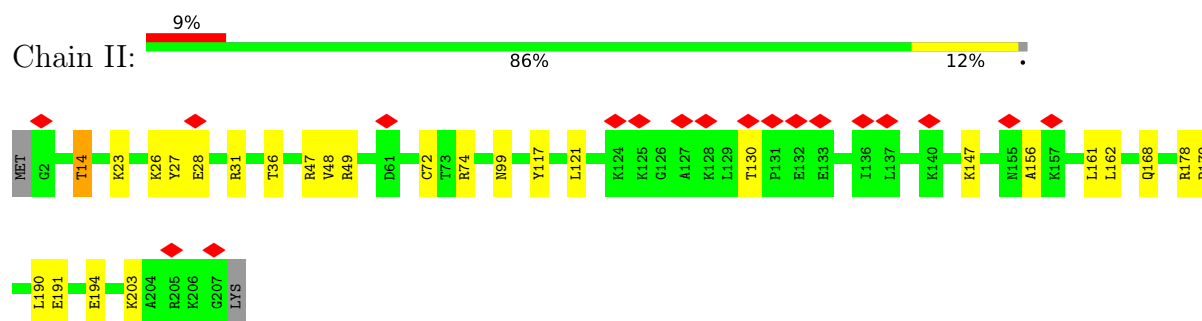
• Molecule 58: eS6



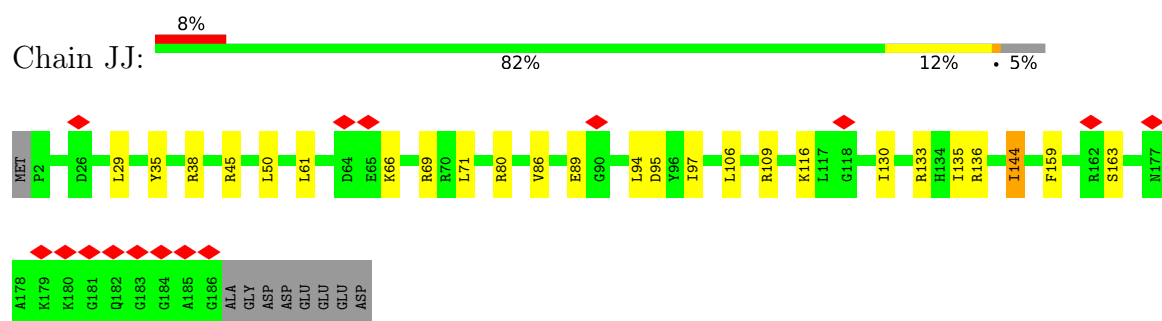
• Molecule 59: eS7



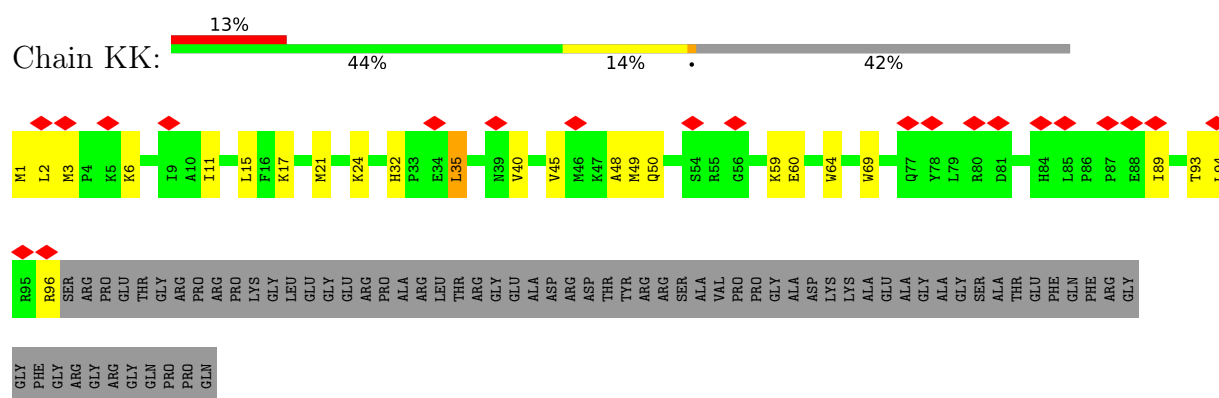
- Molecule 60: eS8



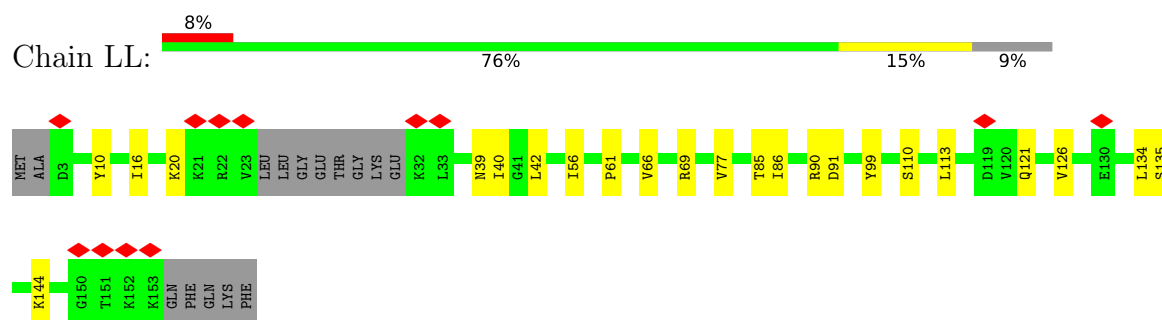
- Molecule 61: uS4



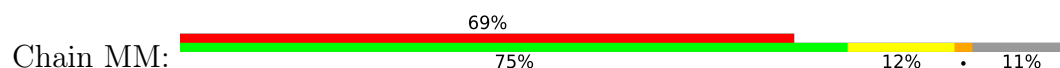
- Molecule 62: eS10



- Molecule 63: uS17

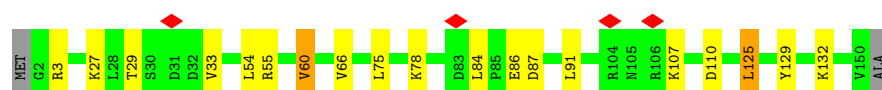


- Molecule 64: eS12

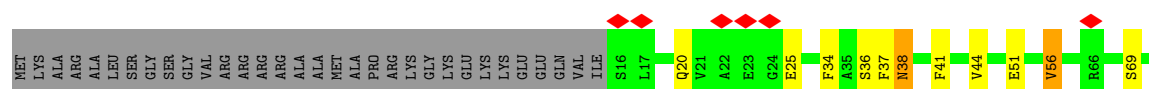




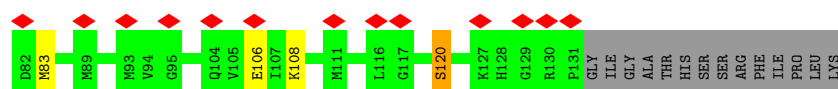
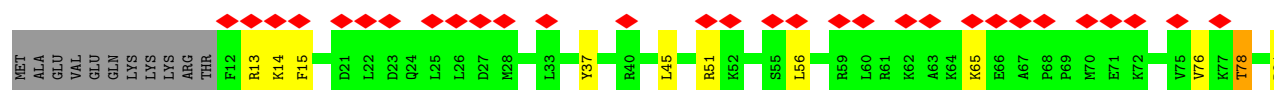
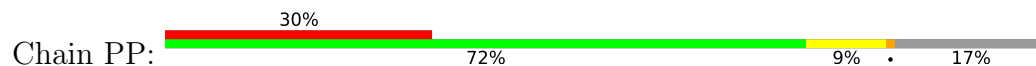
• Molecule 65: uS15



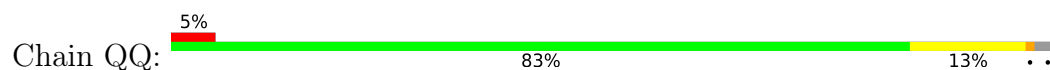
• Molecule 66: uS11



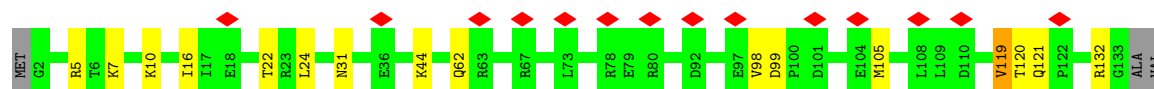
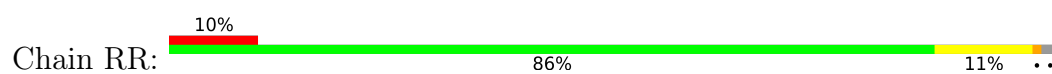
• Molecule 67: uS19



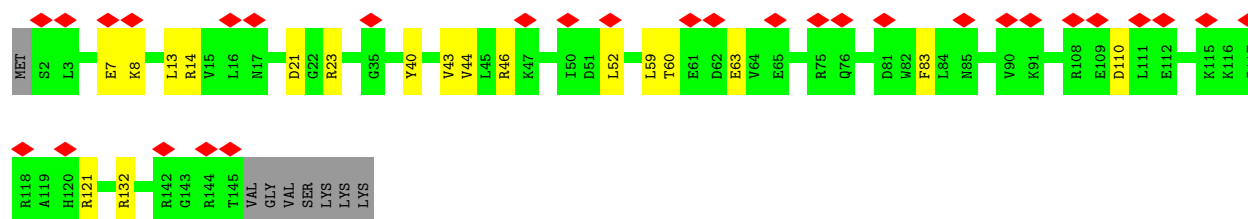
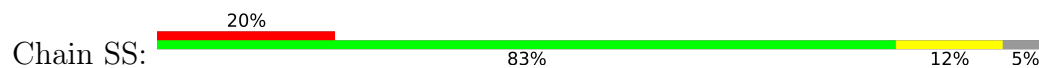
• Molecule 68: uS9



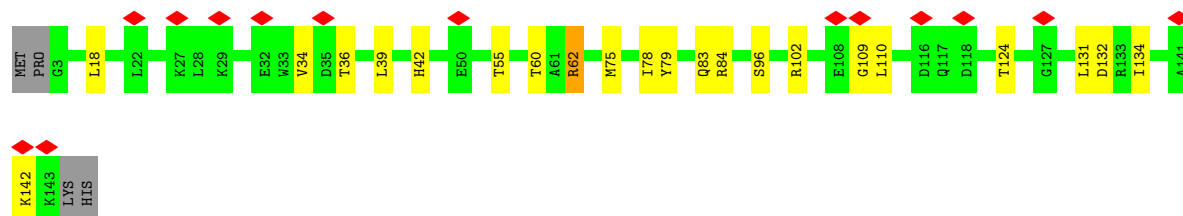
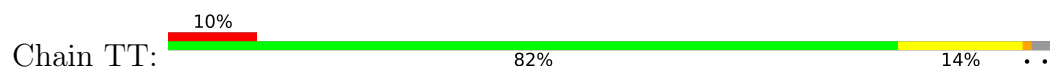
• Molecule 69: eS17



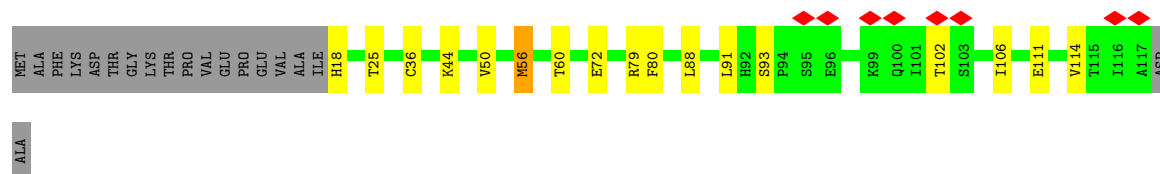
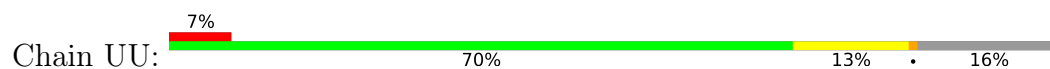
• Molecule 70: uS13



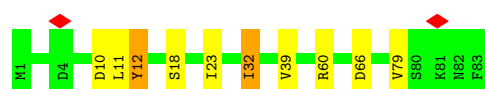
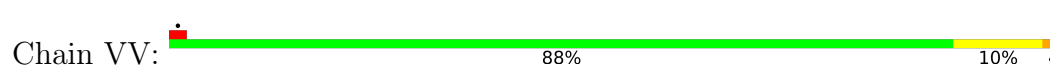
• Molecule 71: eS19



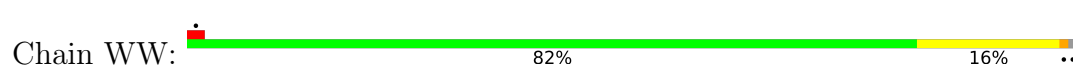
• Molecule 72: uS10

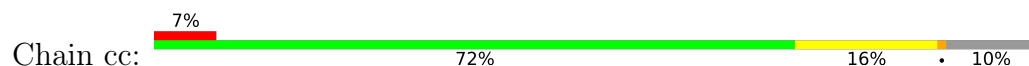


• Molecule 73: eS21

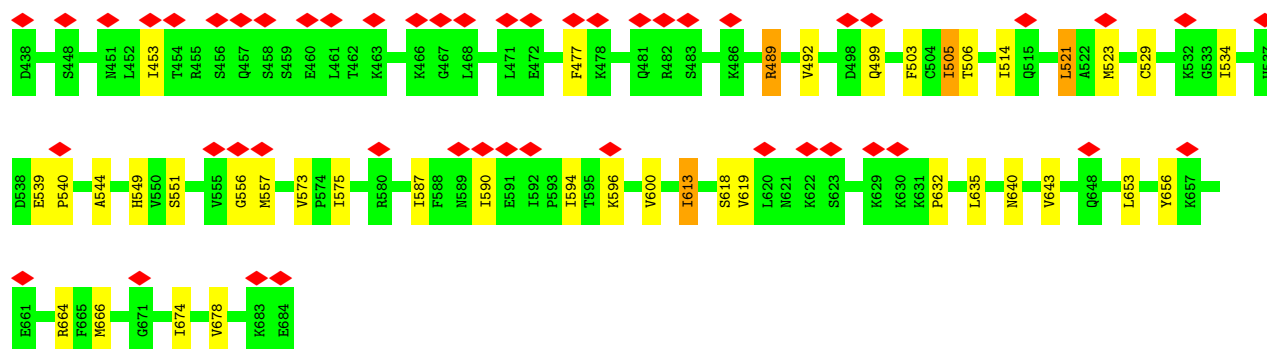


• Molecule 74: uS8









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	42011	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.703	Depositor
Minimum map value	-0.451	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	562.8, 562.8, 562.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3399999, 1.3399999, 1.3399999	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GCP, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.49	0/1936	0.80	0/2596
2	B	0.45	0/3240	0.77	1/4339 (0.0%)
3	C	0.47	0/2937	0.81	3/3946 (0.1%)
4	D	0.45	0/2437	0.80	0/3264
5	E	0.48	0/1762	0.77	0/2362
6	F	0.48	0/1911	0.83	0/2549
7	G	0.49	0/1910	0.81	0/2569
8	H	0.43	0/1535	0.72	0/2063
9	I	0.45	0/1702	0.77	0/2272
10	J	0.44	0/1385	0.75	0/1852
11	L	0.48	0/1733	0.80	0/2316
12	M	0.48	0/1158	0.86	0/1547
13	N	0.46	0/1746	0.82	0/2338
14	O	0.49	0/1662	0.84	1/2222 (0.0%)
15	P	0.47	0/1268	0.78	0/1700
16	Q	0.49	0/1539	0.80	0/2054
17	R	0.48	0/1524	0.81	0/2013
18	S	0.46	0/1501	0.76	0/2012
19	T	0.47	0/1326	0.76	0/1770
20	U	0.46	0/823	0.73	0/1104
21	V	0.50	0/993	0.79	0/1332
22	W	0.48	0/873	0.79	0/1158
23	X	0.44	0/984	0.77	0/1323
24	Y	0.45	0/1132	0.76	0/1504
25	Z	0.47	0/1130	0.76	0/1507
26	a	0.47	0/1191	0.79	1/1590 (0.1%)
27	b	0.45	0/861	0.79	0/1138
28	c	0.45	0/771	0.74	0/1034
29	d	0.47	0/903	0.77	0/1216
30	e	0.48	0/1071	0.80	0/1429
31	f	0.48	0/895	0.78	0/1198
32	g	0.46	0/916	0.81	1/1220 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.44	0/1021	0.80	0/1348
34	i	0.45	0/841	0.76	0/1112
35	j	0.45	0/720	0.81	0/952
36	k	0.43	0/575	0.73	0/761
37	l	0.43	0/459	0.75	0/608
38	m	0.48	0/435	0.80	0/575
39	n	0.43	0/240	0.85	0/305
40	o	0.42	0/864	0.71	0/1140
41	p	0.45	0/718	0.80	0/953
42	r	0.52	0/1010	0.82	0/1354
43	s	0.55	0/1530	0.74	0/2064
44	t	0.58	0/1174	0.82	0/1582
45	1	0.55	0/129	0.84	0/173
46	2	0.36	0/1805	0.68	0/2809
47	3	0.37	0/1777	0.68	0/2763
48	5	0.48	17/84961 (0.0%)	0.76	130/132460 (0.1%)
49	7	0.37	0/2858	0.71	0/4455
50	8	0.37	0/3581	0.70	2/5577 (0.0%)
51	9	0.38	0/40523	0.76	38/63130 (0.1%)
52	AA	0.50	0/1747	0.83	0/2374
53	BB	0.45	0/1756	0.82	0/2350
54	CC	0.48	0/1753	0.86	0/2369
55	DD	0.51	0/1796	0.80	0/2417
56	EE	0.50	0/2118	0.82	2/2849 (0.1%)
57	FF	0.47	0/1492	0.84	0/2005
58	GG	0.52	0/1946	0.85	2/2590 (0.1%)
59	HH	0.51	0/1510	0.80	0/2022
60	II	0.49	0/1715	0.78	0/2287
61	JJ	0.47	0/1550	0.88	2/2069 (0.1%)
62	KK	0.53	0/834	0.83	0/1125
63	LL	0.44	0/1195	0.74	1/1597 (0.1%)
64	MM	0.55	0/918	0.85	0/1233
65	NN	0.50	0/1226	0.83	0/1649
66	OO	0.50	0/1029	0.89	0/1380
67	PP	0.54	0/1017	0.85	0/1358
68	QQ	0.48	0/1146	0.79	0/1534
69	RR	0.49	0/1082	0.80	0/1452
70	SS	0.53	0/1208	0.83	0/1618
71	TT	0.54	0/1115	0.89	0/1493
72	UU	0.48	0/805	0.88	2/1081 (0.2%)
73	VV	0.52	0/643	0.84	0/860
74	WW	0.49	0/1051	0.83	0/1406
75	XX	0.46	0/1116	0.81	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	YY	0.50	0/1028	0.79	0/1366
77	ZZ	0.55	1/604 (0.2%)	0.84	0/810
78	aa	0.50	0/828	0.87	0/1109
79	bb	0.49	0/665	0.76	0/891
80	cc	0.50	0/490	0.82	0/656
81	dd	0.50	0/470	0.77	0/623
82	ee	0.48	0/447	0.80	0/587
83	ff	0.52	0/567	0.74	0/753
84	gg	0.47	0/2493	0.69	0/3394
85	hh	0.39	0/188	0.86	0/290
86	ii	0.48	0/2996	0.81	1/4050 (0.0%)
87	jj	0.50	0/3352	0.78	0/4523
All	All	0.46	18/237872 (0.0%)	0.77	187/348318 (0.1%)

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	2
6	F	0	1
48	5	0	3
75	XX	0	1
86	ii	0	2
All	All	0	9

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	935	A	C6-N6	77.14	2.88	1.33
48	5	922(A)	G	O3'-P	17.07	1.81	1.61
48	5	1411(C)	C	O5'-C5'	13.16	1.62	1.42
48	5	922	C	O3'-P	13.02	1.76	1.61
48	5	935	A	C5-C6	-9.29	1.22	1.41
48	5	1411	C	P-OP1	-7.59	1.33	1.49
48	5	922(B)	C	O5'-C5'	7.47	1.53	1.42
48	5	1411	C	P-O5'	7.15	1.70	1.59
48	5	922(A)	G	C3'-O3'	6.05	1.51	1.42
48	5	922(B)	C	O3'-P	5.99	1.70	1.61
48	5	971	U	C2-O2	-5.99	1.10	1.22
48	5	922	C	C3'-O3'	5.80	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	ZZ	62	VAL	CA-CB	5.70	1.56	1.54
48	5	922	C	O5'-C5'	5.65	1.50	1.42
48	5	1411	C	C5'-C4'	5.62	1.59	1.51
48	5	1411(B)	C	O3'-P	5.59	1.67	1.61
48	5	481	G	C2-N3	-5.40	1.22	1.32
48	5	923	C	O5'-C5'	5.31	1.50	1.42

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	481	G	C8-N9-C1'	-26.46	47.63	127.00
48	5	922	C	C2'-C3'-O3'	16.68	138.72	113.70
48	5	481	G	C4-N9-C1'	-15.80	79.09	126.50
51	9	1835	A	C2'-C3'-O3'	12.28	127.93	109.50
48	5	481	G	N1-C2-N2	-11.54	81.59	116.20
48	5	1411(C)	C	P-O5'-C5'	11.37	137.95	120.90
48	5	935	A	C5-C6-N6	-10.41	92.47	123.70
48	5	47	A	C4'-C3'-O3'	10.39	124.98	109.40
48	5	385	A	C4'-C3'-O3'	10.38	124.97	109.40
51	9	1820	G	C1'-C2'-O2'	-9.72	93.81	108.40
48	5	2046	G	C2'-C3'-O3'	9.55	123.83	109.50
48	5	922	C	C3'-C2'-O2'	9.46	124.89	110.70
48	5	922	C	C4'-C3'-C2'	-9.39	93.21	102.60
48	5	2695	A	C2'-C3'-O3'	9.17	123.25	109.50
48	5	3888	G	C2'-C3'-O3'	9.07	127.30	113.70
51	9	1394	G	C2'-C3'-O3'	9.05	127.28	113.70
48	5	922(B)	C	C1'-C2'-O2'	-8.97	94.94	108.40
48	5	1411	C	C4'-C3'-O3'	8.78	126.17	113.00
48	5	481	G	N3-C2-N2	-8.76	93.63	119.90
48	5	481	G	N9-C1'-C2'	8.40	124.60	112.00
48	5	922(B)	C	C2'-C3'-O3'	-8.24	101.34	113.70
48	5	2474	G	C2'-C3'-O3'	8.24	121.86	109.50
48	5	2068	C	C4'-C3'-O3'	8.21	121.71	109.40
48	5	922(B)	C	C4'-C3'-O3'	8.13	125.19	113.00
48	5	1834	U	C2'-C3'-O3'	8.06	121.58	109.50
48	5	935	A	C6-N1-C2	-7.99	94.62	118.60
48	5	1370	G	C2'-C3'-O3'	7.97	121.45	109.50
14	O	110	PRO	N-CA-C	7.96	120.41	110.70
51	9	1664	A	C4'-C3'-O3'	7.94	121.31	109.40
48	5	1485	C	C2'-C3'-O3'	7.83	121.24	109.50
48	5	48	G	C2'-C3'-O3'	7.70	121.05	109.50
48	5	922	C	O4'-C4'-C3'	-7.64	96.36	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	3619	G	C4'-C3'-O3'	-7.63	101.55	113.00
48	5	2468	U	C4'-C3'-O3'	7.61	120.82	109.40
48	5	4942	C	C4'-C3'-O3'	7.49	120.63	109.40
51	9	870	A	C4'-C3'-O3'	7.46	120.60	109.40
48	5	498	C	C4'-C3'-O3'	7.36	120.44	109.40
58	GG	134	GLY	CA-C-N	7.30	128.97	119.84
58	GG	134	GLY	C-N-CA	7.30	128.97	119.84
51	9	1821	U	N1-C1'-C2'	-7.30	101.05	112.00
51	9	1820	G	C4'-C3'-O3'	7.19	123.79	113.00
48	5	3697	U	C2'-C3'-O3'	7.13	124.39	113.70
48	5	922(A)	G	P-O3'-C3'	7.11	128.23	119.70
51	9	688	U	C2'-C3'-O3'	7.09	120.14	109.50
48	5	1477	C	C2'-C3'-O3'	7.08	124.33	113.70
48	5	922(A)	G	N9-C1'-C2'	7.07	122.61	112.00
48	5	4232	U	C4'-C3'-O3'	7.07	120.00	109.40
51	9	1253	A	C2'-C3'-O3'	7.04	120.06	109.50
48	5	922(B)	C	P-O5'-C5'	7.02	131.44	120.90
48	5	4448	G	C4'-C3'-O3'	6.98	123.47	113.00
48	5	2587	A	C2'-C3'-O3'	-6.91	103.33	113.70
51	9	1130	G	C4'-C3'-O3'	6.88	123.32	113.00
48	5	1329	G	C2'-C3'-O3'	6.87	124.00	113.70
48	5	922	C	C5'-C4'-O4'	6.84	120.06	109.80
51	9	72	C	C4'-C3'-O3'	6.84	119.66	109.40
48	5	406	C	C2'-C3'-O3'	6.81	123.92	113.70
48	5	1455	G	C2'-C3'-O3'	6.80	123.89	113.70
48	5	971(A)	G	C4'-C3'-O3'	6.78	123.17	113.00
51	9	1061	U	C2'-C3'-O3'	-6.77	103.55	113.70
48	5	4925	U	C2'-C3'-O3'	6.65	119.48	109.50
48	5	1211	G	C2'-C3'-O3'	6.62	123.62	113.70
48	5	696	C	C2'-C3'-O3'	6.60	119.40	109.50
48	5	492	U	C2'-C3'-O3'	6.55	119.33	109.50
3	C	340	ILE	N-CA-C	-6.54	105.93	111.56
48	5	1411	C	C5'-C4'-C3'	6.54	125.81	116.00
61	JJ	163	SER	N-CA-C	6.50	113.98	108.13
51	9	1520	G	C4'-C3'-O3'	6.41	122.62	113.00
48	5	922	C	C1'-C2'-O2'	-6.39	98.82	108.40
48	5	923	C	P-O5'-C5'	6.34	130.41	120.90
48	5	935	A	C1'-O4'-C4'	-6.33	103.37	109.70
48	5	935(A)	G	C2'-C3'-O3'	6.33	123.19	113.70
51	9	1395	C	C4'-C3'-O3'	6.30	122.45	113.00
51	9	1646	C	C2'-C3'-O3'	6.28	123.12	113.70
48	5	4075	U	C2'-C3'-O3'	6.27	118.91	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	922	C	N1-C1'-C2'	-6.25	102.62	112.00
50	8	124	U	C4'-C3'-O3'	6.22	118.72	109.40
48	5	4947	U	C2'-C3'-O3'	6.21	123.02	113.70
48	5	747	A	C4'-C3'-O3'	6.21	118.71	109.40
48	5	2266	C	C2'-C3'-O3'	6.21	118.81	109.50
48	5	1358	G	C4'-C3'-O3'	6.18	118.67	109.40
48	5	1804	A	C2'-C3'-O3'	6.15	118.72	109.50
48	5	959	G	C2'-C3'-O3'	6.15	118.72	109.50
48	5	38	A	C4'-C3'-O3'	-6.14	103.79	113.00
48	5	2089	G	C2'-C3'-O3'	6.14	118.71	109.50
48	5	935	A	C4-C5-C6	-6.13	98.61	117.00
48	5	1406(C)	G	C3'-C2'-O2'	6.12	119.88	110.70
48	5	922(B)	C	N1-C1'-C2'	6.11	121.17	112.00
48	5	1072	C	C2'-C3'-O3'	6.11	118.67	109.50
48	5	935	A	O4'-C4'-C3'	-6.08	100.02	106.10
48	5	449	C	C2'-C3'-O3'	6.07	118.60	109.50
51	9	1264	C	C4'-C3'-O3'	6.07	118.50	109.40
48	5	2661	U	C2'-C3'-O3'	6.05	118.58	109.50
51	9	1313	A	C4'-C3'-O3'	6.04	118.45	109.40
48	5	1291	G	C2'-C3'-O3'	6.03	122.75	113.70
51	9	752	G	C2'-C3'-O3'	6.02	118.53	109.50
48	5	4378	A	C2'-C3'-O3'	6.01	118.51	109.50
48	5	245	C	C2'-C3'-O3'	5.99	122.68	113.70
48	5	125	C	C2'-C3'-O3'	5.97	122.65	113.70
48	5	1287	G	C4'-C3'-O3'	5.96	118.34	109.40
48	5	738	C	C1'-C2'-O2'	5.94	120.71	111.80
26	a	61	TYR	N-CA-C	5.93	117.55	111.14
48	5	971	U	O4'-C1'-C2'	-5.92	101.69	107.60
48	5	922(B)	C	C5'-C4'-C3'	5.91	124.86	116.00
48	5	4170	A	C2'-C3'-O3'	5.91	118.36	109.50
51	9	160	U	C4'-C3'-O3'	5.87	118.21	109.40
51	9	642	U	C4'-C3'-O3'	5.82	121.73	113.00
48	5	3876	A	C2'-C3'-O3'	5.81	118.22	109.50
48	5	924	C	C2'-C3'-O3'	-5.80	105.00	113.70
48	5	2089	G	C4'-C3'-O3'	5.79	118.08	109.40
48	5	1732	C	C4'-C3'-O3'	-5.78	104.33	113.00
48	5	1921	C	C2'-C3'-O3'	5.76	118.14	109.50
51	9	1820	G	N9-C1'-C2'	-5.75	103.38	112.00
51	9	110	U	C2'-C3'-O3'	5.72	122.29	113.70
61	JJ	144	ILE	N-CA-C	5.71	114.24	107.73
48	5	90	G	C4'-C3'-O3'	-5.67	104.50	113.00
51	9	434	G	C4'-C3'-O3'	5.66	121.49	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	74	ALA	N-CA-C	5.66	119.66	112.87
48	5	1411	C	O4'-C4'-C3'	-5.63	98.37	104.00
48	5	4699	U	C4'-C3'-O3'	5.62	117.84	109.40
48	5	1445	U	C2'-C3'-O3'	5.62	122.13	113.70
48	5	4335	C	C4'-C3'-O3'	-5.62	104.57	113.00
48	5	1406	G	O4'-C4'-C3'	-5.59	100.51	106.10
48	5	484	U	C4'-C3'-O3'	5.58	117.77	109.40
51	9	594	A	C4'-C3'-O3'	5.58	117.77	109.40
48	5	2452	G	C4'-C3'-O3'	-5.57	104.64	113.00
50	8	94	G	C2'-C3'-O3'	5.55	117.83	109.50
48	5	738	C	C4'-C3'-O3'	-5.54	101.08	109.40
48	5	3603	G	C2'-C3'-O3'	5.53	122.00	113.70
48	5	3603	G	C4'-C3'-O3'	-5.52	104.72	113.00
56	EE	108	ARG	N-CA-C	5.51	117.19	110.41
48	5	48	G	C4'-C3'-O3'	5.50	117.65	109.40
51	9	687	C	C2'-C3'-O3'	5.50	117.75	109.50
51	9	434	G	C2'-C3'-O3'	5.49	121.93	113.70
86	ii	209	SER	N-CA-C	5.47	112.94	108.07
51	9	170	A	C4'-C3'-O3'	-5.47	104.80	113.00
51	9	1130	G	C3'-C2'-O2'	5.46	118.89	110.70
51	9	501	C	N1-C1'-C2'	5.45	120.17	112.00
51	9	1137	U	C2'-C3'-O3'	5.44	121.86	113.70
48	5	1428	U	C4'-C3'-O3'	-5.43	104.85	113.00
51	9	532	C	C2'-C3'-O3'	5.43	121.84	113.70
51	9	1821	U	C3'-C2'-O2'	5.42	118.84	110.70
48	5	1670	G	C2'-C3'-O3'	-5.42	105.58	113.70
48	5	3697	U	C3'-C2'-O2'	5.40	118.80	110.70
48	5	971	U	N3-C2-O2	-5.37	106.11	122.20
56	EE	156	VAL	N-CA-C	5.33	116.06	110.62
51	9	1825	A	C4'-C3'-O3'	-5.32	105.02	113.00
63	LL	99	TYR	N-CA-C	-5.31	100.51	108.96
48	5	3710	G	C4'-C3'-O3'	5.31	117.36	109.40
51	9	553	U	C3'-C2'-O2'	5.29	118.64	110.70
48	5	935	A	C1'-C2'-O2'	5.28	119.72	111.80
51	9	874	G	C2'-C3'-O3'	5.25	121.58	113.70
72	UU	72	GLU	N-CA-C	5.25	117.23	107.99
48	5	4884	G	C2'-C3'-O3'	5.25	121.57	113.70
48	5	1428	U	C2'-C3'-O3'	5.25	121.57	113.70
48	5	1818	G	C2'-C3'-O3'	5.25	121.57	113.70
48	5	3625	G	C2'-C3'-O3'	5.24	121.56	113.70
48	5	1835	G	C2'-C3'-O3'	5.24	117.36	109.50
48	5	275	C	C2'-C3'-O3'	5.22	121.54	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	922(B)	C	C3'-C2'-O2'	5.22	118.53	110.70
48	5	275	C	C4'-C3'-O3'	5.20	120.80	113.00
48	5	2088	A	C2'-C3'-O3'	5.19	117.28	109.50
48	5	2313	A	C2'-C3'-O3'	5.16	117.25	109.50
48	5	4632	U	C4'-C3'-O3'	-5.16	105.26	113.00
72	UU	93	SER	N-CA-C	5.15	112.65	108.07
3	C	232	VAL	CB-CA-C	-5.14	105.30	112.04
48	5	1485	C	C4'-C3'-O3'	5.14	117.11	109.40
51	9	126	G	C4'-C3'-O3'	5.14	117.11	109.40
48	5	4525	C	C3'-C2'-O2'	5.12	118.38	110.70
48	5	485	C	C3'-C2'-O2'	5.09	118.34	110.70
2	B	262	VAL	N-CA-CB	5.09	116.27	110.72
48	5	1072	C	C4'-C3'-O3'	5.08	117.02	109.40
48	5	1238	A	C3'-C2'-O2'	5.06	118.29	110.70
48	5	2265	G	C4'-C3'-O3'	5.06	116.99	109.40
48	5	2299	G	C2'-C3'-O3'	-5.06	106.11	113.70
51	9	1489	A	C4'-C3'-O3'	5.05	120.58	113.00
48	5	1237	C	C2'-C3'-O3'	-5.05	106.12	113.70
48	5	481	G	C6-N1-C2	-5.05	109.95	125.10
48	5	1236	C	C4'-C3'-O3'	5.05	120.57	113.00
48	5	922	C	P-O5'-C5'	5.04	128.47	120.90
48	5	1406(C)	G	C4'-C3'-O3'	5.04	120.56	113.00
48	5	4232	U	C2'-C3'-O3'	5.03	117.04	109.50
51	9	553	U	C2'-C3'-O3'	5.02	121.23	113.70
48	5	971	U	N1-C2-O2	-5.01	107.77	122.80
48	5	3761	C	N1-C1'-C2'	-5.01	104.48	112.00
32	g	5	LEU	N-CA-C	5.01	116.67	108.76
48	5	1445	U	C3'-C2'-O2'	5.01	118.22	110.70
48	5	1633	G	C4'-C3'-O3'	5.01	120.52	113.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	5	481	G	Sidechain
48	5	935	A	Sidechain
48	5	971	U	Sidechain
2	B	16	PHE	Peptide
2	B	258	HIS	Peptide
6	F	235	ARG	Peptide
75	XX	61	GLN	Peptide
86	ii	45	ARG	Sidechain

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Mol	Chain	Res	Type	Group
86	ii	62	ARG	Sidechain

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	18	0
2	B	3172	0	3310	19	0
3	C	2883	0	3053	16	0
4	D	2391	0	2424	16	0
5	E	1729	0	1887	10	0
6	F	1875	0	1995	12	0
7	G	1879	0	2027	5	0
8	H	1516	0	1597	8	0
9	I	1664	0	1712	4	0
10	J	1362	0	1399	3	0
11	L	1702	0	1820	7	0
12	M	1137	0	1211	14	0
13	N	1701	0	1749	7	0
14	O	1630	0	1778	17	0
15	P	1242	0	1274	6	0
16	Q	1515	0	1634	10	0
17	R	1508	0	1664	7	0
18	S	1462	0	1508	11	0
19	T	1298	0	1366	7	0
20	U	809	0	833	5	0
21	V	979	0	1039	11	0
22	W	860	0	903	2	0
23	X	967	0	1040	2	0
24	Y	1115	0	1205	1	0
25	Z	1107	0	1182	5	0
26	a	1162	0	1209	8	0
27	b	848	0	920	0	0
28	c	761	0	794	2	0
29	d	888	0	930	11	0
30	e	1053	0	1147	10	0
31	f	876	0	912	4	0
32	g	906	0	1000	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	h	1013	0	1147	3	0
34	i	830	0	916	2	0
35	j	705	0	737	5	0
36	k	569	0	637	0	0
37	l	447	0	480	3	0
38	m	429	0	465	1	0
39	n	239	0	289	0	0
40	o	851	0	920	4	0
41	p	708	0	756	3	0
42	r	994	0	1051	3	0
43	s	1507	0	1564	3	0
44	t	1160	0	1218	2	0
45	1	125	0	117	1	0
46	2	1616	0	824	2	0
47	3	1593	0	811	2	0
48	5	75972	0	38402	303	0
49	7	2558	0	1296	3	0
50	8	3208	0	1629	6	0
51	9	36249	0	18314	218	0
52	AA	1710	0	1708	19	0
53	BB	1729	0	1803	10	0
54	CC	1716	0	1806	15	0
55	DD	1768	0	1866	28	0
56	EE	2076	0	2177	14	0
57	FF	1471	0	1522	7	0
58	GG	1923	0	2089	12	0
59	HH	1488	0	1582	12	0
60	II	1686	0	1772	10	0
61	JJ	1525	0	1640	7	0
62	KK	810	0	836	10	0
63	LL	1175	0	1249	3	0
64	MM	908	0	939	6	0
65	NN	1202	0	1289	6	0
66	OO	1016	0	1039	12	0
67	PP	997	0	1045	2	0
68	QQ	1128	0	1195	8	0
69	RR	1068	0	1121	3	0
70	SS	1190	0	1249	4	0
71	TT	1097	0	1132	7	0
72	UU	795	0	862	4	0
73	VV	636	0	637	5	0
74	WW	1034	0	1080	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	XX	1098	0	1167	7	0
76	YY	1011	0	1083	7	0
77	ZZ	598	0	656	5	0
78	aa	814	0	865	11	0
79	bb	651	0	672	3	0
80	cc	488	0	514	9	0
81	dd	459	0	449	2	0
82	ee	443	0	492	0	0
83	ff	555	0	567	5	0
84	gg	2436	0	2393	7	0
85	hh	169	0	86	0	0
86	ii	2947	0	2957	65	0
87	jj	3292	0	3371	34	0
88	5	188	0	0	0	0
88	7	5	0	0	0	0
88	8	6	0	0	0	0
88	9	71	0	0	0	0
88	B	1	0	0	0	0
88	I	1	0	0	0	0
88	P	2	0	0	0	0
88	Q	1	0	0	0	0
88	V	1	0	0	0	0
88	a	1	0	0	0	0
88	e	1	0	0	0	0
88	g	1	0	0	0	0
88	j	1	0	0	0	0
88	jj	1	0	0	0	0
89	aa	1	0	0	0	0
89	dd	1	0	0	0	0
89	ff	1	0	0	2	0
89	g	1	0	0	2	0
89	j	1	0	0	0	0
89	m	1	0	0	0	0
89	o	1	0	0	0	0
89	p	1	0	0	0	0
90	9	32	0	14	28	0
90	jj	32	0	14	0	0
All	All	222130	0	167026	1037	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 (1037) 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)
48:5:922:C:C5'	48:5:922(A):G:H3'	1.47	1.45
48:5:922:C:H5'	48:5:922(A):G:C3'	1.56	1.34
48:5:922:C:H2'	48:5:922(B):C:C2	1.62	1.33
51:9:1137:U:O4	51:9:1148:A:N1	1.64	1.29
51:9:614:C:C4'	51:9:626:G:H21	1.45	1.29
48:5:2367:A:N1	48:5:2788:U:O4	1.64	1.28
51:9:628:A:OP1	90:9:1972:GCP:N2	1.67	1.25
48:5:922:C:H2'	48:5:922(B):C:N1	1.52	1.25
51:9:614:C:N3	86:ii:45:ARG:HG3	1.50	1.23
48:5:935:A:H62	48:5:935:A:C1'	1.52	1.23
48:5:922:C:C5'	48:5:922(B):C:P	2.27	1.22
51:9:1137:U:C4	51:9:1148:A:N1	2.07	1.22
48:5:935:A:N6	48:5:935:A:H1'	1.53	1.21
48:5:922:C:H3'	48:5:922(B):C:C6	1.75	1.20
86:ii:222:PHE:HB3	86:ii:237:ARG:NH1	1.55	1.20
48:5:922:C:C3'	48:5:922(B):C:C6	2.26	1.19
86:ii:222:PHE:CE1	86:ii:237:ARG:HG2	1.75	1.19
48:5:922:C:H5''	48:5:922(B):C:P	1.72	1.18
48:5:922:C:O3'	48:5:922(B):C:C6	1.97	1.17
51:9:628:A:N6	51:9:1332:A:O4'	1.80	1.13
48:5:935:A:N6	48:5:935(A):G:OP1	1.82	1.11
48:5:922:C:O3'	48:5:922(B):C:O4'	1.67	1.11
86:ii:225:ALA:HB2	86:ii:233:LEU:HD23	1.28	1.10
90:9:1972:GCP:C3B	55:DD:179:GLN:HE22	1.64	1.09
48:5:922:C:C3'	48:5:922(B):C:O4'	2.00	1.09
86:ii:199:PHE:HB3	86:ii:236:ASN:ND2	1.69	1.07
86:ii:222:PHE:HB3	86:ii:237:ARG:HH11	1.06	1.07
55:DD:179:GLN:HA	55:DD:179:GLN:HE21	1.19	1.07
51:9:614:C:H4'	51:9:626:G:H21	1.18	1.06
51:9:614:C:C4'	51:9:626:G:N2	2.18	1.05
48:5:935:A:H62	48:5:935:A:C2'	1.68	1.05
48:5:935:A:C1'	48:5:935:A:N6	2.14	1.05
48:5:922(A):G:P	48:5:922(B):C:H6	1.79	1.05
48:5:922:C:O3'	48:5:922(B):C:H6	1.29	1.04
51:9:614:C:O4'	51:9:626:G:N2	1.91	1.04
48:5:922:C:C2'	48:5:922(B):C:N1	2.21	1.03
51:9:1137:U:O4	51:9:1148:A:C2	2.12	1.02
51:9:613:G:N2	51:9:629:A:OP2	1.93	1.02
48:5:922:C:C2'	48:5:922(B):C:C1'	2.38	1.01
51:9:613:G:H4'	51:9:615:C:C5	1.97	0.99
48:5:922:C:C3'	48:5:922(B):C:C1'	2.40	0.99
48:5:922:C:C2'	48:5:922(B):C:H1'	1.93	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:615:C:H2'	51:9:616:A:C8	1.99	0.97
48:5:922:C:O2'	48:5:922(B):C:H1'	1.65	0.97
51:9:614:C:H4'	51:9:626:G:N2	1.78	0.96
48:5:922:C:H5'	48:5:922(A):G:H3'	1.00	0.95
90:9:1972:GCP:C3B	55:DD:179:GLN:NE2	2.29	0.95
51:9:1711:U:N3	51:9:1822:A:N1	2.14	0.94
51:9:615:C:O2'	51:9:616:A:O4'	1.84	0.94
48:5:1411:C:O2'	48:5:1411(C):C:C3'	2.16	0.94
51:9:1679:A:OP1	80:cc:20:ARG:NH2	2.00	0.92
48:5:1411:C:O2'	48:5:1411(C):C:C6	2.22	0.91
51:9:1825:A:C2	86:ii:62:ARG:NH1	2.38	0.91
51:9:628:A:P	90:9:1972:GCP:HN22	1.94	0.91
48:5:922:C:C5'	48:5:922(A):G:C3'	2.29	0.90
86:ii:222:PHE:CB	86:ii:237:ARG:HH11	1.84	0.90
83:ff:144:CYS:HG	89:ff:200:ZN:ZN	0.79	0.90
48:5:922:C:C3'	48:5:922(B):C:N1	2.35	0.89
48:5:922:C:P	48:5:922(A):G:OP2	2.30	0.89
48:5:922(A):G:P	48:5:922(B):C:C6	2.66	0.88
90:9:1972:GCP:H3B1	55:DD:179:GLN:NE2	1.87	0.88
86:ii:199:PHE:HB3	86:ii:236:ASN:HD22	1.37	0.88
48:5:3760:A:H2	51:9:1825:A:N3	1.72	0.87
51:9:1501:C:O2'	90:9:1972:GCP:H2'	1.75	0.87
51:9:627:U:O4	86:ii:99:TYR:HB3	1.73	0.87
32:g:49:CYS:HG	89:g:201:ZN:ZN	0.75	0.87
51:9:628:A:H61	51:9:1332:A:C1'	1.86	0.87
86:ii:225:ALA:HB2	86:ii:233:LEU:CD2	2.06	0.86
48:5:922:C:O5'	48:5:922(A):G:H3'	1.74	0.86
48:5:922(B):C:O2'	48:5:923:C:OP1	1.94	0.86
48:5:1411:C:O4'	48:5:1411(B):C:H2'	1.75	0.86
51:9:1821:U:O2'	51:9:1822:A:O4'	1.95	0.85
51:9:1137:U:O4	51:9:1148:A:C6	2.30	0.85
51:9:1501:C:O2'	90:9:1972:GCP:N9	2.11	0.84
48:5:2367:A:N1	48:5:2788:U:C4	2.46	0.84
48:5:1411:C:O2'	48:5:1411(C):C:H3'	1.78	0.83
51:9:1824:A:N3	51:9:1824:A:H2'	1.92	0.83
48:5:1411:C:C5'	48:5:1411(C):C:H5'	2.08	0.83
51:9:627:U:C4	86:ii:99:TYR:CB	2.62	0.82
62:KK:15:LEU:HD22	62:KK:49:MET:HE1	1.59	0.82
48:5:1411:C:O2'	48:5:1411(C):C:O4'	1.96	0.82
51:9:614:C:N3	86:ii:45:ARG:CG	2.40	0.82
83:ff:144:CYS:SG	89:ff:200:ZN:ZN	1.69	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:922:C:C2'	48:5:922(B):C:C2	2.58	0.81
48:5:1411:C:O2'	48:5:1411(C):C:C4'	2.29	0.81
48:5:2367:A:N6	48:5:2788:U:N3	2.30	0.80
51:9:1823:A:H3'	51:9:1824:A:H5'	1.61	0.80
48:5:1406:G:O4'	48:5:1406(C):G:O2'	1.99	0.80
48:5:1411:C:O2'	48:5:1411(C):C:H6	1.62	0.80
86:ii:222:PHE:CB	86:ii:237:ARG:NH1	2.43	0.80
48:5:922(B):C:O2'	48:5:923:C:P	2.38	0.79
48:5:1406:G:O4'	48:5:1406(C):G:C2'	2.30	0.79
48:5:3760:A:H2	51:9:1825:A:C4	2.00	0.79
51:9:612:U:O2	51:9:629:A:N6	2.15	0.79
48:5:3914:U:H3	48:5:4378:A:N6	1.80	0.78
86:ii:199:PHE:CB	86:ii:236:ASN:ND2	2.45	0.78
48:5:3760:A:O2'	86:ii:108:ARG:NH2	2.17	0.78
48:5:1411:C:O2'	48:5:1411(C):C:C1'	2.32	0.78
55:DD:70:THR:HG22	55:DD:86:LEU:HD13	1.65	0.77
12:M:44:ARG:HB2	48:5:935:A:OP2	1.84	0.77
51:9:615:C:O2'	51:9:616:A:O5'	2.04	0.76
48:5:1411:C:C5'	48:5:1411(C):C:C5'	2.42	0.76
51:9:615:C:H2'	51:9:616:A:H8	1.51	0.76
48:5:738:C:O2'	48:5:738(A):C:O4'	2.01	0.75
90:9:1972:GCP:O3G	90:9:1972:GCP:O2A	2.05	0.75
48:5:1411:C:O4'	48:5:1411(B):C:C2'	2.35	0.74
58:GG:5:ILE:HD12	58:GG:16:ILE:HD13	1.69	0.74
1:A:82:ILE:HD11	1:A:99:GLY:HA3	1.68	0.74
51:9:628:A:C2	55:DD:145:GLN:OE1	2.41	0.74
1:A:158:ILE:HG23	1:A:162:ASN:HD21	1.52	0.74
86:ii:44:ILE:CG2	86:ii:60:ARG:HD2	2.17	0.74
86:ii:225:ALA:CB	86:ii:233:LEU:HD23	2.13	0.73
51:9:615:C:O2'	51:9:616:A:C5'	2.36	0.73
51:9:1137:U:C4	51:9:1148:A:C6	2.77	0.73
51:9:1501:C:O2'	90:9:1972:GCP:C4	2.36	0.73
90:9:1972:GCP:H3B2	55:DD:179:GLN:HE22	1.52	0.73
51:9:614:C:O4'	51:9:626:G:C2	2.41	0.73
48:5:1406:G:C8	48:5:1406(C):G:H2'	2.23	0.73
48:5:1406:G:O5'	48:5:1406(C):G:O3'	2.07	0.73
51:9:1091:C:HO2'	74:WW:2:VAL:N	1.85	0.73
84:gg:87:LEU:HD21	84:gg:108:VAL:HG11	1.70	0.73
51:9:612:U:O2'	51:9:615:C:N3	2.19	0.73
51:9:627:U:C5	86:ii:99:TYR:HB2	2.25	0.72
48:5:922:C:O5'	48:5:922(A):G:P	2.48	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:922(A):G:OP1	48:5:922(B):C:C6	2.42	0.72
90:9:1972:GCP:O2B	55:DD:179:GLN:NE2	2.23	0.72
51:9:1500:G:N2	90:9:1972:GCP:O6	2.23	0.71
48:5:922:C:C6	48:5:922(A):G:C5	2.79	0.71
42:r:32:LEU:HD21	42:r:106:LEU:HD12	1.73	0.70
87:jj:613:ILE:HD12	87:jj:643:VAL:HG21	1.72	0.70
51:9:1501:C:H5'	90:9:1972:GCP:O1A	1.91	0.70
48:5:1411:C:O5'	48:5:1411(C):C:H5'	1.90	0.70
90:9:1972:GCP:O1G	55:DD:178:ARG:NH1	2.17	0.70
48:5:3914:U:N3	48:5:4378:A:N6	2.37	0.70
48:5:922:C:H2'	48:5:922(B):C:C6	2.27	0.70
51:9:96:C:O2	51:9:473:A:O2'	2.10	0.70
51:9:1501:C:C5'	90:9:1972:GCP:O1A	2.40	0.70
48:5:922:C:H5'	48:5:922(A):G:O3'	1.92	0.69
51:9:627:U:C4	86:ii:99:TYR:HB2	2.27	0.69
51:9:628:A:C2	55:DD:145:GLN:CD	2.71	0.69
14:O:54:TYR:CD1	14:O:145:VAL:HG21	2.26	0.69
51:9:1501:C:HO2'	90:9:1972:GCP:H2'	1.55	0.69
48:5:922:C:H5'	48:5:922(A):G:C2'	2.20	0.69
55:DD:179:GLN:HA	55:DD:179:GLN:NE2	1.98	0.69
51:9:1501:C:O2'	90:9:1972:GCP:C8	2.42	0.68
48:5:3760:A:C2	51:9:1825:A:N3	2.60	0.68
51:9:613:G:H4'	51:9:615:C:C4	2.28	0.68
51:9:1130:G:H2'	51:9:1130:G:N3	2.08	0.68
48:5:1411:C:HO2'	48:5:1411(C):C:H6	0.78	0.68
51:9:629:A:O2'	51:9:631:U:OP2	2.12	0.68
19:T:80:VAL:HG21	19:T:85:LEU:HD12	1.75	0.67
57:FF:102:LEU:HD22	77:ZZ:110:THR:HG21	1.77	0.67
86:ii:217:PHE:CZ	86:ii:221:MET:HE2	2.29	0.67
56:EE:44:LEU:HD13	56:EE:72:ILE:HD11	1.77	0.67
48:5:935:A:N6	48:5:935:A:O2'	2.27	0.67
51:9:627:U:O4	86:ii:99:TYR:CB	2.42	0.67
55:DD:179:GLN:HE21	55:DD:179:GLN:CA	2.00	0.67
48:5:922:C:O3'	48:5:922(B):C:C1'	2.40	0.67
48:5:1411:C:O5'	48:5:1411(C):C:C5'	2.43	0.67
48:5:1411:C:H1'	48:5:1411(C):C:O4'	1.95	0.66
64:MM:22:LEU:HD11	64:MM:89:VAL:HA	1.76	0.66
52:AA:63:ARG:HG3	52:AA:185:MET:HE1	1.78	0.66
6:F:227:VAL:HA	18:S:39:VAL:HG12	1.78	0.66
15:P:127:ARG:NH2	48:5:2422:C:OP1	2.29	0.66
51:9:1825:A:N3	86:ii:62:ARG:HD3	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:23:LYS:NZ	48:5:935:A:O3'	2.25	0.66
48:5:4723:A:H2'	48:5:4724:A:C8	2.31	0.65
48:5:922:C:H5'	48:5:922(B):C:P	2.31	0.65
51:9:945:U:H2'	51:9:946:U:C6	2.31	0.65
48:5:2395:A:O2'	48:5:2806:A:N3	2.28	0.65
51:9:1825:A:C4	86:ii:62:ARG:CZ	2.80	0.65
48:5:922:C:C2'	48:5:922(B):C:C6	2.76	0.65
48:5:1406(B):C:H2'	48:5:1406(C):G:O4'	1.95	0.65
87:jj:343:MET:HE2	87:jj:361:GLN:HE22	1.61	0.65
48:5:971:U:N3	48:5:971(A):G:C4	2.65	0.64
90:9:1972:GCP:PB	55:DD:179:GLN:HE22	2.20	0.64
17:R:74:ARG:NH2	48:5:2891:U:OP2	2.30	0.64
51:9:613:G:C4'	51:9:615:C:C4	2.80	0.64
86:ii:217:PHE:CE2	86:ii:221:MET:CE	2.80	0.64
48:5:922:C:C5'	48:5:922(A):G:O3'	2.44	0.64
48:5:922(B):C:H2'	48:5:923:C:H5''	1.79	0.64
48:5:4579:U:H2'	48:5:4580:U:C6	2.32	0.64
48:5:1411:C:P	48:5:1411(C):C:OP1	2.56	0.64
56:EE:56:LEU:HD11	76:YY:74:MET:HE1	1.80	0.64
18:S:34:ALA:HB1	18:S:39:VAL:HG23	1.77	0.64
59:HH:61:ILE:HD11	59:HH:95:ILE:HD12	1.80	0.63
30:e:38:PRO:HD2	30:e:55:MET:HE3	1.81	0.63
32:g:49:CYS:SG	89:g:201:ZN:ZN	1.84	0.63
48:5:481:G:O6	48:5:481(A):C:H3'	1.97	0.63
48:5:1406:G:O4'	48:5:1406(C):G:H2'	1.97	0.63
30:e:81:ASN:HA	30:e:111:ILE:HD11	1.80	0.63
14:O:27:VAL:HG12	14:O:98:ALA:HB1	1.79	0.63
51:9:1825:A:N1	86:ii:62:ARG:NH1	2.45	0.63
55:DD:176:LEU:N	55:DD:176:LEU:HD12	2.13	0.63
48:5:922:C:C5	48:5:922(A):G:C5	2.87	0.63
51:9:1589:A:N3	51:9:1653:U:O2'	2.27	0.63
11:L:169:ILE:HD13	26:a:142:GLY:HA2	1.81	0.62
86:ii:222:PHE:CD1	86:ii:237:ARG:NE	2.66	0.62
48:5:935:A:C6	48:5:935(A):G:C8	2.87	0.62
51:9:1407:U:H2'	51:9:1408:U:C6	2.33	0.62
52:AA:63:ARG:CG	52:AA:185:MET:HE1	2.28	0.62
54:CC:209:VAL:HG21	54:CC:233:LEU:HD13	1.80	0.62
78:aa:73:TYR:CE2	78:aa:83:VAL:HG21	2.34	0.62
48:5:922(B):C:N3	48:5:923:C:C5	2.67	0.62
48:5:922(A):G:OP1	48:5:922(B):C:C5	2.53	0.62
48:5:1411(C):C:H2'	48:5:1412:G:O4'	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2367:A:C2	48:5:2788:U:O4	2.51	0.62
3:C:101:MET:SD	3:C:104:PRO:HA	2.39	0.62
48:5:481:G:C6	48:5:481(A):C:H3'	2.35	0.62
48:5:3723:A:H2'	48:5:3724:A:C8	2.35	0.62
51:9:1825:A:N1	86:ii:108:ARG:HG2	2.14	0.62
86:ii:222:PHE:CE1	86:ii:237:ARG:CG	2.69	0.62
59:HH:27:LEU:HD13	59:HH:45:ILE:HD13	1.81	0.61
1:A:101:VAL:HB	1:A:165:VAL:HG12	1.82	0.61
51:9:943:U:OP2	53:BB:216:LYS:NZ	2.32	0.61
6:F:152:LEU:HD21	6:F:243:ILE:HG23	1.83	0.61
51:9:627:U:C4	86:ii:99:TYR:HB3	2.35	0.61
51:9:1568:C:OP1	71:TT:96:SER:OG	2.17	0.61
20:U:87:THR:HG23	20:U:102:VAL:HG21	1.83	0.61
84:gg:79:LEU:HD22	84:gg:111:VAL:HG21	1.80	0.61
2:B:174:ARG:NH1	48:5:4985:U:O2	2.34	0.60
48:5:738(A):C:H5''	48:5:739:G:H5''	1.81	0.60
48:5:922:C:O5'	48:5:922(A):G:C3'	2.46	0.60
87:jj:392:LEU:HD23	87:jj:666:MET:HE2	1.82	0.60
48:5:935:A:H61	48:5:935(A):G:P	2.22	0.60
51:9:183:G:O2'	51:9:184:G:O5'	2.19	0.60
51:9:1129:G:C6	51:9:1130:G:O6	2.54	0.60
12:M:15:VAL:HG22	12:M:50:MET:HE1	1.82	0.60
48:5:922:C:C4'	48:5:922(B):C:O4'	2.49	0.60
86:ii:222:PHE:CZ	86:ii:237:ARG:HG2	2.31	0.60
2:B:254:ILE:HG23	2:B:266:VAL:HG11	1.81	0.60
51:9:980:A:H2'	51:9:981:A:C8	2.36	0.60
90:9:1972:GCP:PB	55:DD:179:GLN:NE2	2.74	0.60
48:5:922:C:O3'	48:5:922:C:O5'	2.20	0.60
86:ii:222:PHE:HE1	86:ii:237:ARG:HG2	1.55	0.60
31:f:47:CYS:HB3	31:f:103:VAL:HG12	1.84	0.60
51:9:1823:A:C3'	51:9:1824:A:H5'	2.32	0.60
48:5:4942:C:H4'	48:5:4943:A:OP1	2.01	0.60
48:5:934:C:O4'	48:5:935(A):G:O4'	2.19	0.59
51:9:1825:A:C4	86:ii:62:ARG:NH2	2.70	0.59
48:5:1411:C:C1'	48:5:1411(C):C:O4'	2.50	0.59
86:ii:33:VAL:HG22	86:ii:112:LEU:HD21	1.82	0.59
87:jj:283:LEU:HB3	87:jj:453:ILE:HD11	1.84	0.59
40:o:68:LEU:HD11	40:o:85:ILE:HD11	1.85	0.59
51:9:1825:A:N1	86:ii:108:ARG:CG	2.65	0.59
48:5:1370:G:O2'	48:5:1371:A:OP2	2.12	0.59
48:5:738:C:O3'	48:5:738(A):C:H5'	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BB:103:MET:HE1	53:BB:212:VAL:HG23	1.85	0.59
48:5:922(B):C:H2'	48:5:923:C:C5'	2.33	0.59
48:5:3766:A:N1	51:9:1827:U:O2'	2.35	0.58
83:ff:130:VAL:HG11	83:ff:143:LYS:HZ2	1.68	0.58
51:9:1501:C:O2'	90:9:1972:GCP:C2'	2.50	0.58
52:AA:38:ILE:HD11	52:AA:150:THR:HG22	1.84	0.58
48:5:922:C:C6	48:5:922(A):G:C4	2.91	0.58
69:RR:16:ILE:HG22	69:RR:24:LEU:HD11	1.84	0.58
48:5:738:C:O2'	48:5:738(A):C:C6	2.57	0.58
55:DD:21:LEU:HD21	55:DD:48:ILE:HD11	1.86	0.58
62:KK:11:ILE:HD12	62:KK:45:VAL:HG22	1.85	0.58
51:9:501:C:H2'	51:9:501:C:O2	2.03	0.58
48:5:922(B):C:HO2'	48:5:923:C:P	2.24	0.57
51:9:628:A:P	90:9:1972:GCP:N2	2.66	0.57
14:O:193:THR:HG23	14:O:202:LEU:HD23	1.84	0.57
76:YY:34:THR:HG23	76:YY:69:THR:HG21	1.87	0.57
86:ii:199:PHE:HB3	86:ii:236:ASN:HD21	1.66	0.57
6:F:89:ALA:HB2	6:F:124:LEU:HD21	1.87	0.57
51:9:1680:G:H4'	80:cc:20:ARG:HH11	1.69	0.57
4:D:152:ARG:HG3	4:D:154:THR:HG23	1.87	0.57
51:9:1825:A:C5	86:ii:62:ARG:NH2	2.73	0.57
48:5:3761:C:H2'	48:5:3762:U:C6	2.40	0.57
51:9:1130:G:O2'	51:9:1131:G:O5'	2.23	0.57
48:5:922(B):C:C2'	48:5:923:C:H5''	2.35	0.56
51:9:1117:C:O2'	51:9:1118:C:O4'	2.23	0.56
54:CC:88:ILE:HG21	54:CC:94:ILE:CD1	2.36	0.56
86:ii:217:PHE:CZ	86:ii:221:MET:CE	2.87	0.56
4:D:23:ARG:NH2	48:5:4280:A:OP2	2.38	0.56
18:S:82:LEU:HB2	18:S:93:MET:HB2	1.88	0.56
20:U:23:LEU:HD11	20:U:83:LEU:CD2	2.35	0.56
13:N:6:TYR:CZ	34:i:40:VAL:HG22	2.41	0.56
51:9:615:C:O2'	51:9:616:A:C4'	2.54	0.56
1:A:234:LYS:HG2	1:A:238:ILE:HD12	1.87	0.56
46:2:16:C:O4'	46:2:16:C:O2	2.24	0.56
51:9:613:G:O4'	51:9:615:C:N4	2.38	0.56
80:cc:21:THR:HG22	80:cc:68:LEU:HD13	1.87	0.56
2:B:249:ARG:NH1	48:5:2837:U:OP1	2.38	0.56
48:5:922:C:OP2	48:5:922(A):G:OP2	2.23	0.56
12:M:24:LEU:HD11	12:M:86:TRP:CG	2.41	0.56
16:Q:11:ARG:NH2	48:5:1690:C:OP2	2.39	0.56
51:9:824:C:C2	61:JJ:144:ILE:HD13	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:127:MET:HE1	19:T:155:PRO:HA	1.86	0.55
48:5:1411:C:O4'	48:5:1411(B):C:C3'	2.55	0.55
48:5:2395:A:O2'	48:5:2806:A:H1'	2.07	0.55
51:9:614:C:C1'	51:9:626:G:N2	2.69	0.55
70:SS:43:VAL:HG21	70:SS:83:PHE:CZ	2.42	0.55
78:aa:11:ALA:HB3	78:aa:33:ASP:HB2	1.88	0.55
6:F:161:ILE:HD12	6:F:166:ILE:HB	1.89	0.55
44:t:81:ILE:HD11	44:t:132:ILE:HG23	1.87	0.55
48:5:1411:C:O5'	48:5:1411(C):C:OP1	2.24	0.55
55:DD:175:VAL:C	55:DD:176:LEU:HD12	2.32	0.55
60:II:36:THR:HG21	60:II:179:PRO:HB2	1.88	0.55
43:s:43:ILE:HD13	43:s:187:LEU:HD21	1.87	0.55
48:5:245:C:O4'	48:5:245:C:O2	2.24	0.55
48:5:1411:C:C2'	48:5:1411(C):C:O4'	2.54	0.55
78:aa:44:ILE:HD12	78:aa:45:VAL:HG13	1.89	0.55
31:f:50:VAL:HG22	31:f:69:VAL:HG12	1.87	0.55
48:5:742:G:C2	48:5:922(A):G:C6	2.94	0.55
13:N:76:PRO:O	13:N:79:ALA:HB3	2.06	0.55
48:5:2031:C:O3'	48:5:2032:U:P	2.65	0.54
51:9:1438:A:H2'	51:9:1439:A:C8	2.41	0.54
19:T:87:LYS:NZ	48:5:4301:U:OP2	2.40	0.54
51:9:627:U:C4	86:ii:99:TYR:CD2	2.96	0.54
51:9:1130:G:O2'	51:9:1131:G:P	2.65	0.54
14:O:27:VAL:CG1	14:O:98:ALA:HB1	2.37	0.54
54:CC:209:VAL:HG21	54:CC:233:LEU:CD1	2.38	0.54
59:HH:36:LEU:HD23	59:HH:40:LEU:HD12	1.90	0.54
62:KK:35:LEU:HD13	62:KK:40:VAL:HG21	1.89	0.54
48:5:2627:C:O4'	48:5:2627:C:O2	2.26	0.54
51:9:614:C:C5	51:9:626:G:O2'	2.58	0.54
86:ii:175:CYS:HB2	87:jj:316:THR:HG22	1.88	0.54
51:9:853:C:O4'	51:9:853:C:O2	2.25	0.54
6:F:97:ILE:HD11	16:Q:4:ASP:CG	2.33	0.54
51:9:627:U:C4	86:ii:99:TYR:CG	2.96	0.54
54:CC:253:PRO:HA	54:CC:256:TRP:CD1	2.43	0.54
78:aa:45:VAL:CG2	78:aa:64:LEU:HD13	2.38	0.54
1:A:104:VAL:CG1	1:A:146:THR:HG21	2.38	0.54
6:F:88:LEU:HD22	6:F:89:ALA:N	2.23	0.54
21:V:26:ILE:HG22	21:V:101:ASN:HB3	1.90	0.54
29:d:33:ILE:HD11	29:d:41:ARG:HB3	1.89	0.54
48:5:1411:C:C2'	48:5:1411(C):C:C6	2.91	0.54
51:9:628:A:OP2	90:9:1972:GCP:N3	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:jj:594:ILE:HD11	87:jj:674:ILE:CG2	2.38	0.53
51:9:1502:C:H5'	90:9:1972:GCP:H2'	1.89	0.53
51:9:1825:A:N3	86:ii:62:ARG:CD	2.71	0.53
8:H:41:ILE:HG21	8:H:73:ILE:HD11	1.90	0.53
12:M:112:VAL:HG11	14:O:201:LEU:HD11	1.90	0.53
48:5:4459:U:H2'	48:5:4460:U:C6	2.43	0.53
14:O:58:LEU:HD11	14:O:145:VAL:HG22	1.89	0.53
48:5:2505:C:O2	48:5:2505:C:O4'	2.24	0.53
51:9:958:G:C6	51:9:959:G:C6	2.97	0.53
59:HH:118:ARG:O	59:HH:121:THR:HG22	2.08	0.53
78:aa:25:ASN:HB3	78:aa:77:CYS:SG	2.48	0.53
14:O:23:VAL:HG13	14:O:33:VAL:HG11	1.91	0.53
25:Z:53:VAL:HG21	25:Z:62:ILE:HG23	1.89	0.53
48:5:114:G:N2	48:5:276:C:O2'	2.41	0.53
48:5:935:A:N6	48:5:935(A):G:P	2.81	0.53
59:HH:145:ARG:HA	74:WW:51:GLU:HB2	1.91	0.53
71:TT:75:MET:HA	71:TT:78:ILE:HG22	1.91	0.53
87:jj:330:MET:HE3	87:jj:549:HIS:CD2	2.42	0.53
48:5:747:A:H4'	48:5:748:G:OP1	2.09	0.53
51:9:15:U:H2'	51:9:16:G:O4'	2.08	0.53
52:AA:134:LEU:HD21	52:AA:144:THR:HG21	1.91	0.53
29:d:36:VAL:HG23	29:d:41:ARG:HG3	1.91	0.53
48:5:294:G:O6	48:5:315:G:H1'	2.08	0.53
51:9:501:C:O2	51:9:501:C:C2'	2.57	0.53
71:TT:42:HIS:HB2	71:TT:83:GLN:HA	1.91	0.53
37:l:2:SER:N	48:5:2406:G:N7	2.57	0.53
51:9:490:C:O2'	51:9:574:A:N1	2.37	0.53
56:EE:182:MET:HE1	56:EE:192:ILE:HD11	1.91	0.53
66:OO:116:LEU:HD22	78:aa:53:ILE:HD11	1.91	0.53
48:5:922:C:H3'	48:5:922:C:C6	2.44	0.53
48:5:935:A:N6	48:5:935(A):G:H3'	2.23	0.53
48:5:1406:G:N9	48:5:1406(C):G:H2'	2.24	0.52
48:5:4989:U:O2	48:5:4989:U:O4'	2.27	0.52
51:9:1351:G:O2'	51:9:1378:A:N1	2.31	0.52
61:JJ:130:ILE:HG12	61:JJ:135:ILE:HD11	1.91	0.52
87:jj:261:LEU:HD23	87:jj:364:VAL:HG21	1.90	0.52
48:5:1411:C:O2'	48:5:1411(C):C:C2'	2.57	0.52
48:5:1483:C:O2	48:5:1483:C:O4'	2.25	0.52
51:9:1137:U:N3	51:9:1148:A:N6	2.57	0.52
51:9:1315:U:O2	51:9:1315:U:O4'	2.28	0.52
71:TT:60:THR:HG23	71:TT:75:MET:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:106:ALA:HB1	4:D:171:LEU:HD13	1.91	0.52
19:T:85:LEU:HD13	48:5:4305:G:C2	2.45	0.52
48:5:3810:C:O4'	48:5:3810:C:O2	2.26	0.52
61:JJ:130:ILE:CG1	61:JJ:135:ILE:HD11	2.39	0.52
48:5:3760:A:C2	51:9:1825:A:C4	2.90	0.52
53:BB:139:CYS:SG	53:BB:140:VAL:N	2.83	0.52
48:5:224:U:O2	48:5:224:U:O4'	2.28	0.52
87:jj:492:VAL:HG23	87:jj:505:ILE:HG23	1.91	0.52
48:5:922:C:H5''	48:5:922(B):C:OP1	2.06	0.52
29:d:46:LEU:HD13	29:d:64:ILE:HD13	1.92	0.52
51:9:1012:A:H2'	51:9:1013:U:O4'	2.09	0.52
55:DD:176:LEU:N	55:DD:176:LEU:CD1	2.73	0.52
63:LL:61:PRO:HA	63:LL:66:VAL:HG13	1.92	0.52
75:XX:61:GLN:HB3	75:XX:62:PRO:CD	2.39	0.52
48:5:2097:A:OP1	48:5:2107:A:N6	2.43	0.52
51:9:627:U:N3	86:ii:99:TYR:CD2	2.78	0.52
51:9:1139:C:O4'	51:9:1139:C:O2	2.23	0.52
57:FF:72:LEU:HD22	57:FF:112:LEU:HD11	1.92	0.52
76:YY:20:ARG:CZ	76:YY:74:MET:HE2	2.40	0.52
4:D:16:TYR:O	49:7:11:A:N6	2.43	0.52
48:5:222:C:H2'	48:5:223:G:O4'	2.09	0.52
51:9:1543:U:OP2	71:TT:62:ARG:NH1	2.42	0.52
17:R:44:LEU:HD22	17:R:49:LEU:HD12	1.91	0.51
29:d:22:THR:HG22	29:d:89:SER:CB	2.40	0.51
8:H:18:ILE:HG22	8:H:27:VAL:HG22	1.92	0.51
48:5:5047:C:O2'	48:5:5050:C:OP2	2.28	0.51
51:9:1058:A:C6	51:9:1059:G:C6	2.98	0.51
86:ii:40:ARG:HB3	86:ii:66:THR:HG22	1.93	0.51
14:O:18:ARG:NH2	48:5:2057:A:OP1	2.43	0.51
48:5:113:A:H2'	48:5:114:G:O4'	2.11	0.51
48:5:1961:G:O2'	48:5:2025:A:N6	2.44	0.51
51:9:1535:U:H2'	51:9:1535:U:O2	2.10	0.51
52:AA:183:LEU:HD22	52:AA:188:THR:HG21	1.92	0.51
47:3:16:C:O2	47:3:16:C:O4'	2.24	0.51
58:GG:132:ARG:HB3	58:GG:133:LEU:HD12	1.92	0.51
66:OO:56:VAL:HG12	66:OO:81:VAL:HG23	1.92	0.51
30:e:31:ILE:HD11	48:5:2347:A:C4	2.45	0.51
51:9:1823:A:H2'	51:9:1824:A:H5''	1.93	0.51
52:AA:167:GLY:O	52:AA:171:VAL:HG23	2.11	0.51
56:EE:11:ARG:HA	56:EE:28:ALA:HB2	1.92	0.51
87:jj:619:VAL:HG23	87:jj:632:PRO:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1872:G:O2'	48:5:4219:A:N3	2.38	0.51
50:8:125:C:O2	50:8:125:C:O4'	2.29	0.51
51:9:613:G:C4'	51:9:615:C:C5	2.83	0.51
65:NN:91:LEU:HD12	65:NN:125:LEU:HD12	1.93	0.51
51:9:92:A:O4'	56:EE:3:ARG:NH1	2.44	0.51
51:9:1139:C:H2'	51:9:1140:G:O4'	2.11	0.51
59:HH:144:ILE:HB	74:WW:52:ILE:HG12	1.93	0.51
68:QQ:49:TYR:O	68:QQ:53:GLU:N	2.43	0.51
7:G:101:LYS:HB3	23:X:42:THR:HG23	1.93	0.51
18:S:34:ALA:HB1	18:S:39:VAL:CG2	2.41	0.51
51:9:1488:C:O2'	51:9:1490:G:OP2	2.28	0.51
55:DD:21:LEU:CD2	55:DD:48:ILE:HD11	2.41	0.51
21:V:60:MET:HE1	21:V:78:PRO:CB	2.40	0.50
87:jj:266:ILE:HD11	87:jj:393:VAL:HG21	1.93	0.50
51:9:612:U:C2'	51:9:615:C:H42	2.25	0.50
57:FF:92:ILE:HD13	57:FF:169:ILE:HG21	1.93	0.50
31:f:28:LEU:HG	31:f:101:ILE:HD11	1.93	0.50
51:9:919:A:C2	51:9:1020:A:C4	2.98	0.50
48:5:922(B):C:H2'	48:5:923:C:O5'	2.12	0.50
51:9:1824:A:N3	51:9:1824:A:C2'	2.72	0.50
35:j:63:ARG:NH2	50:8:58:G:N7	2.60	0.50
48:5:922(B):C:C2	48:5:923:C:C6	2.99	0.50
51:9:1489:A:H4'	51:9:1490:G:OP2	2.10	0.50
75:XX:51:VAL:HG13	75:XX:70:VAL:HG13	1.93	0.50
12:M:119:ARG:NH1	14:O:202:LEU:HD21	2.27	0.50
51:9:1162:C:H2'	51:9:1163:C:O4'	2.11	0.50
3:C:164:THR:HG21	48:5:223:G:H2'	1.94	0.49
21:V:80:VAL:HG23	21:V:106:VAL:HG21	1.94	0.49
24:Y:49:ILE:HD11	24:Y:55:VAL:HG21	1.92	0.49
48:5:4515:G:C2	48:5:4516:G:C8	3.00	0.49
51:9:1501:C:HO2'	90:9:1972:GCP:C4	2.25	0.49
51:9:1863:A:H1'	78:aa:79:ILE:HD13	1.93	0.49
86:ii:217:PHE:CE2	86:ii:221:MET:HE1	2.46	0.49
26:a:103:VAL:HG12	26:a:108:TYR:HB2	1.94	0.49
35:j:66:HIS:O	35:j:70:VAL:HG23	2.12	0.49
48:5:1237:C:O2	48:5:1237:C:O4'	2.28	0.49
1:A:77:ILE:HD13	1:A:128:ARG:HB2	1.94	0.49
9:I:97:ILE:HD13	9:I:126:VAL:HG11	1.94	0.49
22:W:45:ASN:HB3	22:W:48:GLN:HE21	1.78	0.49
48:5:2094:C:O2	48:5:2094:C:O4'	2.30	0.49
63:LL:77:VAL:HG22	63:LL:86:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:ARG:HD2	3:C:36:ILE:HD12	1.94	0.49
8:H:92:MET:SD	8:H:161:ILE:HD11	2.52	0.49
30:e:47:ARG:NH1	48:5:1883:G:OP1	2.45	0.49
48:5:922:C:P	48:5:922(A):G:P	3.10	0.49
51:9:67:C:C6	58:GG:162:LEU:HD23	2.47	0.49
2:B:89:ILE:HD13	2:B:153:MET:HE1	1.94	0.49
48:5:2763:U:O2	48:5:2763:U:O4'	2.31	0.49
48:5:1328:G:O2'	48:5:2349:A:OP1	2.28	0.49
51:9:62:G:H4'	51:9:172:U:C5	2.48	0.49
53:BB:79:VAL:HG21	53:BB:81:PHE:CZ	2.48	0.49
66:OO:34:PHE:HB3	66:OO:41:PHE:HB2	1.93	0.49
12:M:72:TYR:CE1	48:5:738:C:H4'	2.48	0.49
12:M:72:TYR:CE1	48:5:918:G:H5'	2.47	0.49
56:EE:182:MET:CE	56:EE:192:ILE:HD11	2.42	0.49
62:KK:32:HIS:CD2	62:KK:45:VAL:HG21	2.47	0.49
76:YY:44:LEU:HB3	76:YY:55:ILE:HD13	1.94	0.49
86:ii:193:ILE:HG23	86:ii:197:ILE:HD12	1.95	0.49
2:B:89:ILE:CD1	2:B:153:MET:HE1	2.43	0.49
48:5:1381:U:O2	48:5:1381:U:O4'	2.31	0.49
3:C:130:ALA:HB3	3:C:246:VAL:HG12	1.94	0.49
3:C:302:LEU:HD22	16:Q:38:ARG:HB3	1.95	0.49
51:9:1825:A:N3	86:ii:62:ARG:CZ	2.76	0.49
60:II:31:ARG:NH2	60:II:48:VAL:HG12	2.28	0.49
48:5:935:A:N6	48:5:935:A:C2'	2.53	0.49
48:5:1406:G:C1'	48:5:1406(C):G:HO2'	2.24	0.49
48:5:1818:G:O2'	48:5:1819:G:OP1	2.24	0.49
51:9:830:A:OP2	51:9:846:G:N2	2.46	0.49
64:MM:22:LEU:HD21	64:MM:89:VAL:HG23	1.94	0.49
74:WW:26:LEU:HD11	74:WW:60:LYS:HB3	1.94	0.49
86:ii:42:SER:HB2	86:ii:62:ARG:HH11	1.77	0.49
19:T:48:VAL:HG21	19:T:94:GLU:HG2	1.94	0.48
51:9:1156:U:O4	54:CC:194:ARG:NH1	2.46	0.48
51:9:1624:U:O2	51:9:1624:U:O4'	2.31	0.48
65:NN:125:LEU:HD22	65:NN:129:TYR:CE2	2.48	0.48
86:ii:150:CYS:SG	86:ii:159:THR:HG22	2.52	0.48
86:ii:225:ALA:HB1	86:ii:234:LEU:CD2	2.43	0.48
26:a:12:ARG:NH1	48:5:2345:G:OP2	2.47	0.48
48:5:3839:G:N2	48:5:3843:C:O2'	2.47	0.48
48:5:4928:C:O4'	48:5:4928:C:O2	2.29	0.48
51:9:146:G:O2'	51:9:147:A:O5'	2.27	0.48
51:9:396:U:O2'	60:II:14:THR:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:cc:46:VAL:HG11	80:cc:50:VAL:HG21	1.96	0.48
2:B:181:MET:HE1	2:B:346:THR:HG23	1.94	0.48
5:E:164:ARG:O	5:E:185:ASN:ND2	2.45	0.48
16:Q:55:ARG:NH1	48:5:1351:G:N7	2.60	0.48
58:GG:63:MET:SD	58:GG:63:MET:N	2.86	0.48
74:WW:55:ASP:O	74:WW:57:ARG:N	2.47	0.48
87:jj:266:ILE:CD1	87:jj:393:VAL:HG21	2.43	0.48
48:5:971:U:O4	48:5:971(A):G:C5	2.66	0.48
48:5:2268:A:H4'	48:5:2269:C:H5'	1.95	0.48
48:5:3724:A:N6	48:5:3725:G:C6	2.81	0.48
52:AA:58:LEU:CD1	52:AA:174:MET:HE1	2.44	0.48
28:c:82:GLY:HA2	28:c:91:VAL:HG12	1.95	0.48
48:5:922:C:H2'	48:5:922(B):C:C1'	2.18	0.48
48:5:4305:G:C2'	48:5:4305:G:N3	2.76	0.48
87:jj:402:ALA:HB2	87:jj:477:PHE:CE2	2.49	0.48
1:A:112:ILE:HG23	1:A:133:TYR:CD2	2.49	0.48
48:5:1411:C:H4'	48:5:1411(C):C:C4'	1.98	0.48
62:KK:11:ILE:CD1	62:KK:45:VAL:HG22	2.43	0.48
1:A:104:VAL:HG12	1:A:146:THR:HG21	1.96	0.48
51:9:1238:U:H2'	51:9:1239:U:O4'	2.14	0.48
51:9:1364:U:O4'	51:9:1364:U:O2	2.28	0.48
51:9:1823:A:N6	51:9:1824:A:N7	2.61	0.48
3:C:325:MET:HE1	6:F:154:TYR:CE2	2.49	0.48
5:E:165:VAL:HG11	5:E:178:VAL:HG13	1.94	0.48
14:O:55:LEU:HD23	14:O:58:LEU:HD12	1.95	0.48
32:g:83:CYS:O	32:g:87:VAL:HG23	2.14	0.48
51:9:612:U:H2'	51:9:615:C:H42	1.78	0.48
59:HH:66:VAL:HG22	59:HH:96:ALA:HB1	1.95	0.48
18:S:35:PRO:HD2	18:S:39:VAL:HG21	1.96	0.48
48:5:1665:C:H2'	48:5:1666:C:H6	1.78	0.48
51:9:823:U:O2	51:9:823:U:O4'	2.32	0.48
48:5:961:G:C6	48:5:971(A):G:C4	3.02	0.48
48:5:1411(A):G:C6	48:5:1411(B):C:C4	3.02	0.48
59:HH:39:GLN:HB3	59:HH:75:ILE:HD12	1.96	0.48
60:II:72:CYS:SG	60:II:72:CYS:O	2.71	0.48
77:ZZ:92:LEU:HD11	77:ZZ:99:LEU:HD12	1.96	0.48
1:A:207:VAL:HG12	48:5:3919:C:C5'	2.44	0.47
1:A:242:ARG:HD2	48:5:3658:C:OP1	2.14	0.47
48:5:922(B):C:C2'	48:5:923:C:O5'	2.62	0.47
51:9:427:U:O2	51:9:427:U:O4'	2.33	0.47
74:WW:6:VAL:HG12	74:WW:34:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:cc:46:VAL:HG11	80:cc:50:VAL:CG2	2.44	0.47
87:jj:330:MET:HE2	87:jj:343:MET:SD	2.54	0.47
5:E:179:THR:OG1	5:E:189:LEU:HD23	2.13	0.47
17:R:173:ARG:NH2	51:9:910:G:OP2	2.47	0.47
37:l:23:ILE:HG22	50:8:52:A:C4	2.49	0.47
48:5:922(B):C:N3	48:5:923:C:C6	2.82	0.47
48:5:922(B):C:C2'	48:5:923:C:C5'	2.91	0.47
48:5:1942:A:N3	48:5:4432:C:O2'	2.43	0.47
51:9:628:A:C6	90:9:1972:GCP:O6	2.67	0.47
52:AA:94:THR:HG23	52:AA:182:VAL:HG21	1.96	0.47
64:MM:40:LYS:HE3	83:ff:130:VAL:HG22	1.95	0.47
8:H:117:PHE:CE1	8:H:118:LEU:HD23	2.49	0.47
29:d:22:THR:HG22	29:d:89:SER:HB2	1.95	0.47
48:5:961:G:C6	48:5:962:C:C4	3.02	0.47
51:9:612:U:H3	51:9:629:A:H62	1.62	0.47
51:9:1599:U:H2'	57:FF:166:ILE:HD11	1.96	0.47
53:BB:134:LEU:CD2	53:BB:218:LEU:HD12	2.44	0.47
60:II:117:TYR:CD1	60:II:156:ALA:HB2	2.49	0.47
75:XX:51:VAL:HG22	75:XX:70:VAL:HG11	1.96	0.47
40:o:15:CYS:SG	40:o:19:GLN:NE2	2.88	0.47
80:cc:21:THR:HG22	80:cc:68:LEU:CD1	2.44	0.47
87:jj:534:ILE:HD11	87:jj:544:ALA:HB3	1.97	0.47
30:e:44:ARG:NH2	48:5:1312:A:O2'	2.48	0.47
48:5:2367:A:N6	48:5:2788:U:C4	2.78	0.47
48:5:4723:A:C2	48:5:4724:A:C6	3.03	0.47
51:9:29:G:H4'	75:XX:129:SER:HB3	1.97	0.47
54:CC:88:ILE:HG21	54:CC:94:ILE:HD12	1.96	0.47
58:GG:52:ILE:HG23	58:GG:52:ILE:O	2.15	0.47
21:V:87:SER:HA	21:V:97:TYR:HB3	1.97	0.47
35:j:12:ARG:NH2	48:5:1617:G:O3'	2.48	0.47
44:t:98:ILE:HG23	44:t:98:ILE:O	2.14	0.47
48:5:1332:C:H2'	48:5:1333:A:C8	2.49	0.47
51:9:887:U:O2	51:9:887:U:O4'	2.31	0.47
51:9:1543:U:OP1	68:QQ:37:ARG:NH1	2.46	0.47
51:9:1825:A:C2	86:ii:62:ARG:CZ	2.97	0.47
66:OO:56:VAL:HG13	66:OO:77:ALA:HB1	1.97	0.47
4:D:62:CYS:HB3	4:D:105:LEU:HD22	1.96	0.47
25:Z:11:VAL:HG11	25:Z:80:LEU:HD22	1.97	0.47
48:5:498:C:O2	48:5:498:C:O4'	2.28	0.47
48:5:923:C:N4	48:5:926:G:C8	2.83	0.47
48:5:4510:A:O2'	48:5:4511:A:O4'	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:CC:196:ILE:HB	54:CC:223:TYR:HB2	1.97	0.47
1:A:27:ALA:O	1:A:128:ARG:NH2	2.48	0.47
48:5:5008:C:H2'	48:5:5009:G:O4'	2.14	0.47
51:9:958:G:H2'	51:9:959:G:O4'	2.15	0.47
59:HH:134:VAL:HG12	59:HH:173:PHE:CE2	2.50	0.47
66:OO:74:ALA:HB1	66:OO:115:ALA:HB2	1.97	0.47
48:5:2459:G:N2	48:5:2462:C:OP2	2.47	0.47
51:9:1336:C:H2'	51:9:1337:C:O4'	2.15	0.47
84:gg:91:ASP:HB2	84:gg:98:THR:HG23	1.96	0.47
87:jj:514:ILE:HD12	87:jj:534:ILE:HD12	1.96	0.47
11:L:116:ARG:NH1	11:L:155:MET:O	2.48	0.46
21:V:82:ILE:HD12	21:V:104:VAL:HG13	1.96	0.46
26:a:82:VAL:HG21	26:a:101:ILE:HG12	1.98	0.46
48:5:2367:A:C6	48:5:2788:U:C4	3.04	0.46
48:5:4579:U:O2	48:5:4580:U:C2	2.67	0.46
59:HH:122:LEU:C	59:HH:122:LEU:HD13	2.40	0.46
21:V:117:ILE:HD11	21:V:132:ILE:HG23	1.97	0.46
56:EE:87:MET:HE1	56:EE:236:ILE:HD13	1.96	0.46
57:FF:99:ILE:HG23	77:ZZ:67:LEU:HD21	1.97	0.46
67:PP:56:LEU:HD13	67:PP:78:THR:HG21	1.97	0.46
10:J:141:ILE:HD11	49:7:55:A:N3	2.31	0.46
68:QQ:51:LEU:HD21	68:QQ:81:ILE:HG12	1.96	0.46
3:C:101:MET:HE2	48:5:2343:G:C4	2.50	0.46
48:5:738:C:O3'	48:5:738(A):C:C5'	2.62	0.46
51:9:584:A:C6	51:9:585:C:C4	3.03	0.46
51:9:612:U:H2'	51:9:615:C:N4	2.31	0.46
58:GG:16:ILE:HD12	58:GG:16:ILE:N	2.31	0.46
87:jj:266:ILE:HG23	87:jj:389:HIS:HB3	1.97	0.46
21:V:60:MET:HE1	21:V:78:PRO:HB3	1.98	0.46
30:e:103:VAL:O	30:e:108:ARG:NH2	2.49	0.46
51:9:1097:G:C6	51:9:1098:C:C4	3.04	0.46
51:9:1823:A:H2'	51:9:1824:A:C5'	2.45	0.46
60:II:162:LEU:HD11	60:II:191:GLU:HG2	1.97	0.46
76:YY:56:PHE:CE2	76:YY:82:ALA:HB1	2.50	0.46
12:M:11:ARG:HD2	12:M:57:LEU:HD12	1.97	0.46
18:S:83:ARG:HB2	18:S:127:MET:HE3	1.98	0.46
29:d:33:ILE:HD11	29:d:41:ARG:CB	2.45	0.46
37:l:44:TRP:CZ3	37:l:45:ARG:HD3	2.51	0.46
48:5:4289:U:H2'	48:5:4290:U:C6	2.50	0.46
70:SS:40:TYR:O	70:SS:44:VAL:HG23	2.16	0.46
18:S:80:ILE:HG22	18:S:82:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:935:A:N1	48:5:935(A):G:H2'	2.31	0.46
48:5:1665:C:H2'	48:5:1666:C:C6	2.50	0.46
48:5:2046:G:C2	48:5:2047:A:C2	3.03	0.46
48:5:4872:G:H4'	48:5:4873:G:H5''	1.97	0.46
48:5:4977:A:H2'	48:5:4978:G:O4'	2.16	0.46
51:9:183:G:N3	51:9:183:G:C2'	2.77	0.46
51:9:1499:U:H5'	55:DD:176:LEU:HD21	1.98	0.46
48:5:1411:C:C2'	48:5:1411(C):C:C4'	2.93	0.46
48:5:4187:G:H2'	48:5:4188:U:O4'	2.16	0.46
51:9:1130:G:N3	51:9:1130:G:C2'	2.78	0.46
51:9:1228:A:O2'	51:9:1634:A:N3	2.34	0.46
51:9:1245:G:O2'	51:9:1492:U:OP1	2.24	0.46
52:AA:185:MET:HE3	73:VV:39:VAL:HG21	1.97	0.46
60:II:27:TYR:CE1	60:II:28:GLU:HG3	2.51	0.46
62:KK:93:THR:HG23	62:KK:94:LEU:HD12	1.98	0.46
43:s:34:ASN:N	43:s:34:ASN:HD22	2.14	0.46
48:5:1964:A:C6	48:5:4694:G:C6	3.03	0.46
48:5:3723:A:C2	48:5:3724:A:C6	3.03	0.46
48:5:3928:A:H2'	48:5:3929:G:O4'	2.16	0.46
48:5:4467:A:O2'	48:5:4510:A:N3	2.45	0.46
48:5:4525:C:H2'	48:5:4526:U:O4'	2.16	0.46
51:9:92:A:H2'	51:9:446:G:N2	2.31	0.46
51:9:434:G:H2'	51:9:435:A:C8	2.51	0.46
51:9:1719:A:N6	51:9:1814:G:O2'	2.49	0.46
66:OO:44:VAL:HG11	66:OO:85:CYS:SG	2.56	0.46
67:PP:81:ARG:NH1	67:PP:120:SER:OG	2.48	0.46
86:ii:17:THR:HG21	86:ii:109:GLN:HE21	1.81	0.46
18:S:84:TYR:CE1	18:S:93:MET:HE3	2.51	0.45
48:5:356:G:O2'	50:8:25:G:N3	2.46	0.45
51:9:1291:A:N3	83:ff:140:TYR:OH	2.49	0.45
61:JJ:35:TYR:CD2	61:JJ:106:LEU:HD23	2.51	0.45
5:E:180:GLY:O	5:E:181:PRO:C	2.59	0.45
19:T:80:VAL:CG2	19:T:85:LEU:HD12	2.45	0.45
23:X:80:PRO:HD2	33:h:33:VAL:HG22	1.99	0.45
40:o:41:TYR:CD1	47:3:75:C:O2	2.69	0.45
87:jj:263:LEU:HD23	87:jj:264:VAL:N	2.31	0.45
10:J:103:GLY:O	10:J:134:LEU:HD12	2.16	0.45
51:9:614:C:H5	51:9:626:G:O2'	1.97	0.45
51:9:1823:A:C3'	51:9:1824:A:C5'	2.94	0.45
55:DD:96:LEU:HD22	55:DD:198:ILE:HG13	1.98	0.45
61:JJ:94:LEU:HB2	61:JJ:97:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:ii:40:ARG:CB	86:ii:66:THR:HG22	2.47	0.45
87:jj:396:LEU:C	87:jj:396:LEU:HD23	2.41	0.45
26:a:21:ARG:NH1	48:5:1317:U:OP1	2.49	0.45
51:9:1554:C:O2	62:KK:24:LYS:NZ	2.43	0.45
9:I:61:SER:HA	9:I:126:VAL:HG23	1.98	0.45
48:5:1279:A:O2'	48:5:1281:G:N7	2.49	0.45
51:9:1303:C:O2	51:9:1303:C:O4'	2.33	0.45
52:AA:134:LEU:CD2	52:AA:144:THR:HG21	2.46	0.45
13:N:50:ARG:NH2	48:5:279:A:OP1	2.49	0.45
51:9:1284:A:C6	64:MM:91:LEU:HD22	2.52	0.45
53:BB:66:VAL:HG22	53:BB:87:ILE:HG22	1.98	0.45
55:DD:162:ASP:N	55:DD:163:PRO:CD	2.80	0.45
58:GG:32:MET:HE2	58:GG:63:MET:HG2	1.98	0.45
8:H:118:LEU:HD21	8:H:177:ASP:HB2	1.98	0.45
41:p:4:ARG:NH1	48:5:1554:A:OP2	2.45	0.45
48:5:1667:A:N1	48:5:2281:U:OP2	2.49	0.45
48:5:2758:G:O2'	48:5:2765:A:N3	2.48	0.45
51:9:1551:U:O2	51:9:1551:U:O4'	2.35	0.45
66:OO:38:ASN:HD22	66:OO:38:ASN:C	2.24	0.45
80:cc:14:VAL:HG13	80:cc:30:VAL:HG13	1.97	0.45
17:R:105:LEU:HD21	17:R:139:MET:HE2	1.99	0.45
26:a:98:ALA:HB2	26:a:121:PRO:HB2	1.99	0.45
53:BB:107:ARG:NH1	66:OO:133:THR:O	2.50	0.45
54:CC:191:VAL:HG11	54:CC:236:PHE:HA	1.99	0.45
4:D:4:VAL:HG11	48:5:4247:G:C5'	2.47	0.45
4:D:208:MET:HE1	4:D:236:MET:HE1	1.99	0.45
16:Q:104:ARG:NH2	48:5:1353:G:N7	2.62	0.45
30:e:31:ILE:HD11	48:5:2347:A:C5	2.51	0.45
51:9:161:U:O2'	58:GG:87:ARG:NH1	2.50	0.45
51:9:1834:A:C2'	51:9:1834:A:N3	2.80	0.45
80:cc:21:THR:O	80:cc:27:CYS:HB2	2.16	0.45
86:ii:225:ALA:HB1	86:ii:234:LEU:HD21	1.99	0.45
9:I:60:LEU:HD22	9:I:160:PRO:HD2	2.00	0.44
28:c:85:CYS:SG	28:c:94:LEU:HD22	2.57	0.44
29:d:36:VAL:HG23	29:d:41:ARG:CG	2.46	0.44
48:5:2816:G:N2	48:5:3622:C:O2	2.50	0.44
48:5:4476:C:O2'	48:5:4478:G:OP2	2.34	0.44
51:9:183:G:O2'	51:9:183:G:N3	2.50	0.44
51:9:933:G:H1'	51:9:1001:A:O4'	2.15	0.44
54:CC:251:LEU:HD23	73:VV:23:ILE:HG23	1.98	0.44
57:FF:88:MET:HE1	57:FF:92:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:ii:44:ILE:HG21	86:ii:60:ARG:HH11	1.82	0.44
86:ii:199:PHE:CB	86:ii:236:ASN:HD21	2.24	0.44
30:e:97:ALA:O	30:e:123:THR:HG23	2.17	0.44
51:9:1035:A:H2'	51:9:1036:A:O4'	2.17	0.44
71:TT:75:MET:HE3	71:TT:79:TYR:CE2	2.53	0.44
12:M:97:ALA:HB2	14:O:203:VAL:HB	1.99	0.44
51:9:1374:C:H2'	51:9:1375:G:O4'	2.18	0.44
51:9:1520:G:H2'	51:9:1520:G:N3	2.32	0.44
84:gg:81:GLY:HA2	84:gg:87:LEU:HD23	2.00	0.44
3:C:95:MET:SD	3:C:95:MET:N	2.82	0.44
6:F:161:ILE:HB	6:F:166:ILE:HD12	1.99	0.44
8:H:41:ILE:CG2	8:H:73:ILE:HD11	2.48	0.44
11:L:100:PRO:O	34:i:25:ARG:NH2	2.49	0.44
15:P:95:LEU:HD12	15:P:148:MET:HE1	1.99	0.44
51:9:987:A:N1	53:BB:120:MET:HE1	2.32	0.44
87:jj:343:MET:HE2	87:jj:361:GLN:NE2	2.31	0.44
2:B:84:MET:HE1	2:B:183:ILE:HD11	1.99	0.44
48:5:922:C:C5	48:5:922(A):G:N7	2.85	0.44
75:XX:68:LYS:CG	75:XX:91:LEU:HD22	2.48	0.44
15:P:69:ARG:NH2	48:5:4568:A:N3	2.66	0.44
48:5:922(A):G:OP1	48:5:922(B):C:H6	1.85	0.44
48:5:1990:A:H3'	48:5:1991:A:H5''	2.00	0.44
51:9:1395:C:H2'	51:9:1396:A:N3	2.33	0.44
72:UU:80:PHE:HB3	81:dd:52:PHE:HB3	1.98	0.44
79:bb:53:VAL:HG23	79:bb:53:VAL:O	2.18	0.44
3:C:334:THR:HG21	6:F:50:TYR:OH	2.17	0.44
3:C:341:LEU:HD21	5:E:52:LEU:HD21	2.00	0.44
4:D:4:VAL:HG11	48:5:4247:G:H5'	1.99	0.44
43:s:47:LEU:HB3	43:s:51:ALA:HB3	2.00	0.44
52:AA:185:MET:HE3	73:VV:39:VAL:CG2	2.48	0.44
78:aa:71:LEU:HD13	78:aa:73:TYR:OH	2.17	0.44
1:A:117:GLU:HB2	1:A:162:ASN:HB2	2.00	0.44
3:C:150:LEU:HB3	3:C:151:PRO:HD3	1.99	0.44
48:5:5066:U:H2'	48:5:5067:U:C6	2.53	0.44
55:DD:16:ILE:HD11	81:dd:36:LEU:HD23	1.99	0.44
55:DD:105:LEU:HD23	55:DD:184:ILE:HG23	2.00	0.44
78:aa:45:VAL:HG11	78:aa:53:ILE:CD1	2.48	0.44
2:B:47:LEU:HD23	2:B:166:THR:HG23	1.99	0.44
20:U:84:LYS:HA	20:U:87:THR:HG22	2.00	0.44
22:W:4:GLU:OE1	22:W:20:ARG:NH2	2.51	0.44
29:d:29:ILE:HG21	29:d:80:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:922:C:O3'	48:5:922(B):C:N1	2.44	0.44
48:5:1634:A:C6	48:5:1635:C:C4	3.06	0.44
48:5:4305:G:N3	48:5:4305:G:H2'	2.33	0.44
56:EE:122:LYS:CG	56:EE:162:ILE:HD11	2.48	0.44
71:TT:18:LEU:HD13	71:TT:134:ILE:HD13	2.00	0.44
48:5:1888:A:N6	48:5:3873:G:O2'	2.50	0.43
48:5:2439:G:C6	48:5:2440:U:C4	3.06	0.43
51:9:297:A:H4'	56:EE:132:GLY:O	2.17	0.43
51:9:1220:A:N6	51:9:1221:G:C6	2.86	0.43
54:CC:176:LYS:O	54:CC:200:ARG:NH1	2.51	0.43
62:KK:49:MET:HB3	62:KK:69:TRP:CE2	2.53	0.43
87:jj:587:ILE:HD11	87:jj:635:LEU:HD13	1.99	0.43
3:C:152:LEU:HD23	3:C:251:ILE:HG12	2.00	0.43
11:L:47:ALA:HB3	11:L:48:PRO:HD3	2.01	0.43
12:M:29:ASP:OD1	12:M:30:VAL:N	2.51	0.43
48:5:4966:A:C2	48:5:4967:A:C2	3.06	0.43
51:9:149:A:H2'	51:9:150:A:C8	2.53	0.43
51:9:628:A:N3	55:DD:145:GLN:CD	2.76	0.43
51:9:1667:U:H2'	51:9:1668:U:C6	2.52	0.43
74:WW:55:ASP:HB3	79:bb:25:VAL:HG13	2.00	0.43
87:jj:489:ARG:NH2	87:jj:573:VAL:O	2.46	0.43
5:E:204:ILE:HD13	5:E:264:ILE:HG22	1.99	0.43
38:m:72:LYS:HD3	38:m:92:THR:HG21	1.99	0.43
51:9:1057:C:O2	51:9:1057:C:O4'	2.37	0.43
56:EE:192:ILE:HD13	56:EE:238:LEU:HD23	2.00	0.43
58:GG:41:LEU:O	58:GG:41:LEU:HD22	2.18	0.43
60:II:190:LEU:HD12	60:II:194:GLU:HB3	2.00	0.43
86:ii:167:ILE:HD13	86:ii:182:LEU:HD23	1.99	0.43
14:O:15:LEU:HD11	14:O:129:LEU:HD13	1.99	0.43
48:5:922:C:C3'	48:5:922:C:C6	3.02	0.43
48:5:4423:U:O2	48:5:4423:U:O4'	2.37	0.43
51:9:314:U:O2	51:9:314:U:H2'	2.19	0.43
51:9:958:G:N1	51:9:959:G:C6	2.86	0.43
51:9:980:A:C2	51:9:981:A:C6	3.05	0.43
51:9:1129:G:C6	51:9:1130:G:C6	3.06	0.43
72:UU:50:VAL:HG23	72:UU:91:LEU:HD23	1.99	0.43
32:g:23:SER:CB	32:g:33:LEU:HD12	2.48	0.43
42:r:18:ILE:HG23	42:r:25:TYR:HB2	2.01	0.43
48:5:739:G:O5'	48:5:739:G:H8	2.00	0.43
48:5:923:C:C5	48:5:926:G:O4'	2.71	0.43
51:9:928:G:H2'	51:9:929:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:72:HIS:N	48:5:4586:G:OP1	2.47	0.43
16:Q:67:ILE:HD13	16:Q:98:LEU:HD11	1.99	0.43
31:f:48:ALA:HB2	31:f:71:TRP:CZ3	2.54	0.43
48:5:738:C:HO2'	48:5:738(A):C:C1'	2.20	0.43
48:5:2265:G:O2'	48:5:2266:C:OP1	2.25	0.43
17:R:70:ARG:CG	17:R:76:MET:HE2	2.49	0.43
48:5:2729:C:H2'	48:5:2730:U:O4'	2.18	0.43
51:9:57:U:OP1	51:9:504:G:O2'	2.36	0.43
51:9:604:A:C6	51:9:605:A:N1	2.87	0.43
52:AA:63:ARG:HG2	52:AA:185:MET:HE1	1.99	0.43
52:AA:161:ILE:HG22	52:AA:163:CYS:SG	2.59	0.43
64:MM:26:LEU:HD11	64:MM:89:VAL:O	2.18	0.43
66:OO:36:SER:OG	66:OO:37:PHE:N	2.50	0.43
4:D:146:LEU:HD12	48:5:4323:A:C2	2.53	0.43
21:V:82:ILE:HG12	21:V:121:VAL:HG13	2.00	0.43
26:a:86:THR:HG22	48:5:510:U:H5''	2.00	0.43
48:5:100:C:O2	48:5:100:C:O4'	2.36	0.43
51:9:363:A:N1	51:9:397:G:O2'	2.41	0.43
51:9:1345:G:OP1	51:9:1688:C:O2'	2.35	0.43
65:NN:54:LEU:HB3	65:NN:60:VAL:HG13	2.01	0.43
69:RR:5:ARG:HB2	69:RR:10:LYS:HE2	2.00	0.43
73:VV:11:LEU:HD12	73:VV:12:TYR:N	2.33	0.43
73:VV:32:ILE:HD12	73:VV:60:ARG:HD2	2.00	0.43
86:ii:43:THR:O	86:ii:62:ARG:HA	2.18	0.43
87:jj:263:LEU:HD21	87:jj:366:VAL:CG2	2.48	0.43
18:S:82:LEU:HD12	18:S:124:ILE:HG23	2.01	0.43
25:Z:11:VAL:CG1	25:Z:80:LEU:HD22	2.49	0.43
30:e:89:LEU:C	30:e:89:LEU:HD12	2.44	0.43
33:h:21:LEU:HD21	33:h:58:LEU:HD21	2.01	0.43
48:5:4966:A:H2'	48:5:4967:A:C8	2.53	0.43
65:NN:33:VAL:HG21	65:NN:66:VAL:HG11	2.00	0.43
86:ii:313:ILE:N	86:ii:313:ILE:HD13	2.34	0.43
87:jj:506:THR:HG22	87:jj:551:SER:CB	2.49	0.43
87:jj:529:CYS:SG	87:jj:556:GLY:N	2.91	0.43
6:F:89:ALA:CB	6:F:124:LEU:HD21	2.48	0.43
16:Q:78:LYS:HG2	16:Q:137:VAL:HG23	2.00	0.43
20:U:23:LEU:HD11	20:U:83:LEU:HD21	2.01	0.43
21:V:42:VAL:HG22	21:V:55:ALA:HB2	2.00	0.43
48:5:1074:G:C2	48:5:1238:A:C2	3.06	0.43
48:5:3648:A:H1'	48:5:3785:A:N6	2.34	0.43
51:9:614:C:O4'	51:9:626:G:N3	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:jj:489:ARG:HG2	87:jj:575:ILE:HD11	2.00	0.43
2:B:11:HIS:ND1	2:B:236:HIS:O	2.52	0.42
3:C:76:ILE:HG22	3:C:77:PRO:HD2	2.00	0.42
9:I:14:ASN:O	9:I:128:ARG:NH2	2.51	0.42
12:M:17:PHE:CE2	12:M:54:CYS:HA	2.54	0.42
46:2:38:C:O2'	51:9:1058:A:OP1	2.37	0.42
51:9:1501:C:HO2'	90:9:1972:GCP:C2'	2.26	0.42
69:RR:119:VAL:HG13	69:RR:119:VAL:O	2.18	0.42
80:cc:30:VAL:HG12	80:cc:32:VAL:HG13	2.01	0.42
1:A:181:LYS:HB2	48:5:1577:G:C5	2.54	0.42
2:B:261:ARG:HB2	14:O:64:THR:HG21	2.01	0.42
16:Q:82:VAL:O	16:Q:102:ALA:HA	2.20	0.42
21:V:60:MET:HE1	21:V:78:PRO:HB2	2.00	0.42
29:d:27:ILE:HD12	29:d:86:VAL:HG21	2.01	0.42
48:5:922(B):C:O2'	48:5:923:C:C5'	2.68	0.42
48:5:1301:C:O2	48:5:1301:C:O4'	2.33	0.42
48:5:2693:G:C6	48:5:2694:G:N1	2.87	0.42
58:GG:52:ILE:HD11	58:GG:109:LEU:HD22	1.99	0.42
74:WW:52:ILE:HG22	74:WW:61:ILE:HG23	2.00	0.42
15:P:41:ILE:HD12	15:P:150:LEU:HD13	2.01	0.42
21:V:39:ILE:HG23	21:V:61:VAL:CG2	2.49	0.42
51:9:446:G:OP2	60:II:47:ARG:NH1	2.42	0.42
1:A:179:ILE:O	48:5:3653:A:H4'	2.19	0.42
32:g:97:ILE:HD13	48:5:4120:U:C4	2.55	0.42
65:NN:91:LEU:CD1	65:NN:125:LEU:HD12	2.50	0.42
66:OO:116:LEU:HD22	78:aa:53:ILE:CD1	2.48	0.42
74:WW:14:ILE:HD11	74:WW:41:MET:HE1	2.01	0.42
14:O:160:ARG:NH2	48:5:4760:G:OP1	2.52	0.42
35:j:19:CYS:SG	35:j:20:ARG:N	2.93	0.42
48:5:100:C:H2'	48:5:101:A:O4'	2.19	0.42
48:5:962:C:C4	48:5:963:G:N7	2.87	0.42
48:5:1406:G:C2	48:5:1406(C):G:N2	2.87	0.42
51:9:943:U:H1'	66:OO:137:SER:HB3	2.01	0.42
68:QQ:34:VAL:HG21	68:QQ:84:ILE:HD12	2.00	0.42
76:YY:55:ILE:HG12	76:YY:75:ILE:HG23	2.02	0.42
86:ii:222:PHE:CG	86:ii:237:ARG:NH1	2.87	0.42
1:A:96:LEU:HD22	1:A:166:VAL:HG21	2.01	0.42
48:5:81:C:H2'	48:5:82:U:O4'	2.19	0.42
48:5:935:A:H61	48:5:935(A):G:H3'	1.85	0.42
48:5:1406(C):G:N2	48:5:1411(A):G:C2	2.87	0.42
48:5:2367:A:N6	48:5:2788:U:H3	2.10	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:614:C:O2	51:9:614:C:C2'	2.68	0.42
52:AA:24:HIS:HB3	52:AA:51:LEU:HD21	2.02	0.42
55:DD:162:ASP:N	55:DD:163:PRO:HD2	2.34	0.42
57:FF:116:ILE:HD12	57:FF:151:ILE:HG13	2.00	0.42
84:gg:5:MET:HE1	84:gg:312:VAL:HG22	2.02	0.42
86:ii:159:THR:HG21	86:ii:250:LYS:HD3	2.02	0.42
87:jj:402:ALA:HB2	87:jj:477:PHE:HE2	1.85	0.42
3:C:53:ALA:HB3	50:8:27:U:H4'	2.01	0.42
4:D:56:THR:HG22	49:7:27:G:OP2	2.20	0.42
4:D:64:ILE:HG13	4:D:105:LEU:HD21	2.02	0.42
30:e:66:THR:HA	30:e:69:MET:HE3	2.02	0.42
48:5:2408:U:O4'	48:5:2409:U:C5	2.73	0.42
1:A:142:GLU:O	1:A:143:THR:OG1	2.36	0.42
3:C:95:MET:HE1	48:5:1521:C:H4'	2.02	0.42
7:G:215:ASP:HB3	7:G:216:PRO:HD3	2.01	0.42
25:Z:23:ALA:HA	25:Z:45:GLY:HA2	2.01	0.42
41:p:75:SER:O	41:p:79:VAL:HG23	2.19	0.42
48:5:1633:G:H5'	48:5:1634:A:OP1	2.20	0.42
61:JJ:66:LYS:HA	61:JJ:71:LEU:HD11	2.01	0.42
1:A:82:ILE:HD11	1:A:99:GLY:CA	2.46	0.42
3:C:323:ARG:NH1	48:5:1281:G:C8	2.88	0.42
29:d:64:ILE:HG13	29:d:68:LEU:HD23	2.02	0.42
48:5:922(B):C:O2	48:5:923:C:O4'	2.38	0.42
51:9:1404:U:C6	72:UU:56:MET:HE2	2.54	0.42
87:jj:352:ILE:N	87:jj:353:PRO:CD	2.83	0.42
2:B:95:THR:HB	2:B:96:PRO:HD2	2.02	0.42
4:D:66:TYR:OH	4:D:73:MET:HE3	2.20	0.42
5:E:156:LEU:HD11	5:E:198:ILE:HG13	2.01	0.42
7:G:219:LEU:HD23	13:N:7:ILE:CD1	2.50	0.42
54:CC:78:LEU:HD13	54:CC:82:TYR:CE2	2.55	0.42
54:CC:252:THR:HG22	54:CC:253:PRO:HD2	2.01	0.42
87:jj:503:PHE:CE1	87:jj:505:ILE:HD12	2.55	0.42
2:B:317:LEU:HD21	2:B:381:THR:HA	2.01	0.41
7:G:139:VAL:HG11	7:G:238:LYS:HG3	2.02	0.41
12:M:6:PHE:O	12:M:11:ARG:NE	2.51	0.41
25:Z:75:TYR:CD2	25:Z:80:LEU:HD21	2.55	0.41
29:d:33:ILE:O	29:d:36:VAL:HG22	2.20	0.41
48:5:957:G:N7	48:5:958:G:C6	2.88	0.41
48:5:1406:G:C1'	48:5:1406(C):G:H2'	2.50	0.41
48:5:3798:U:C2	48:5:3801:U:C5	3.08	0.41
51:9:1207:G:C6	51:9:1837:G:C6	3.07	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BB:49:VAL:CG2	53:BB:62:LEU:HD13	2.49	0.41
72:UU:102:THR:HG21	72:UU:114:VAL:HG21	2.02	0.41
84:gg:86:THR:HG22	84:gg:102:VAL:HG22	2.02	0.41
87:jj:539:GLU:N	87:jj:540:PRO:CD	2.83	0.41
51:9:628:A:C4	55:DD:145:GLN:NE2	2.89	0.41
51:9:1611:G:OP2	70:SS:121:ARG:NH1	2.47	0.41
51:9:1825:A:C6	86:ii:62:ARG:NH1	2.88	0.41
78:aa:45:VAL:HG11	78:aa:53:ILE:HD13	2.02	0.41
14:O:168:TYR:CE2	14:O:172:LYS:HD2	2.56	0.41
15:P:122:ALA:HB1	15:P:123:PRO:HD2	2.02	0.41
16:Q:43:PHE:CD2	16:Q:133:GLY:HA3	2.56	0.41
33:h:44:LEU:O	33:h:47:ILE:HG22	2.20	0.41
48:5:964:A:H2'	48:5:965:G:O4'	2.19	0.41
48:5:1236:C:O2'	48:5:1237:C:O5'	2.30	0.41
59:HH:133:LEU:HD21	59:HH:176:VAL:HG11	2.01	0.41
87:jj:395:SER:CB	87:jj:666:MET:HE1	2.50	0.41
2:B:29:VAL:HG13	2:B:348:ARG:HD3	2.03	0.41
11:L:58:ILE:HG12	11:L:157:ILE:HG23	2.02	0.41
13:N:38:ARG:NH1	50:8:142:U:OP2	2.43	0.41
18:S:30:MET:HE1	18:S:47:PHE:CB	2.50	0.41
35:j:52:LYS:NZ	48:5:375:G:OP2	2.51	0.41
48:5:37:U:H2'	48:5:38:A:O4'	2.20	0.41
74:WW:62:VAL:HG11	79:bb:8:LEU:HG	2.01	0.41
10:J:53:ALA:HB2	10:J:68:ILE:CD1	2.50	0.41
14:O:84:VAL:HG11	14:O:102:LEU:HD22	2.02	0.41
45:1:66:LEU:HD12	48:5:3908:A:C2	2.55	0.41
51:9:1531:A:H2'	51:9:1532:C:C6	2.56	0.41
90:9:1972:GCP:O2A	90:9:1972:GCP:PG	2.79	0.41
52:AA:76:VAL:C	52:AA:77:ILE:HG13	2.45	0.41
52:AA:137:ALA:HB1	52:AA:142:LEU:HB3	2.03	0.41
61:JJ:136:ARG:NH1	61:JJ:159:PHE:O	2.53	0.41
6:F:242:LEU:O	6:F:246:MET:HG3	2.21	0.41
51:9:944:A:C5	51:9:945:U:C5	3.08	0.41
51:9:981:A:H2'	51:9:982:G:O4'	2.20	0.41
87:jj:656:TYR:CD2	87:jj:678:VAL:HG13	2.54	0.41
26:a:61:TYR:N	48:5:4354:U:O4	2.50	0.41
40:o:81:ARG:NH2	48:5:4293:U:O2'	2.54	0.41
51:9:495:U:H2'	51:9:496:C:O4'	2.21	0.41
51:9:1666:C:H2'	51:9:1667:U:O4'	2.21	0.41
52:AA:122:LEU:HD13	52:AA:142:LEU:HD22	2.03	0.41
56:EE:31:PRO:HG2	56:EE:38:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:NN:87:ASP:OD2	65:NN:125:LEU:HD11	2.21	0.41
2:B:14:LEU:HD23	2:B:17:LEU:CD2	2.51	0.41
7:G:207:LEU:HD23	7:G:208:VAL:N	2.35	0.41
8:H:12:ILE:HG22	8:H:81:ILE:CD1	2.50	0.41
13:N:48:ALA:HB1	13:N:53:TYR:CB	2.50	0.41
15:P:36:ILE:HD12	15:P:48:LEU:HD11	2.02	0.41
20:U:27:HIS:N	20:U:28:PRO:HD2	2.36	0.41
48:5:1632:A:H2'	48:5:1632:A:N3	2.35	0.41
48:5:4724:A:C6	48:5:4725:C:C4	3.08	0.41
51:9:35:C:O2	51:9:520:A:N1	2.54	0.41
52:AA:60:LEU:HD13	52:AA:159:ILE:HD11	2.03	0.41
55:DD:138:VAL:CG1	55:DD:182:LEU:HD23	2.51	0.41
59:HH:133:LEU:HD22	59:HH:173:PHE:CD1	2.56	0.41
87:jj:263:LEU:HD21	87:jj:366:VAL:HG23	2.03	0.41
2:B:86:VAL:HG13	2:B:162:VAL:HG22	2.02	0.41
2:B:252:ALA:HB3	48:5:4457:U:H1'	2.03	0.41
4:D:83:LEU:N	4:D:84:PRO:CD	2.84	0.41
5:E:129:LEU:HD13	48:5:973:G:C8	2.56	0.41
5:E:131:HIS:HB2	48:5:1281:G:C6	2.55	0.41
6:F:90:PHE:CD2	6:F:243:ILE:HD11	2.56	0.41
12:M:36:ALA:HB2	12:M:52:PHE:CZ	2.56	0.41
48:5:2396:A:N6	48:5:2814:C:O2	2.54	0.41
48:5:4310:A:H2'	48:5:4311:A:O4'	2.21	0.41
48:5:4966:A:C2	48:5:5067:U:N3	2.86	0.41
51:9:627:U:O4	86:ii:99:TYR:CD2	2.74	0.41
51:9:1673:U:H2'	51:9:1674:G:O4'	2.20	0.41
51:9:1825:A:C6	86:ii:108:ARG:NH2	2.83	0.41
51:9:1855:G:OP2	66:OO:147:ARG:NH1	2.53	0.41
52:AA:180:ARG:HG2	52:AA:195:TRP:CE3	2.56	0.41
54:CC:161:SER:O	54:CC:163:VAL:HG13	2.21	0.41
58:GG:76:LEU:HD22	58:GG:92:ARG:HB3	2.03	0.41
62:KK:3:MET:HE1	62:KK:48:ALA:CA	2.51	0.41
62:KK:21:MET:HE1	62:KK:45:VAL:HG13	2.02	0.41
4:D:129:GLU:HB2	4:D:177:THR:HG21	2.03	0.41
48:5:35:U:O2'	48:5:1525:A:N1	2.53	0.41
48:5:738:C:O3'	48:5:738(A):C:C4'	2.69	0.41
48:5:922(B):C:C4	48:5:923:C:C5	3.09	0.41
51:9:356:C:O2	51:9:356:C:C2'	2.69	0.41
51:9:1546:G:C5'	68:QQ:18:THR:HG21	2.50	0.41
54:CC:180:VAL:HG22	54:CC:219:ILE:HD13	2.03	0.41
58:GG:5:ILE:HD12	58:GG:16:ILE:CD1	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:II:194:GLU:HG2	63:LL:10:TYR:CD2	2.56	0.41
75:XX:90:CYS:SG	75:XX:130:LEU:HD21	2.61	0.41
84:gg:173:LEU:HD22	84:gg:189:ILE:HG12	2.02	0.41
5:E:286:PRO:HA	5:E:289:LEU:CD2	2.52	0.40
8:H:7:ASN:OD1	8:H:7:ASN:N	2.54	0.40
13:N:158:HIS:HB3	13:N:161:MET:HG2	2.03	0.40
48:5:1787:A:N3	48:5:4210:U:O2'	2.52	0.40
51:9:617:G:N7	75:XX:67:ARG:NH1	2.69	0.40
68:QQ:51:LEU:HD22	68:QQ:84:ILE:HD11	2.04	0.40
70:SS:23:ARG:HB3	77:ZZ:48:VAL:HG21	2.03	0.40
87:jj:521:LEU:HD11	87:jj:523:MET:HE2	2.03	0.40
2:B:299:ILE:N	2:B:299:ILE:HD12	2.36	0.40
4:D:75:VAL:O	4:D:112:ARG:NH1	2.54	0.40
11:L:27:ASN:O	11:L:28:GLN:C	2.64	0.40
11:L:71:ARG:NH2	48:5:74:G:O3'	2.54	0.40
19:T:57:TYR:CD1	19:T:76:VAL:HG21	2.56	0.40
51:9:191:A:C2'	51:9:192:C:OP1	2.69	0.40
51:9:625:G:O5'	51:9:626:G:OP2	2.39	0.40
51:9:1100:A:H2'	51:9:1101:U:O4'	2.22	0.40
51:9:1485:U:H2'	51:9:1486:A:O4'	2.21	0.40
90:9:1972:GCP:O3G	90:9:1972:GCP:PA	2.79	0.40
54:CC:123:ARG:NH2	54:CC:143:CYS:SG	2.94	0.40
2:B:92:TYR:CE1	2:B:101:THR:HB	2.57	0.40
17:R:70:ARG:HG3	17:R:76:MET:HE2	2.03	0.40
41:p:61:MET:HE2	48:5:2652:G:N1	2.37	0.40
42:r:18:ILE:HD11	42:r:20:ARG:NH2	2.36	0.40
48:5:976:G:C2	48:5:977:C:C5	3.09	0.40
48:5:3891:A:H2'	48:5:3892:U:O4'	2.21	0.40
48:5:4371:G:O2'	48:5:4372:U:OP2	2.34	0.40
48:5:4871:C:O2	48:5:4871:C:O4'	2.38	0.40
56:EE:185:GLY:N	56:EE:189:LEU:HD13	2.36	0.40
68:QQ:70:VAL:HG11	68:QQ:84:ILE:HG22	2.03	0.40
76:YY:56:PHE:HE2	76:YY:82:ALA:HB1	1.86	0.40
1:A:90:CYS:HB2	1:A:101:VAL:HG13	2.04	0.40
17:R:21:LYS:NZ	48:5:2821:U:OP1	2.51	0.40
51:9:613:G:N2	51:9:626:G:OP1	2.54	0.40
51:9:1824:A:H3'	51:9:1824:A:OP2	2.20	0.40
51:9:1825:A:C5	86:ii:108:ARG:NH2	2.89	0.40
64:MM:17:ALA:C	64:MM:124:ILE:HD11	2.47	0.40
68:QQ:22:VAL:HG11	68:QQ:71:ARG:NH2	2.37	0.40
77:ZZ:79:ILE:HB	77:ZZ:83:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:ASP:OD1	2:B:36:ASP:N	2.54	0.40
4:D:22:ARG:NH1	4:D:28:THR:OG1	2.55	0.40
16:Q:67:ILE:CD1	16:Q:98:LEU:HD11	2.51	0.40
48:5:716:C:H2'	48:5:717:U:O4'	2.22	0.40
48:5:1411:C:C4	48:5:1411(B):C:C4	3.09	0.40
48:5:2363:A:C2	48:5:3860:A:C4	3.10	0.40
51:9:51:U:H2'	51:9:52:G:C8	2.56	0.40
53:BB:71:LEU:HD12	53:BB:82:ARG:HB3	2.04	0.40
56:EE:45:ILE:HD12	56:EE:80:ILE:HD12	2.04	0.40
56:EE:126:VAL:HG23	56:EE:156:VAL:O	2.22	0.40
74:WW:3:ARG:HD3	74:WW:6:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/257 (96%)	222 (90%)	23 (9%)	1 (0%)	30	61
2	B	392/403 (97%)	363 (93%)	26 (7%)	3 (1%)	16	50
3	C	360/425 (85%)	339 (94%)	20 (6%)	1 (0%)	36	66
4	D	291/297 (98%)	276 (95%)	13 (4%)	2 (1%)	18	52
5	E	208/291 (72%)	190 (91%)	17 (8%)	1 (0%)	24	58
6	F	223/247 (90%)	209 (94%)	12 (5%)	2 (1%)	14	47
7	G	229/319 (72%)	222 (97%)	7 (3%)	0	100	100
8	H	188/192 (98%)	178 (95%)	10 (5%)	0	100	100
9	I	201/214 (94%)	182 (90%)	19 (10%)	0	100	100
10	J	168/178 (94%)	162 (96%)	6 (4%)	0	100	100
11	L	208/211 (99%)	200 (96%)	7 (3%)	1 (0%)	24	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M	136/218 (62%)	126 (93%)	10 (7%)	0	100	100
13	N	201/204 (98%)	187 (93%)	13 (6%)	1 (0%)	24	58
14	O	197/203 (97%)	188 (95%)	9 (5%)	0	100	100
15	P	151/184 (82%)	143 (95%)	7 (5%)	1 (1%)	18	52
16	Q	185/188 (98%)	169 (91%)	15 (8%)	1 (0%)	24	58
17	R	178/196 (91%)	172 (97%)	6 (3%)	0	100	100
18	S	174/176 (99%)	164 (94%)	8 (5%)	2 (1%)	11	44
19	T	157/160 (98%)	145 (92%)	12 (8%)	0	100	100
20	U	97/128 (76%)	85 (88%)	12 (12%)	0	100	100
21	V	129/140 (92%)	114 (88%)	15 (12%)	0	100	100
22	W	102/157 (65%)	96 (94%)	6 (6%)	0	100	100
23	X	116/156 (74%)	110 (95%)	6 (5%)	0	100	100
24	Y	132/145 (91%)	122 (92%)	10 (8%)	0	100	100
25	Z	133/136 (98%)	127 (96%)	4 (3%)	2 (2%)	8	37
26	a	145/148 (98%)	130 (90%)	15 (10%)	0	100	100
27	b	100/245 (41%)	92 (92%)	7 (7%)	1 (1%)	12	45
28	c	96/115 (84%)	90 (94%)	5 (5%)	1 (1%)	12	45
29	d	105/125 (84%)	89 (85%)	15 (14%)	1 (1%)	12	45
30	e	126/135 (93%)	120 (95%)	6 (5%)	0	100	100
31	f	107/110 (97%)	99 (92%)	6 (6%)	2 (2%)	6	33
32	g	112/116 (97%)	105 (94%)	7 (6%)	0	100	100
33	h	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
34	i	100/105 (95%)	93 (93%)	7 (7%)	0	100	100
35	j	84/97 (87%)	78 (93%)	6 (7%)	0	100	100
36	k	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
37	l	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
38	m	50/102 (49%)	49 (98%)	0	1 (2%)	6	32
39	n	23/25 (92%)	23 (100%)	0	0	100	100
40	o	102/106 (96%)	96 (94%)	6 (6%)	0	100	100
41	p	89/92 (97%)	82 (92%)	6 (7%)	1 (1%)	11	44
42	r	122/137 (89%)	111 (91%)	10 (8%)	1 (1%)	16	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	s	194/318 (61%)	175 (90%)	17 (9%)	2 (1%)	12	45
44	t	151/165 (92%)	135 (89%)	14 (9%)	2 (1%)	9	40
45	1	13/15 (87%)	10 (77%)	3 (23%)	0	100	100
52	AA	215/295 (73%)	200 (93%)	13 (6%)	2 (1%)	14	47
53	BB	211/264 (80%)	197 (93%)	14 (7%)	0	100	100
54	CC	219/293 (75%)	206 (94%)	13 (6%)	0	100	100
55	DD	226/243 (93%)	209 (92%)	14 (6%)	3 (1%)	9	40
56	EE	260/263 (99%)	242 (93%)	18 (7%)	0	100	100
57	FF	181/204 (89%)	170 (94%)	11 (6%)	0	100	100
58	GG	235/249 (94%)	227 (97%)	7 (3%)	1 (0%)	30	61
59	HH	181/194 (93%)	170 (94%)	11 (6%)	0	100	100
60	II	204/208 (98%)	192 (94%)	12 (6%)	0	100	100
61	JJ	183/194 (94%)	173 (94%)	10 (6%)	0	100	100
62	KK	94/165 (57%)	85 (90%)	8 (8%)	1 (1%)	11	44
63	LL	139/158 (88%)	129 (93%)	10 (7%)	0	100	100
64	MM	115/132 (87%)	103 (90%)	12 (10%)	0	100	100
65	NN	147/151 (97%)	141 (96%)	6 (4%)	0	100	100
66	OO	134/168 (80%)	122 (91%)	10 (8%)	2 (2%)	8	37
67	PP	118/145 (81%)	106 (90%)	12 (10%)	0	100	100
68	QQ	140/146 (96%)	131 (94%)	9 (6%)	0	100	100
69	RR	130/135 (96%)	122 (94%)	7 (5%)	1 (1%)	16	50
70	SS	142/152 (93%)	135 (95%)	7 (5%)	0	100	100
71	TT	139/145 (96%)	130 (94%)	8 (6%)	1 (1%)	18	52
72	UU	98/119 (82%)	91 (93%)	7 (7%)	0	100	100
73	VV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
74	WW	127/130 (98%)	118 (93%)	7 (6%)	2 (2%)	7	36
75	XX	139/143 (97%)	129 (93%)	7 (5%)	3 (2%)	5	30
76	YY	122/130 (94%)	112 (92%)	10 (8%)	0	100	100
77	ZZ	73/125 (58%)	71 (97%)	2 (3%)	0	100	100
78	aa	99/115 (86%)	92 (93%)	6 (6%)	1 (1%)	12	45
79	bb	81/84 (96%)	74 (91%)	6 (7%)	1 (1%)	10	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	cc	60/69 (87%)	57 (95%)	3 (5%)	0	100	100
81	dd	53/56 (95%)	47 (89%)	5 (9%)	1 (2%)	6	33
82	ee	53/133 (40%)	51 (96%)	2 (4%)	0	100	100
83	ff	66/156 (42%)	60 (91%)	6 (9%)	0	100	100
84	gg	311/317 (98%)	285 (92%)	23 (7%)	3 (1%)	12	45
86	ii	370/403 (92%)	338 (91%)	31 (8%)	1 (0%)	36	66
87	jj	423/710 (60%)	387 (92%)	32 (8%)	4 (1%)	14	47
All	All	12325/14502 (85%)	11474 (93%)	794 (6%)	57 (0%)	26	58

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
75	XX	62	PRO
1	A	14	SER
3	C	83	GLY
11	L	63	THR
15	P	114	ILE
18	S	155	PRO
31	f	107	PRO
43	s	142	GLY
44	t	125	LEU
75	XX	86	PRO
13	N	89	VAL
27	b	102	PRO
28	c	92	CYS
29	d	58	GLY
31	f	106	TYR
38	m	94	ASN
62	KK	64	TRP
66	OO	20	GLN
66	OO	149	ARG
79	bb	6	ASP
86	ii	12	ASN
87	jj	618	SER
2	B	17	LEU
4	D	44	TYR
25	Z	90	PRO
25	Z	91	LEU
52	AA	102	ARG
52	AA	159	ILE

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Mol	Chain	Res	Type
55	DD	93	THR
81	dd	7	TYR
87	jj	268	HIS
87	jj	596	LYS
18	S	165	PRO
42	r	33	LYS
44	t	54	LYS
55	DD	44	THR
55	DD	48	ILE
58	GG	135	PRO
71	TT	109	GLY
78	aa	47	ALA
87	jj	269	VAL
2	B	258	HIS
6	F	196	VAL
74	WW	56	HIS
75	XX	61	GLN
16	Q	92	VAL
43	s	25	PRO
4	D	125	VAL
69	RR	119	VAL
84	gg	61	GLY
84	gg	224	GLY
5	E	181	PRO
6	F	99	GLY
41	p	9	GLY
84	gg	13	GLY
2	B	90	VAL
74	WW	29	PRO

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%)	174 (92%)	16 (8%)	10	35
2	B	342/348 (98%)	320 (94%)	22 (6%)	16	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	302/347 (87%)	285 (94%)	17 (6%)	19	46
4	D	247/250 (99%)	234 (95%)	13 (5%)	20	47
5	E	190/251 (76%)	180 (95%)	10 (5%)	20	47
6	F	196/215 (91%)	187 (95%)	9 (5%)	24	50
7	G	200/272 (74%)	189 (94%)	11 (6%)	19	46
8	H	169/171 (99%)	157 (93%)	12 (7%)	13	39
9	I	175/181 (97%)	164 (94%)	11 (6%)	16	43
10	J	143/149 (96%)	137 (96%)	6 (4%)	26	52
11	L	175/176 (99%)	172 (98%)	3 (2%)	53	69
12	M	117/161 (73%)	110 (94%)	7 (6%)	17	44
13	N	171/172 (99%)	166 (97%)	5 (3%)	37	60
14	O	171/173 (99%)	161 (94%)	10 (6%)	18	45
15	P	134/163 (82%)	128 (96%)	6 (4%)	24	51
16	Q	164/165 (99%)	154 (94%)	10 (6%)	17	44
17	R	159/175 (91%)	149 (94%)	10 (6%)	16	43
18	S	157/157 (100%)	149 (95%)	8 (5%)	21	48
19	T	139/140 (99%)	130 (94%)	9 (6%)	15	42
20	U	89/114 (78%)	88 (99%)	1 (1%)	65	74
21	V	101/107 (94%)	90 (89%)	11 (11%)	6	27
22	W	86/126 (68%)	85 (99%)	1 (1%)	63	73
23	X	106/134 (79%)	100 (94%)	6 (6%)	18	46
24	Y	124/135 (92%)	119 (96%)	5 (4%)	28	53
25	Z	117/118 (99%)	115 (98%)	2 (2%)	53	69
26	a	119/120 (99%)	117 (98%)	2 (2%)	53	69
27	b	84/184 (46%)	81 (96%)	3 (4%)	31	57
28	c	84/98 (86%)	81 (96%)	3 (4%)	31	57
29	d	98/110 (89%)	92 (94%)	6 (6%)	17	44
30	e	114/121 (94%)	105 (92%)	9 (8%)	11	37
31	f	88/89 (99%)	84 (96%)	4 (4%)	24	51
32	g	98/99 (99%)	92 (94%)	6 (6%)	17	44
33	h	109/110 (99%)	107 (98%)	2 (2%)	51	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	i	86/89 (97%)	83 (96%)	3 (4%)	32	57
35	j	73/80 (91%)	71 (97%)	2 (3%)	39	62
36	k	64/65 (98%)	62 (97%)	2 (3%)	35	60
37	l	47/48 (98%)	46 (98%)	1 (2%)	47	66
38	m	48/90 (53%)	45 (94%)	3 (6%)	16	43
39	n	24/24 (100%)	22 (92%)	2 (8%)	10	35
40	o	92/94 (98%)	87 (95%)	5 (5%)	20	47
41	p	74/75 (99%)	72 (97%)	2 (3%)	39	62
42	r	108/121 (89%)	101 (94%)	7 (6%)	15	42
43	s	164/258 (64%)	157 (96%)	7 (4%)	26	51
44	t	126/137 (92%)	122 (97%)	4 (3%)	34	59
45	1	13/13 (100%)	13 (100%)	0	100	100
52	AA	180/245 (74%)	162 (90%)	18 (10%)	7	30
53	BB	194/231 (84%)	176 (91%)	18 (9%)	8	32
54	CC	187/225 (83%)	167 (89%)	20 (11%)	6	28
55	DD	190/202 (94%)	177 (93%)	13 (7%)	14	41
56	EE	224/225 (100%)	209 (93%)	15 (7%)	15	41
57	FF	158/170 (93%)	150 (95%)	8 (5%)	21	48
58	GG	207/218 (95%)	191 (92%)	16 (8%)	12	38
59	HH	165/174 (95%)	146 (88%)	19 (12%)	5	25
60	II	178/180 (99%)	165 (93%)	13 (7%)	13	39
61	JJ	161/168 (96%)	148 (92%)	13 (8%)	11	35
62	KK	87/136 (64%)	77 (88%)	10 (12%)	5	25
63	LL	130/142 (92%)	113 (87%)	17 (13%)	4	21
64	MM	99/108 (92%)	86 (87%)	13 (13%)	4	21
65	NN	130/131 (99%)	117 (90%)	13 (10%)	7	30
66	OO	106/130 (82%)	95 (90%)	11 (10%)	7	29
67	PP	109/130 (84%)	96 (88%)	13 (12%)	5	24
68	QQ	117/121 (97%)	105 (90%)	12 (10%)	7	29
69	RR	119/121 (98%)	108 (91%)	11 (9%)	8	32
70	SS	125/132 (95%)	113 (90%)	12 (10%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	TT	111/115 (96%)	99 (89%)	12 (11%)	6	28
72	UU	92/107 (86%)	82 (89%)	10 (11%)	6	27
73	VV	67/67 (100%)	61 (91%)	6 (9%)	9	33
74	WW	112/113 (99%)	105 (94%)	7 (6%)	16	43
75	XX	113/115 (98%)	107 (95%)	6 (5%)	20	47
76	YY	107/112 (96%)	93 (87%)	14 (13%)	4	21
77	ZZ	66/103 (64%)	59 (89%)	7 (11%)	6	28
78	aa	88/98 (90%)	75 (85%)	13 (15%)	3	17
79	bb	75/76 (99%)	68 (91%)	7 (9%)	8	32
80	cc	55/62 (89%)	51 (93%)	4 (7%)	13	39
81	dd	48/49 (98%)	47 (98%)	1 (2%)	47	66
82	ee	46/106 (43%)	41 (89%)	5 (11%)	6	27
83	ff	61/140 (44%)	55 (90%)	6 (10%)	7	30
84	gg	272/275 (99%)	263 (97%)	9 (3%)	33	58
86	ii	326/353 (92%)	304 (93%)	22 (7%)	15	41
87	jj	358/608 (59%)	333 (93%)	25 (7%)	14	40
All	All	10740/12312 (87%)	10027 (93%)	713 (7%)	17	42

All (713) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	109	GLU
1	A	115	CYS
1	A	128	ARG
1	A	142	GLU
1	A	149	LYS
1	A	163	ARG
1	A	165	VAL
1	A	175	ILE
1	A	200	ARG
1	A	209	HIS
1	A	221	LYS
1	A	226	ARG
1	A	233	ARG
1	A	235	VAL

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Mol	Chain	Res	Type
1	A	242	ARG
2	B	10	ARG
2	B	17	LEU
2	B	53	MET
2	B	56	ILE
2	B	60	VAL
2	B	66	LYS
2	B	74	GLU
2	B	95	THR
2	B	97	ARG
2	B	135	LYS
2	B	248	LEU
2	B	262	VAL
2	B	268	ARG
2	B	279	GLU
2	B	294	LYS
2	B	314	ILE
2	B	333	LEU
2	B	351	LEU
2	B	356	LYS
2	B	366	LYS
2	B	381	THR
2	B	383	GLU
3	C	20	LYS
3	C	45	ARG
3	C	95	MET
3	C	124	ILE
3	C	144	ILE
3	C	150	LEU
3	C	165	LYS
3	C	175	LYS
3	C	193	LYS
3	C	208	CYS
3	C	232	VAL
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	22	ARG
4	D	33	ARG

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Mol	Chain	Res	Type
4	D	37	VAL
4	D	50	ARG
4	D	56	THR
4	D	89	LYS
4	D	104	LEU
4	D	124	GLU
4	D	128	ASP
4	D	202	GLN
4	D	262	LYS
4	D	264	LYS
4	D	268	ARG
5	E	52	LEU
5	E	58	ARG
5	E	112	LEU
5	E	123	ASP
5	E	143	LEU
5	E	169	LYS
5	E	178	VAL
5	E	197	VAL
5	E	213	LYS
5	E	291	PHE
6	F	38	GLN
6	F	46	ARG
6	F	65	ARG
6	F	88	LEU
6	F	106	LYS
6	F	134	ILE
6	F	151	GLU
6	F	198	LYS
6	F	211	LYS
7	G	163	LYS
7	G	184	LYS
7	G	201	GLU
7	G	203	LYS
7	G	204	LYS
7	G	220	VAL
7	G	223	LEU
7	G	226	LEU
7	G	230	MET
7	G	293	ASN
7	G	312	LYS
8	H	1	MET

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Mol	Chain	Res	Type
8	H	23	ARG
8	H	52	LYS
8	H	57	VAL
8	H	59	LYS
8	H	66	GLU
8	H	105	ILE
8	H	106	GLN
8	H	108	ASN
8	H	128	MET
8	H	141	LYS
8	H	173	ARG
9	I	36	LEU
9	I	39	LYS
9	I	76	MET
9	I	97	ILE
9	I	116	ARG
9	I	153	ARG
9	I	163	GLN
9	I	164	LYS
9	I	168	SER
9	I	208	LYS
9	I	212	LEU
10	J	16	ARG
10	J	28	GLU
10	J	81	GLU
10	J	96	LYS
10	J	113	ILE
10	J	175	LEU
11	L	63	THR
11	L	162	LYS
11	L	186	ARG
12	M	2	VAL
12	M	37	LEU
12	M	57	LEU
12	M	62	LEU
12	M	89	THR
12	M	96	GLU
12	M	112	VAL
13	N	9	GLU
13	N	64	ILE
13	N	72	LYS
13	N	77	LYS

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Mol	Chain	Res	Type
13	N	89	VAL
14	O	16	LEU
14	O	27	VAL
14	O	49	ARG
14	O	128	ARG
14	O	130	LYS
14	O	145	VAL
14	O	165	LYS
14	O	175	MET
14	O	179	LYS
14	O	202	LEU
15	P	24	VAL
15	P	69	ARG
15	P	86	LYS
15	P	91	LEU
15	P	128	ARG
15	P	147	GLU
16	Q	3	VAL
16	Q	5	ILE
16	Q	13	VAL
16	Q	42	THR
16	Q	61	LEU
16	Q	63	LEU
16	Q	78	LYS
16	Q	91	ARG
16	Q	95	VAL
16	Q	143	ARG
17	R	15	LEU
17	R	36	ASN
17	R	50	ILE
17	R	82	LYS
17	R	89	MET
17	R	99	MET
17	R	103	ARG
17	R	113	LYS
17	R	138	LEU
17	R	178	GLN
18	S	7	LEU
18	S	9	GLU
18	S	24	THR
18	S	70	LYS
18	S	77	ASN

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Mol	Chain	Res	Type
18	S	149	LYS
18	S	159	LEU
18	S	174	THR
19	T	5	LYS
19	T	33	ILE
19	T	45	MET
19	T	60	LYS
19	T	80	VAL
19	T	88	ARG
19	T	96	ILE
19	T	144	ASN
19	T	159	MET
20	U	33	ILE
21	V	15	ARG
21	V	16	ILE
21	V	18	LEU
21	V	35	LYS
21	V	45	ILE
21	V	60	MET
21	V	69	LYS
21	V	82	ILE
21	V	91	LYS
21	V	109	LYS
21	V	123	LYS
22	W	41	LEU
23	X	39	LYS
23	X	53	ARG
23	X	59	LYS
23	X	63	LYS
23	X	91	GLU
23	X	111	GLN
24	Y	2	LYS
24	Y	8	THR
24	Y	55	VAL
24	Y	72	GLN
24	Y	104	VAL
25	Z	11	VAL
25	Z	33	THR
26	a	4	ARG
26	a	84	GLU
27	b	22	LYS
27	b	40	LEU

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Mol	Chain	Res	Type
27	b	101	HIS
28	c	37	MET
28	c	52	CYS
28	c	78	ASN
29	d	23	ARG
29	d	26	THR
29	d	48	GLU
29	d	78	ARG
29	d	98	SER
29	d	102	LEU
30	e	11	LYS
30	e	21	ILE
30	e	22	ARG
30	e	64	LYS
30	e	78	LEU
30	e	86	GLU
30	e	89	LEU
30	e	106	LYS
30	e	128	ARG
31	f	23	GLU
31	f	33	VAL
31	f	52	LYS
31	f	101	ILE
32	g	5	LEU
32	g	43	LYS
32	g	54	ARG
32	g	60	ARG
32	g	66	ARG
32	g	114	GLN
33	h	28	LEU
33	h	67	GLU
34	i	33	LEU
34	i	86	LYS
34	i	89	GLU
35	j	3	LYS
35	j	58	THR
36	k	69	LEU
36	k	70	LYS
37	l	49	LEU
38	m	71	ARG
38	m	72	LYS
38	m	92	THR

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Mol	Chain	Res	Type
39	n	1	MET
39	n	13	LEU
40	o	17	LYS
40	o	28	LYS
40	o	36	GLN
40	o	61	LYS
40	o	83	LEU
41	p	8	VAL
41	p	84	ARG
42	r	8	MET
42	r	20	ARG
42	r	32	LEU
42	r	35	ARG
42	r	39	ARG
42	r	67	ARG
42	r	118	LEU
43	s	34	ASN
43	s	38	LYS
43	s	95	LEU
43	s	105	ASN
43	s	146	LYS
43	s	187	LEU
43	s	191	GLN
44	t	37	LEU
44	t	72	GLU
44	t	98	ILE
44	t	133	LEU
52	AA	5	LEU
52	AA	23	THR
52	AA	25	LEU
52	AA	46	ILE
52	AA	50	ASN
52	AA	56	GLU
52	AA	58	LEU
52	AA	59	LEU
52	AA	60	LEU
52	AA	89	LYS
52	AA	122	LEU
52	AA	124	VAL
52	AA	132	GLN
52	AA	136	GLU
52	AA	142	LEU

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Mol	Chain	Res	Type
52	AA	155	ARG
52	AA	178	LEU
52	AA	198	MET
53	BB	29	ASP
53	BB	38	MET
53	BB	63	LYS
53	BB	71	LEU
53	BB	78	GLU
53	BB	82	ARG
53	BB	96	CYS
53	BB	105	LEU
53	BB	125	VAL
53	BB	157	GLN
53	BB	172	MET
53	BB	180	ASP
53	BB	181	LEU
53	BB	184	VAL
53	BB	207	LEU
53	BB	209	ASP
53	BB	213	ARG
53	BB	231	LEU
54	CC	78	LEU
54	CC	79	GLU
54	CC	94	ILE
54	CC	105	GLU
54	CC	114	LYS
54	CC	120	GLN
54	CC	121	ARG
54	CC	132	ASP
54	CC	144	SER
54	CC	160	LEU
54	CC	167	ARG
54	CC	185	THR
54	CC	188	CYS
54	CC	192	LEU
54	CC	196	ILE
54	CC	244	ILE
54	CC	248	TYR
54	CC	252	THR
54	CC	255	LEU
54	CC	271	ASP
55	DD	28	GLU

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Mol	Chain	Res	Type
55	DD	31	GLU
55	DD	72	VAL
55	DD	127	MET
55	DD	142	LEU
55	DD	145	GLN
55	DD	146	ARG
55	DD	168	VAL
55	DD	179	GLN
55	DD	182	LEU
55	DD	190	LEU
55	DD	218	LEU
55	DD	220	THR
56	EE	17	HIS
56	EE	33	THR
56	EE	42	LEU
56	EE	51	ARG
56	EE	66	MET
56	EE	67	GLN
56	EE	77	ARG
56	EE	162	ILE
56	EE	181	CYS
56	EE	222	LEU
56	EE	227	VAL
56	EE	232	ASN
56	EE	245	ARG
56	EE	246	LEU
56	EE	247	THR
57	FF	63	LYS
57	FF	71	ARG
57	FF	88	MET
57	FF	89	THR
57	FF	127	ARG
57	FF	128	ILE
57	FF	169	ILE
57	FF	204	ARG
58	GG	34	THR
58	GG	41	LEU
58	GG	63	MET
58	GG	64	LYS
58	GG	67	VAL
58	GG	75	LEU
58	GG	95	LYS

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Mol	Chain	Res	Type
58	GG	103	ASP
58	GG	135	PRO
58	GG	171	THR
58	GG	183	ARG
58	GG	190	ARG
58	GG	191	ARG
58	GG	199	THR
58	GG	216	ARG
58	GG	230	LYS
59	HH	8	ILE
59	HH	17	ASP
59	HH	27	LEU
59	HH	36	LEU
59	HH	40	LEU
59	HH	45	ILE
59	HH	46	THR
59	HH	53	VAL
59	HH	75	ILE
59	HH	76	GLN
59	HH	79	LEU
59	HH	82	GLU
59	HH	100	ILE
59	HH	105	THR
59	HH	119	SER
59	HH	160	LYS
59	HH	172	THR
59	HH	188	GLU
59	HH	193	GLN
60	II	14	THR
60	II	23	LYS
60	II	26	LYS
60	II	49	ARG
60	II	74	ARG
60	II	99	ASN
60	II	121	LEU
60	II	130	THR
60	II	147	LYS
60	II	161	LEU
60	II	168	GLN
60	II	178	ARG
60	II	203	LYS
61	JJ	29	LEU

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Mol	Chain	Res	Type
61	JJ	38	ARG
61	JJ	45	ARG
61	JJ	50	LEU
61	JJ	61	LEU
61	JJ	69	ARG
61	JJ	80	ARG
61	JJ	86	VAL
61	JJ	89	GLU
61	JJ	95	ASP
61	JJ	109	ARG
61	JJ	116	LYS
61	JJ	133	ARG
62	KK	1	MET
62	KK	2	LEU
62	KK	6	LYS
62	KK	17	LYS
62	KK	35	LEU
62	KK	50	GLN
62	KK	59	LYS
62	KK	60	GLU
62	KK	89	ILE
62	KK	96	ARG
63	LL	16	ILE
63	LL	20	LYS
63	LL	39	ASN
63	LL	40	ILE
63	LL	42	LEU
63	LL	56	ILE
63	LL	69	ARG
63	LL	85	THR
63	LL	90	ARG
63	LL	91	ASP
63	LL	110	SER
63	LL	113	LEU
63	LL	121	GLN
63	LL	126	VAL
63	LL	134	LEU
63	LL	135	SER
63	LL	144	LYS
64	MM	22	LEU
64	MM	31	LEU
64	MM	33	ARG

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Mol	Chain	Res	Type
64	MM	40	LYS
64	MM	42	LEU
64	MM	45	ARG
64	MM	49	LEU
64	MM	55	ASN
64	MM	64	LEU
64	MM	76	LEU
64	MM	85	LEU
64	MM	99	LYS
64	MM	101	ARG
65	NN	3	ARG
65	NN	27	LYS
65	NN	29	THR
65	NN	55	ARG
65	NN	60	VAL
65	NN	75	LEU
65	NN	78	LYS
65	NN	84	LEU
65	NN	86	GLU
65	NN	107	LYS
65	NN	110	ASP
65	NN	125	LEU
65	NN	132	LYS
66	OO	25	GLU
66	OO	38	ASN
66	OO	51	GLU
66	OO	56	VAL
66	OO	69	SER
66	OO	85	CYS
66	OO	104	ARG
66	OO	133	THR
66	OO	137	SER
66	OO	150	ARG
66	OO	151	LEU
67	PP	13	ARG
67	PP	14	LYS
67	PP	15	PHE
67	PP	37	TYR
67	PP	45	LEU
67	PP	51	ARG
67	PP	65	LYS
67	PP	76	VAL

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Mol	Chain	Res	Type
67	PP	78	THR
67	PP	83	MET
67	PP	106	GLU
67	PP	108	LYS
67	PP	120	SER
68	QQ	26	LYS
68	QQ	31	LEU
68	QQ	37	ARG
68	QQ	41	MET
68	QQ	47	LEU
68	QQ	60	LYS
68	QQ	67	ASP
68	QQ	81	ILE
68	QQ	90	LYS
68	QQ	100	VAL
68	QQ	127	CYS
68	QQ	140	ARG
69	RR	7	LYS
69	RR	22	THR
69	RR	31	ASN
69	RR	44	LYS
69	RR	62	GLN
69	RR	98	VAL
69	RR	99	ASP
69	RR	105	MET
69	RR	120	THR
69	RR	121	GLN
69	RR	132	ARG
70	SS	7	GLU
70	SS	8	LYS
70	SS	13	LEU
70	SS	14	ARG
70	SS	21	ASP
70	SS	46	ARG
70	SS	52	LEU
70	SS	59	LEU
70	SS	60	THR
70	SS	63	GLU
70	SS	110	ASP
70	SS	132	ARG
71	TT	34	VAL
71	TT	36	THR

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Mol	Chain	Res	Type
71	TT	39	LEU
71	TT	55	THR
71	TT	62	ARG
71	TT	84	ARG
71	TT	102	ARG
71	TT	110	LEU
71	TT	124	THR
71	TT	131	LEU
71	TT	132	ASP
71	TT	142	LYS
72	UU	18	HIS
72	UU	25	THR
72	UU	36	CYS
72	UU	44	LYS
72	UU	56	MET
72	UU	60	THR
72	UU	79	ARG
72	UU	88	LEU
72	UU	106	ILE
72	UU	111	GLU
73	VV	10	ASP
73	VV	12	TYR
73	VV	18	SER
73	VV	32	ILE
73	VV	66	ASP
73	VV	79	VAL
74	WW	7	LEU
74	WW	23	ARG
74	WW	51	GLU
74	WW	84	LYS
74	WW	92	ASN
74	WW	103	VAL
74	WW	104	LEU
75	XX	8	ARG
75	XX	29	LYS
75	XX	34	THR
75	XX	67	ARG
75	XX	115	ILE
75	XX	125	VAL
76	YY	16	ARG
76	YY	17	LEU
76	YY	20	ARG

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Mol	Chain	Res	Type
76	YY	32	LYS
76	YY	40	ILE
76	YY	44	LEU
76	YY	46	LYS
76	YY	51	THR
76	YY	54	VAL
76	YY	74	MET
76	YY	88	LYS
76	YY	101	LYS
76	YY	104	ARG
76	YY	115	LYS
77	ZZ	49	LEU
77	ZZ	52	LYS
77	ZZ	89	GLN
77	ZZ	90	GLU
77	ZZ	92	LEU
77	ZZ	99	LEU
77	ZZ	110	THR
78	aa	2	THR
78	aa	12	LYS
78	aa	15	ARG
78	aa	18	VAL
78	aa	19	GLN
78	aa	21	ILE
78	aa	23	CYS
78	aa	41	ILE
78	aa	42	ARG
78	aa	44	ILE
78	aa	55	GLU
78	aa	74	CYS
78	aa	87	ARG
79	bb	15	GLU
79	bb	37	CYS
79	bb	42	LYS
79	bb	48	SER
79	bb	65	GLN
79	bb	80	ARG
79	bb	81	ARG
80	cc	35	MET
80	cc	40	ARG
80	cc	51	ARG
80	cc	68	LEU

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Mol	Chain	Res	Type
81	dd	4	GLN
82	ee	89	THR
82	ee	99	LYS
82	ee	107	ARG
82	ee	109	MET
82	ee	113	ARG
83	ff	83	LYS
83	ff	94	LYS
83	ff	99	LYS
83	ff	110	GLU
83	ff	138	ARG
83	ff	140	TYR
84	gg	17	TRP
84	gg	20	GLN
84	gg	36	ARG
84	gg	87	LEU
84	gg	119	GLN
84	gg	198	VAL
84	gg	207	CYS
84	gg	289	LEU
84	gg	306	LEU
86	ii	8	ILE
86	ii	40	ARG
86	ii	44	ILE
86	ii	50	GLU
86	ii	61	VAL
86	ii	63	THR
86	ii	68	CYS
86	ii	81	LEU
86	ii	107	ASN
86	ii	148	HIS
86	ii	149	ILE
86	ii	170	LYS
86	ii	172	LYS
86	ii	183	GLU
86	ii	198	HIS
86	ii	205	ILE
86	ii	243	VAL
86	ii	258	CYS
86	ii	311	LEU
86	ii	313	ILE
86	ii	319	ARG

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Mol	Chain	Res	Type
86	ii	349	LEU
87	jj	269	VAL
87	jj	276	LEU
87	jj	297	GLN
87	jj	298	GLU
87	jj	313	LEU
87	jj	325	THR
87	jj	330	MET
87	jj	361	GLN
87	jj	369	VAL
87	jj	385	GLN
87	jj	408	MET
87	jj	425	LEU
87	jj	434	PHE
87	jj	436	GLU
87	jj	489	ARG
87	jj	499	GLN
87	jj	505	ILE
87	jj	521	LEU
87	jj	557	MET
87	jj	590	ILE
87	jj	600	VAL
87	jj	613	ILE
87	jj	640	ASN
87	jj	653	LEU
87	jj	664	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (148) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	162	ASN
1	A	194	ASN
1	A	205	ASN
1	A	217	GLN
2	B	3	HIS
2	B	167	GLN
2	B	203	GLN
2	B	204	GLN
2	B	258	HIS
2	B	354	GLN
3	C	60	HIS

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Mol	Chain	Res	Type
3	C	203	GLN
3	C	212	ASN
3	C	299	GLN
3	C	310	HIS
4	D	57	ASN
4	D	244	HIS
5	E	45	HIS
5	E	269	GLN
7	G	143	GLN
7	G	147	GLN
7	G	194	ASN
7	G	293	ASN
8	H	76	HIS
8	H	108	ASN
10	J	104	ASN
10	J	112	HIS
11	L	27	ASN
11	L	28	GLN
11	L	87	HIS
11	L	113	ASN
13	N	15	GLN
13	N	57	GLN
13	N	139	HIS
13	N	149	GLN
13	N	182	HIS
13	N	199	GLN
14	O	50	ASN
14	O	65	ASN
14	O	167	HIS
15	P	75	GLN
15	P	137	ASN
16	Q	57	ASN
16	Q	188	ASN
17	R	34	ASN
17	R	40	GLN
17	R	130	ASN
18	S	122	HIS
18	S	125	GLN
18	S	144	GLN
19	T	22	HIS
19	T	70	HIS
19	T	90	ASN

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Mol	Chain	Res	Type
22	W	30	GLN
22	W	48	GLN
23	X	57	GLN
23	X	69	ASN
23	X	73	HIS
23	X	105	ASN
24	Y	61	HIS
27	b	50	ASN
27	b	60	ASN
31	f	99	HIS
32	g	110	GLN
33	h	20	GLN
33	h	107	GLN
33	h	108	GLN
34	i	80	HIS
35	j	48	ASN
38	m	64	ASN
42	r	12	ASN
42	r	70	GLN
42	r	100	ASN
42	r	121	GLN
43	s	34	ASN
43	s	39	GLN
43	s	81	HIS
43	s	126	GLN
43	s	179	ASN
43	s	200	ASN
44	t	65	GLN
44	t	95	GLN
44	t	103	ASN
52	AA	111	GLN
52	AA	113	GLN
53	BB	92	GLN
53	BB	202	GLN
54	CC	136	HIS
55	DD	179	GLN
56	EE	50	ASN
56	EE	157	ASN
56	EE	188	ASN
56	EE	197	ASN
56	EE	260	GLN
57	FF	31	ASN

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Mol	Chain	Res	Type
57	FF	83	ASN
57	FF	101	HIS
58	GG	105	ASN
59	HH	97	GLN
59	HH	114	GLN
59	HH	168	HIS
59	HH	186	ASN
59	HH	193	GLN
60	II	52	ASN
61	JJ	111	GLN
61	JJ	156	HIS
62	KK	44	HIS
62	KK	84	HIS
63	LL	141	ASN
64	MM	19	GLN
64	MM	46	GLN
64	MM	55	ASN
66	OO	20	GLN
66	OO	38	ASN
67	PP	54	HIS
68	QQ	142	GLN
69	RR	26	ASN
69	RR	62	GLN
70	SS	10	GLN
70	SS	72	GLN
71	TT	42	HIS
73	VV	21	ASN
73	VV	47	ASN
73	VV	49	GLN
74	WW	5	ASN
74	WW	92	ASN
76	YY	85	ASN
78	aa	19	GLN
80	cc	29	GLN
80	cc	45	ASN
84	gg	196	ASN
84	gg	215	GLN
84	gg	222	ASN
86	ii	87	ASN
86	ii	109	GLN
86	ii	236	ASN
86	ii	244	HIS

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Mol	Chain	Res	Type
86	ii	355	GLN
86	ii	358	GLN
87	jj	268	HIS
87	jj	361	GLN
87	jj	385	GLN
87	jj	389	HIS
87	jj	537	HIS
87	jj	549	HIS
87	jj	605	GLN
87	jj	639	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	15 (20%)	0
47	3	72/75 (96%)	28 (38%)	2 (2%)
48	5	3511/3543 (99%)	887 (25%)	165 (4%)
49	7	119/120 (99%)	15 (12%)	0
50	8	150/156 (96%)	37 (24%)	7 (4%)
51	9	1683/1869 (90%)	437 (25%)	87 (5%)
85	hh	7/8 (87%)	4 (57%)	0
All	All	5616/5847 (96%)	1423 (25%)	261 (4%)

All (1423) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	8	U
46	2	9	A
46	2	13	U
46	2	16	C
46	2	19	G
46	2	20	U
46	2	21	A
46	2	43	A
46	2	46	G
46	2	47	U
46	2	49	C
46	2	61	C
46	2	64	G
46	2	72	C
46	2	75	C

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Mol	Chain	Res	Type
47	3	7	A
47	3	8	U
47	3	13	C
47	3	14	A
47	3	16	C
47	3	21	A
47	3	25	C
47	3	28	C
47	3	29	A
47	3	34	U
47	3	35	U
47	3	36	U
47	3	40	C
47	3	42	G
47	3	47	U
47	3	49	C
47	3	51	G
47	3	53	G
47	3	58	A
47	3	60	U
47	3	61	C
47	3	63	C
47	3	65	G
47	3	71	G
47	3	72	C
47	3	74	C
47	3	75	C
47	3	76	A
48	5	12	A
48	5	13	U
48	5	15	A
48	5	20	U
48	5	21	G
48	5	25	A
48	5	30	C
48	5	35	U
48	5	39	A
48	5	42	A
48	5	43	U
48	5	44	A
48	5	48	G
48	5	49	U

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Mol	Chain	Res	Type
48	5	56	A
48	5	58	G
48	5	59	A
48	5	64	A
48	5	65	A
48	5	72	C
48	5	73	A
48	5	75	G
48	5	91	G
48	5	93	G
48	5	108	A
48	5	109	G
48	5	110	C
48	5	116	G
48	5	118	C
48	5	119	G
48	5	120	A
48	5	122	U
48	5	126	C
48	5	134	G
48	5	135	G
48	5	136	C
48	5	143	C
48	5	144	G
48	5	157	U
48	5	159	C
48	5	172	C
48	5	173	C
48	5	177	G
48	5	179	G
48	5	200	U
48	5	201	C
48	5	202	C
48	5	203	U
48	5	205	C
48	5	209	U
48	5	216	C
48	5	217	C
48	5	218	A
48	5	220	C
48	5	221	C
48	5	224	U

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Mol	Chain	Res	Type
48	5	226	G
48	5	227	A
48	5	233	U
48	5	234	G
48	5	245	C
48	5	246	G
48	5	253	G
48	5	262	G
48	5	265	C
48	5	266	C
48	5	275	C
48	5	276	C
48	5	279	A
48	5	280	G
48	5	281	U
48	5	297	U
48	5	298	G
48	5	306	A
48	5	309	C
48	5	310	G
48	5	315	G
48	5	316	U
48	5	317	A
48	5	322	C
48	5	328	A
48	5	334	A
48	5	340	C
48	5	350	C
48	5	357	U
48	5	361	C
48	5	363	A
48	5	386	A
48	5	387	G
48	5	388	A
48	5	399	G
48	5	407	A
48	5	408	A
48	5	409	G
48	5	410	A
48	5	412	G
48	5	413	G
48	5	431	G

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Mol	Chain	Res	Type
48	5	432	U
48	5	446	C
48	5	449	C
48	5	450	G
48	5	452	A
48	5	453	G
48	5	454	U
48	5	457	G
48	5	466	A
48	5	467	U
48	5	468	U
48	5	469	C
48	5	482	G
48	5	483	G
48	5	484	U
48	5	485	C
48	5	486	C
48	5	490	C
48	5	492	U
48	5	493	G
48	5	495	C
48	5	497	G
48	5	498	C
48	5	499	G
48	5	505	G
48	5	510	U
48	5	647	G
48	5	649	A
48	5	654	C
48	5	658	C
48	5	667	A
48	5	668	C
48	5	672	C
48	5	683	C
48	5	685	C
48	5	687	U
48	5	696	C
48	5	697	G
48	5	704	C
48	5	705	G
48	5	708	G
48	5	722	G

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Mol	Chain	Res	Type
48	5	729	G
48	5	730	G
48	5	731	G
48	5	734	G
48	5	739	G
48	5	742	G
48	5	744	G
48	5	747	A
48	5	748	G
48	5	749	G
48	5	752	G
48	5	756	G
48	5	758	G
48	5	911	U
48	5	913	U
48	5	914	U
48	5	917	A
48	5	918	G
48	5	922(A)	G
48	5	922(B)	C
48	5	923	C
48	5	924	C
48	5	925	C
48	5	926	G
48	5	929	A
48	5	931	C
48	5	932	A
48	5	933	G
48	5	934	C
48	5	936	C
48	5	939	G
48	5	941	C
48	5	943	A
48	5	944	A
48	5	945	U
48	5	955	G
48	5	956	A
48	5	957	G
48	5	959	G
48	5	960	A
48	5	961	G
48	5	962	C

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Mol	Chain	Res	Type
48	5	963	G
48	5	964	A
48	5	965	G
48	5	966	A
48	5	967	C
48	5	968	C
48	5	969	C
48	5	972	C
48	5	979	C
48	5	983	C
48	5	990	C
48	5	1072	C
48	5	1073	G
48	5	1075	G
48	5	1076	C
48	5	1078	A
48	5	1079	C
48	5	1082	C
48	5	1174	G
48	5	1177	U
48	5	1179	U
48	5	1184	A
48	5	1185	G
48	5	1195	G
48	5	1211	G
48	5	1212	G
48	5	1214	C
48	5	1215	C
48	5	1234	G
48	5	1235	G
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1239	C
48	5	1272	C
48	5	1273	G
48	5	1274	A
48	5	1275	G
48	5	1276	C
48	5	1280	C
48	5	1284	G
48	5	1287	G

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Mol	Chain	Res	Type
48	5	1288	G
48	5	1291	G
48	5	1292	C
48	5	1293	G
48	5	1295	U
48	5	1296	G
48	5	1301	C
48	5	1303	A
48	5	1304	C
48	5	1313	C
48	5	1326	A
48	5	1328	G
48	5	1329	G
48	5	1330	A
48	5	1337	A
48	5	1353	G
48	5	1354	A
48	5	1359	G
48	5	1360	G
48	5	1364	U
48	5	1370	G
48	5	1371	A
48	5	1377	G
48	5	1378	C
48	5	1380	G
48	5	1381	U
48	5	1387	A
48	5	1394	G
48	5	1397	A
48	5	1398	A
48	5	1401	C
48	5	1403	G
48	5	1411(B)	C
48	5	1411(C)	C
48	5	1416	G
48	5	1418	C
48	5	1419	G
48	5	1420	A
48	5	1421	G
48	5	1429	C
48	5	1435	G
48	5	1436	C

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Mol	Chain	Res	Type
48	5	1437	C
48	5	1438	U
48	5	1440	U
48	5	1441	C
48	5	1442	C
48	5	1445	U
48	5	1446	C
48	5	1453	G
48	5	1455	G
48	5	1456	C
48	5	1457	G
48	5	1458	C
48	5	1465	G
48	5	1475	G
48	5	1478	C
48	5	1482	G
48	5	1483	C
48	5	1484	G
48	5	1485	C
48	5	1486	C
48	5	1489	G
48	5	1497	A
48	5	1498	G
48	5	1502	G
48	5	1504	G
48	5	1514	U
48	5	1516	G
48	5	1518	A
48	5	1523	A
48	5	1525	A
48	5	1533	A
48	5	1534	A
48	5	1535	C
48	5	1547	A
48	5	1554	A
48	5	1563	A
48	5	1564	A
48	5	1566	C
48	5	1568	C
48	5	1574	G
48	5	1578	U
48	5	1586	G

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Mol	Chain	Res	Type
48	5	1591	U
48	5	1596	U
48	5	1602	U
48	5	1612	G
48	5	1613	A
48	5	1624	G
48	5	1625	G
48	5	1631	A
48	5	1633	G
48	5	1634	A
48	5	1640	C
48	5	1641	G
48	5	1654	G
48	5	1656	U
48	5	1661	C
48	5	1670	G
48	5	1676	C
48	5	1677	U
48	5	1679	A
48	5	1684	A
48	5	1691	G
48	5	1724	G
48	5	1726	U
48	5	1733	G
48	5	1734	G
48	5	1740	C
48	5	1741	G
48	5	1742	A
48	5	1750	G
48	5	1753	G
48	5	1755	C
48	5	1756	U
48	5	1757	U
48	5	1761	G
48	5	1763	C
48	5	1764	G
48	5	1768	C
48	5	1772	C
48	5	1773	U
48	5	1776	A
48	5	1781	U
48	5	1785	C

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Mol	Chain	Res	Type
48	5	1787	A
48	5	1797	G
48	5	1799	G
48	5	1800	U
48	5	1803	G
48	5	1804	A
48	5	1805	A
48	5	1819	G
48	5	1821	G
48	5	1822	U
48	5	1828	C
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1836	G
48	5	1837	A
48	5	1842	G
48	5	1855	G
48	5	1869	G
48	5	1882	U
48	5	1890	G
48	5	1892	A
48	5	1893	C
48	5	1897	A
48	5	1909	G
48	5	1910	G
48	5	1918	U
48	5	1920	C
48	5	1921	C
48	5	1922	G
48	5	1923	A
48	5	1931	C
48	5	1932	A
48	5	1933	G
48	5	1940	G
48	5	1941	A
48	5	1948	G
48	5	1952	G
48	5	1959	U
48	5	1961	G
48	5	1962	A
48	5	1963	C

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Mol	Chain	Res	Type
48	5	1966	C
48	5	1967	A
48	5	1976	G
48	5	1977	C
48	5	1978	C
48	5	1979	A
48	5	1980	U
48	5	1982	G
48	5	1983	A
48	5	1984	A
48	5	1986	U
48	5	1987	C
48	5	1991	A
48	5	1992	U
48	5	1993	C
48	5	1997	U
48	5	2001	G
48	5	2002	A
48	5	2003	G
48	5	2004	U
48	5	2005	G
48	5	2008	U
48	5	2011	C
48	5	2024	G
48	5	2025	A
48	5	2026	A
48	5	2033	A
48	5	2046	G
48	5	2047	A
48	5	2048	U
48	5	2052	G
48	5	2055	G
48	5	2056	G
48	5	2062	C
48	5	2064	G
48	5	2068	C
48	5	2069	A
48	5	2070	U
48	5	2084	U
48	5	2085	G
48	5	2089	G
48	5	2090	U

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Mol	Chain	Res	Type
48	5	2092	G
48	5	2093	G
48	5	2094	C
48	5	2095	A
48	5	2097	A
48	5	2098	G
48	5	2100	G
48	5	2101	A
48	5	2102	G
48	5	2104	A
48	5	2105	A
48	5	2106	G
48	5	2107	A
48	5	2108	G
48	5	2110	G
48	5	2259	G
48	5	2260	C
48	5	2262	G
48	5	2266	C
48	5	2267	U
48	5	2268	A
48	5	2269	C
48	5	2270	G
48	5	2275	G
48	5	2279	A
48	5	2289	C
48	5	2294	G
48	5	2300	A
48	5	2301	G
48	5	2313	A
48	5	2314	G
48	5	2331	G
48	5	2333	G
48	5	2348	G
48	5	2351	C
48	5	2352	U
48	5	2360	A
48	5	2364	G
48	5	2370	A
48	5	2380	G
48	5	2395	A
48	5	2396	A

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Mol	Chain	Res	Type
48	5	2397	G
48	5	2399	G
48	5	2416	G
48	5	2417	A
48	5	2422	C
48	5	2424	G
48	5	2425	U
48	5	2428	A
48	5	2429	A
48	5	2433	G
48	5	2441	C
48	5	2447	U
48	5	2450	G
48	5	2467	U
48	5	2468	U
48	5	2469	C
48	5	2471	G
48	5	2475	G
48	5	2476	G
48	5	2483	G
48	5	2488	C
48	5	2489	C
48	5	2490	U
48	5	2491	C
48	5	2493	G
48	5	2495	U
48	5	2503	G
48	5	2504	C
48	5	2505	C
48	5	2506	G
48	5	2513	A
48	5	2521	G
48	5	2530	U
48	5	2537	A
48	5	2546	G
48	5	2547	G
48	5	2553	A
48	5	2554	U
48	5	2555	G
48	5	2564	G
48	5	2566	G
48	5	2571	C

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Mol	Chain	Res	Type
48	5	2572	C
48	5	2575	U
48	5	2583	C
48	5	2587	A
48	5	2601	A
48	5	2620	G
48	5	2627	C
48	5	2638	G
48	5	2639	U
48	5	2647	A
48	5	2660	A
48	5	2662	G
48	5	2663	G
48	5	2669	C
48	5	2673	G
48	5	2676	A
48	5	2681	G
48	5	2686	G
48	5	2687	U
48	5	2688	G
48	5	2689	C
48	5	2695	A
48	5	2696	A
48	5	2707	U
48	5	2708	U
48	5	2709	C
48	5	2710	C
48	5	2711	G
48	5	2712	G
48	5	2714	G
48	5	2716	C
48	5	2719	C
48	5	2721	G
48	5	2725	A
48	5	2726	G
48	5	2735	G
48	5	2740	U
48	5	2743	A
48	5	2751	G
48	5	2754	G
48	5	2755	A
48	5	2760	G

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Mol	Chain	Res	Type
48	5	2761	U
48	5	2763	U
48	5	2764	A
48	5	2769	U
48	5	2787	A
48	5	2789	A
48	5	2790	U
48	5	2794	C
48	5	2795	A
48	5	2796	G
48	5	2798	A
48	5	2802	C
48	5	2806	A
48	5	2807	A
48	5	2814	C
48	5	2826	U
48	5	2827	G
48	5	2828	U
48	5	2829	U
48	5	2835	A
48	5	2838	G
48	5	2839	U
48	5	2842	G
48	5	2855	G
48	5	2875	C
48	5	2884	G
48	5	2896	G
48	5	2897	G
48	5	3598	C
48	5	3604	A
48	5	3605	C
48	5	3615	G
48	5	3625	G
48	5	3626	G
48	5	3630	A
48	5	3635	A
48	5	3644	U
48	5	3653	A
48	5	3662	A
48	5	3674	G
48	5	3692	A
48	5	3696	C

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Mol	Chain	Res	Type
48	5	3698	G
48	5	3711	A
48	5	3712	A
48	5	3722	G
48	5	3729	U
48	5	3733	A
48	5	3740	G
48	5	3748	A
48	5	3753	G
48	5	3756	A
48	5	3759	A
48	5	3760	A
48	5	3761	C
48	5	3765	G
48	5	3766	A
48	5	3773	U
48	5	3774	A
48	5	3776	G
48	5	3777	G
48	5	3778	U
48	5	3780	G
48	5	3784	A
48	5	3786	U
48	5	3809	G
48	5	3810	C
48	5	3811	G
48	5	3812	C
48	5	3813	A
48	5	3814	U
48	5	3817	A
48	5	3819	G
48	5	3822	U
48	5	3831	U
48	5	3838	U
48	5	3839	G
48	5	3840	U
48	5	3859	G
48	5	3867	A
48	5	3876	A
48	5	3877	A
48	5	3878	C
48	5	3879	G

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Mol	Chain	Res	Type
48	5	3888	G
48	5	3889	G
48	5	3892	U
48	5	3897	G
48	5	3898	G
48	5	3901	A
48	5	3905	A
48	5	3906	A
48	5	3907	G
48	5	3915	U
48	5	3916	G
48	5	3917	A
48	5	3927	U
48	5	3939	G
48	5	3943	A
48	5	4067	U
48	5	4069	U
48	5	4073	A
48	5	4076	G
48	5	4084	G
48	5	4085	A
48	5	4086	G
48	5	4088	C
48	5	4092	G
48	5	4099	G
48	5	4100	C
48	5	4116	C
48	5	4117	U
48	5	4118	U
48	5	4119	C
48	5	4120	U
48	5	4121	G
48	5	4122	G
48	5	4125	C
48	5	4127	A
48	5	4150	G
48	5	4158	C
48	5	4162	C
48	5	4163	U
48	5	4164	C
48	5	4166	G
48	5	4171	C

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Mol	Chain	Res	Type
48	5	4177	C
48	5	4183	G
48	5	4184	G
48	5	4191	G
48	5	4201	G
48	5	4203	A
48	5	4212	A
48	5	4213	A
48	5	4215	C
48	5	4218	U
48	5	4219	A
48	5	4225	G
48	5	4229	U
48	5	4232	U
48	5	4233	A
48	5	4249	G
48	5	4251	A
48	5	4255	A
48	5	4257	A
48	5	4258	C
48	5	4265	U
48	5	4268	A
48	5	4271	A
48	5	4273	A
48	5	4281	A
48	5	4291	G
48	5	4297	G
48	5	4304	A
48	5	4305	G
48	5	4306	U
48	5	4314	C
48	5	4317	A
48	5	4318	C
48	5	4319	C
48	5	4326	G
48	5	4329	G
48	5	4330	G
48	5	4335	C
48	5	4336	A
48	5	4339	A
48	5	4349	C
48	5	4350	C

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Mol	Chain	Res	Type
48	5	4354	U
48	5	4355	G
48	5	4373	G
48	5	4377	G
48	5	4378	A
48	5	4379	A
48	5	4380	A
48	5	4387	C
48	5	4391	G
48	5	4393	G
48	5	4394	A
48	5	4395	U
48	5	4396	A
48	5	4398	C
48	5	4401	G
48	5	4415	A
48	5	4419	U
48	5	4421	C
48	5	4422	A
48	5	4440	G
48	5	4444	C
48	5	4448	G
48	5	4449	A
48	5	4450	U
48	5	4453	C
48	5	4454	G
48	5	4463	U
48	5	4464	A
48	5	4471	U
48	5	4475	G
48	5	4476	C
48	5	4488	A
48	5	4495	G
48	5	4500	U
48	5	4510	A
48	5	4511	A
48	5	4512	U
48	5	4513	A
48	5	4515	G
48	5	4519	C
48	5	4520	G
48	5	4522	G

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Mol	Chain	Res	Type
48	5	4524	G
48	5	4548	A
48	5	4549	G
48	5	4560	C
48	5	4561	C
48	5	4563	U
48	5	4567	G
48	5	4570	G
48	5	4573	G
48	5	4575	G
48	5	4584	A
48	5	4585	U
48	5	4586	G
48	5	4590	A
48	5	4599	A
48	5	4618	G
48	5	4636	U
48	5	4637	G
48	5	4639	G
48	5	4656	A
48	5	4657	U
48	5	4658	G
48	5	4661	G
48	5	4667	C
48	5	4669	A
48	5	4670	C
48	5	4672	A
48	5	4677	U
48	5	4678	G
48	5	4700	A
48	5	4701	A
48	5	4709	U
48	5	4719	G
48	5	4720	C
48	5	4721	G
48	5	4728	U
48	5	4736	C
48	5	4737	G
48	5	4745	G
48	5	4751	G
48	5	4754	G
48	5	4755	G

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Mol	Chain	Res	Type
48	5	4756	C
48	5	4757	C
48	5	4759	C
48	5	4761	G
48	5	4765	G
48	5	4771	C
48	5	4772	C
48	5	4868	G
48	5	4870	G
48	5	4871	C
48	5	4872	G
48	5	4873	G
48	5	4874	A
48	5	4875	G
48	5	4876	A
48	5	4877	G
48	5	4882	U
48	5	4883	C
48	5	4885	U
48	5	4887	C
48	5	4891	G
48	5	4895	C
48	5	4897	G
48	5	4904	G
48	5	4910	A
48	5	4912	G
48	5	4913	G
48	5	4914	G
48	5	4915	G
48	5	4919	G
48	5	4921	C
48	5	4924	C
48	5	4925	U
48	5	4926	C
48	5	4927	G
48	5	4928	C
48	5	4931	G
48	5	4935	C
48	5	4937	C
48	5	4938	A
48	5	4940	C
48	5	4942	C

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Mol	Chain	Res	Type
48	5	4943	A
48	5	4944	C
48	5	4948	C
48	5	4949	G
48	5	4950	U
48	5	4951	G
48	5	4956	A
48	5	4957	C
48	5	4958	C
48	5	4964	C
48	5	4965	U
48	5	4966	A
48	5	4967	A
48	5	4976	U
48	5	4985	U
48	5	4988	U
48	5	4989	U
48	5	4990	C
48	5	4991	U
48	5	4993	G
48	5	4999	G
48	5	5014	A
48	5	5017	G
48	5	5040	U
48	5	5041	G
48	5	5047	C
48	5	5050	C
48	5	5053	U
48	5	5054	C
48	5	5056	A
48	5	5061	A
48	5	5062	G
48	5	5069	U
49	7	7	G
49	7	25	G
49	7	33	U
49	7	42	A
49	7	53	U
49	7	54	A
49	7	64	G
49	7	66	G
49	7	97	G

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Mol	Chain	Res	Type
49	7	99	G
49	7	100	A
49	7	110	G
49	7	111	C
49	7	117	G
49	7	120	U
50	8	2	G
50	8	3	A
50	8	32	C
50	8	34	U
50	8	35	C
50	8	49	G
50	8	51	U
50	8	52	A
50	8	59	A
50	8	62	A
50	8	63	U
50	8	75	G
50	8	79	G
50	8	86	U
50	8	87	G
50	8	94	G
50	8	95	A
50	8	103	A
50	8	104	A
50	8	105	C
50	8	107	C
50	8	109	C
50	8	110	U
50	8	111	U
50	8	112	G
50	8	114	G
50	8	121	G
50	8	123	U
50	8	124	U
50	8	125	C
50	8	126	C
50	8	127	U
50	8	137	A
50	8	143	G
50	8	147	G
50	8	150	C

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Mol	Chain	Res	Type
50	8	153	C
51	9	2	A
51	9	3	C
51	9	4	C
51	9	17	C
51	9	25	A
51	9	26	U
51	9	33	G
51	9	37	C
51	9	41	G
51	9	44	U
51	9	45	A
51	9	46	A
51	9	56	G
51	9	58	C
51	9	60	A
51	9	65	C
51	9	67	C
51	9	68	A
51	9	70	G
51	9	71	G
51	9	73	C
51	9	74	G
51	9	75	G
51	9	77	A
51	9	79	A
51	9	99	A
51	9	100	U
51	9	103	A
51	9	104	A
51	9	110	U
51	9	111	A
51	9	113	G
51	9	115	U
51	9	116	U
51	9	124	U
51	9	126	G
51	9	127	C
51	9	128	U
51	9	129	C
51	9	130	G
51	9	141	A

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Mol	Chain	Res	Type
51	9	143	U
51	9	147	A
51	9	155	G
51	9	158	A
51	9	161	U
51	9	162	C
51	9	163	U
51	9	167	G
51	9	168	C
51	9	175	A
51	9	182	C
51	9	183	G
51	9	184	G
51	9	188	C
51	9	189	U
51	9	192	C
51	9	200	G
51	9	202	G
51	9	206	G
51	9	213	G
51	9	215	G
51	9	292	A
51	9	294	U
51	9	302	A
51	9	304	C
51	9	307	G
51	9	308	G
51	9	309	G
51	9	312	G
51	9	313	A
51	9	314	U
51	9	317	C
51	9	318	A
51	9	319	C
51	9	322	C
51	9	331	C
51	9	332	G
51	9	335	G
51	9	343	A
51	9	347	G
51	9	351	G
51	9	360	A

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Mol	Chain	Res	Type
51	9	362	C
51	9	364	A
51	9	368	U
51	9	370	G
51	9	379	C
51	9	381	C
51	9	382	C
51	9	385	G
51	9	386	C
51	9	400	C
51	9	407	G
51	9	409	C
51	9	410	G
51	9	417	C
51	9	418	A
51	9	434	G
51	9	435	A
51	9	438	G
51	9	448	A
51	9	449	A
51	9	450	C
51	9	459	C
51	9	460	A
51	9	462	C
51	9	464	A
51	9	465	A
51	9	466	G
51	9	468	A
51	9	472	C
51	9	473	A
51	9	474	G
51	9	476	A
51	9	482	G
51	9	487	U
51	9	492	C
51	9	496	C
51	9	501	C
51	9	503	C
51	9	523	A
51	9	525	A
51	9	528	A
51	9	531	A

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Mol	Chain	Res	Type
51	9	532	C
51	9	533	A
51	9	544	G
51	9	545	A
51	9	546	G
51	9	548	C
51	9	549	C
51	9	550	C
51	9	551	U
51	9	554	A
51	9	555	A
51	9	556	U
51	9	557	U
51	9	559	G
51	9	560	A
51	9	563	G
51	9	564	A
51	9	568	C
51	9	576	A
51	9	583	A
51	9	587	A
51	9	588	G
51	9	589	G
51	9	590	A
51	9	591	U
51	9	592	C
51	9	594	A
51	9	595	U
51	9	597	G
51	9	604	A
51	9	606	G
51	9	607	U
51	9	608	C
51	9	613	G
51	9	614	C
51	9	615	C
51	9	616	A
51	9	617	G
51	9	625	G
51	9	626	G
51	9	627	U
51	9	628	A

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Mol	Chain	Res	Type
51	9	629	A
51	9	630	U
51	9	632	C
51	9	637	U
51	9	643	A
51	9	644	G
51	9	655	A
51	9	659	G
51	9	660	C
51	9	663	C
51	9	668	A
51	9	669	A
51	9	670	A
51	9	671	A
51	9	672	A
51	9	683	G
51	9	684	G
51	9	688	U
51	9	689	U
51	9	732	U
51	9	752	G
51	9	753	C
51	9	754	G
51	9	811	A
51	9	812	A
51	9	821	G
51	9	822	U
51	9	830	A
51	9	834	C
51	9	847	A
51	9	849	A
51	9	861	A
51	9	868	G
51	9	869	A
51	9	870	A
51	9	871	U
51	9	872	A
51	9	873	G
51	9	874	G
51	9	875	A
51	9	877	C
51	9	878	G

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Mol	Chain	Res	Type
51	9	885	U
51	9	887	U
51	9	890	U
51	9	892	U
51	9	911	C
51	9	913	A
51	9	914	U
51	9	920	A
51	9	922	A
51	9	930	C
51	9	933	G
51	9	934	G
51	9	943	U
51	9	971	G
51	9	985	G
51	9	990	A
51	9	992	A
51	9	999	G
51	9	1016	U
51	9	1017	U
51	9	1023	A
51	9	1041	G
51	9	1055	A
51	9	1060	A
51	9	1061	U
51	9	1062	A
51	9	1067	C
51	9	1078	C
51	9	1083	A
51	9	1085	C
51	9	1089	G
51	9	1099	G
51	9	1100	A
51	9	1113	A
51	9	1114	U
51	9	1115	U
51	9	1116	C
51	9	1117	C
51	9	1118	C
51	9	1121	G
51	9	1131	G
51	9	1137	U

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Mol	Chain	Res	Type
51	9	1138	C
51	9	1139	C
51	9	1144	A
51	9	1148	A
51	9	1149	A
51	9	1153	C
51	9	1154	U
51	9	1161	U
51	9	1165	G
51	9	1166	G
51	9	1195	A
51	9	1196	A
51	9	1207	G
51	9	1208	A
51	9	1211	G
51	9	1213	C
51	9	1215	C
51	9	1221	G
51	9	1223	A
51	9	1224	G
51	9	1227	G
51	9	1230	C
51	9	1240	A
51	9	1242	U
51	9	1251	A
51	9	1253	A
51	9	1254	C
51	9	1256	G
51	9	1257	G
51	9	1258	A
51	9	1259	A
51	9	1265	A
51	9	1266	C
51	9	1268	C
51	9	1271	C
51	9	1274	G
51	9	1275	G
51	9	1281	G
51	9	1284	A
51	9	1285	G
51	9	1286	G
51	9	1287	A

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Mol	Chain	Res	Type
51	9	1289	U
51	9	1291	A
51	9	1293	A
51	9	1298	G
51	9	1299	A
51	9	1300	U
51	9	1301	A
51	9	1302	G
51	9	1303	C
51	9	1307	U
51	9	1308	U
51	9	1313	A
51	9	1314	U
51	9	1316	C
51	9	1322	G
51	9	1330	G
51	9	1331	C
51	9	1337	C
51	9	1342	U
51	9	1348	G
51	9	1354	G
51	9	1369	A
51	9	1371	U
51	9	1372	U
51	9	1378	A
51	9	1395	C
51	9	1396	A
51	9	1397	U
51	9	1401	A
51	9	1402	A
51	9	1404	U
51	9	1410	C
51	9	1412	C
51	9	1424	G
51	9	1428	G
51	9	1429	G
51	9	1439	A
51	9	1449	G
51	9	1454	A
51	9	1459	G
51	9	1462	U
51	9	1463	U

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Mol	Chain	Res	Type
51	9	1466	G
51	9	1473	G
51	9	1476	A
51	9	1477	U
51	9	1478	U
51	9	1489	A
51	9	1490	G
51	9	1493	C
51	9	1494	U
51	9	1498	A
51	9	1507	G
51	9	1509	U
51	9	1510	G
51	9	1521	C
51	9	1522	A
51	9	1531	A
51	9	1533	A
51	9	1536	G
51	9	1539	U
51	9	1544	C
51	9	1545	A
51	9	1548	G
51	9	1552	G
51	9	1553	C
51	9	1555	U
51	9	1556	A
51	9	1557	C
51	9	1560	U
51	9	1570	G
51	9	1574	C
51	9	1575	G
51	9	1580	A
51	9	1581	C
51	9	1585	U
51	9	1587	G
51	9	1588	A
51	9	1589	A
51	9	1600	G
51	9	1601	A
51	9	1602	U
51	9	1604	G
51	9	1621	U

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Mol	Chain	Res	Type
51	9	1622	U
51	9	1623	A
51	9	1624	U
51	9	1625	U
51	9	1637	A
51	9	1638	G
51	9	1641	A
51	9	1647	A
51	9	1648	G
51	9	1654	G
51	9	1664	A
51	9	1665	G
51	9	1671	G
51	9	1680	G
51	9	1682	C
51	9	1683	C
51	9	1686	G
51	9	1689	C
51	9	1695	A
51	9	1698	C
51	9	1715	A
51	9	1721	U
51	9	1722	G
51	9	1726	G
51	9	1728	U
51	9	1729	U
51	9	1730	U
51	9	1732	G
51	9	1737	G
51	9	1744	G
51	9	1745	A
51	9	1753	C
51	9	1758	G
51	9	1760	G
51	9	1772	C
51	9	1783	C
51	9	1785	C
51	9	1800	A
51	9	1801	A
51	9	1805	G
51	9	1823	A
51	9	1824	A

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Mol	Chain	Res	Type
51	9	1825	A
51	9	1826	G
51	9	1829	G
51	9	1831	A
51	9	1835	A
51	9	1836	G
51	9	1838	U
51	9	1849	G
51	9	1850	A
51	9	1851	A
51	9	1861	G
51	9	1862	G
51	9	1863	A
51	9	1865	C
51	9	1866	A
51	9	1867	U
51	9	1868	U
51	9	1869	A
85	hh	42	C
85	hh	43	A
85	hh	45	A
85	hh	46	G

All (261) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
47	3	7	A
47	3	74	C
48	5	12	A
48	5	20	U
48	5	47	A
48	5	48	G
48	5	64	A
48	5	119	G
48	5	125	C
48	5	134	G
48	5	143	C
48	5	159	C
48	5	217	C
48	5	226	G
48	5	245	C
48	5	265	C

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Mol	Chain	Res	Type
48	5	275	C
48	5	278	G
48	5	315	G
48	5	385	A
48	5	387	G
48	5	406	C
48	5	408	A
48	5	409	G
48	5	417	G
48	5	449	C
48	5	484	U
48	5	485	C
48	5	492	U
48	5	497	G
48	5	498	C
48	5	504	G
48	5	696	C
48	5	728	U
48	5	729	G
48	5	738(A)	C
48	5	747	A
48	5	748	G
48	5	916	C
48	5	922	C
48	5	922(B)	C
48	5	930	G
48	5	933	G
48	5	935(A)	G
48	5	936	C
48	5	955	G
48	5	956	A
48	5	959	G
48	5	963	G
48	5	965	G
48	5	966	A
48	5	968	C
48	5	969	C
48	5	971(A)	G
48	5	1072	C
48	5	1209	U
48	5	1211	G
48	5	1214	C

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Mol	Chain	Res	Type
48	5	1236	C
48	5	1238	A
48	5	1287	G
48	5	1291	G
48	5	1295	U
48	5	1329	G
48	5	1358	G
48	5	1359	G
48	5	1370	G
48	5	1378	C
48	5	1380	G
48	5	1420	A
48	5	1432	G
48	5	1440	U
48	5	1445	U
48	5	1455	G
48	5	1477	C
48	5	1484	G
48	5	1485	C
48	5	1533	A
48	5	1563	A
48	5	1633	G
48	5	1678	C
48	5	1733	G
48	5	1740	C
48	5	1804	A
48	5	1818	G
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1892	A
48	5	1919	G
48	5	1921	C
48	5	1935	C
48	5	1979	A
48	5	1983	A
48	5	1986	U
48	5	2001	G
48	5	2046	G
48	5	2068	C
48	5	2088	A
48	5	2089	G

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Mol	Chain	Res	Type
48	5	2100	G
48	5	2265	G
48	5	2266	C
48	5	2278	G
48	5	2313	A
48	5	2396	A
48	5	2398	U
48	5	2428	A
48	5	2467	U
48	5	2468	U
48	5	2474	G
48	5	2475	G
48	5	2490	U
48	5	2502	A
48	5	2546	G
48	5	2553	A
48	5	2661	U
48	5	2695	A
48	5	2724	G
48	5	2754	G
48	5	2782	U
48	5	2789	A
48	5	2794	C
48	5	2806	A
48	5	3603	G
48	5	3625	G
48	5	3673	C
48	5	3697	U
48	5	3710	G
48	5	3759	A
48	5	3760	A
48	5	3809	G
48	5	3876	A
48	5	3888	G
48	5	3904	G
48	5	4075	U
48	5	4076	G
48	5	4084	G
48	5	4119	C
48	5	4121	G
48	5	4124	G
48	5	4162	C

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Mol	Chain	Res	Type
48	5	4170	A
48	5	4221	C
48	5	4232	U
48	5	4254	G
48	5	4266	G
48	5	4378	A
48	5	4395	U
48	5	4448	G
48	5	4449	A
48	5	4463	U
48	5	4488	A
48	5	4510	A
48	5	4583	C
48	5	4699	U
48	5	4719	G
48	5	4871	C
48	5	4872	G
48	5	4873	G
48	5	4876	A
48	5	4884	G
48	5	4925	U
48	5	4936	G
48	5	4942	C
48	5	4947	U
48	5	4965	U
50	8	2	G
50	8	51	U
50	8	85	U
50	8	86	U
50	8	94	G
50	8	110	U
50	8	124	U
51	9	2	A
51	9	3	C
51	9	72	C
51	9	110	U
51	9	126	G
51	9	127	C
51	9	128	U
51	9	142	C
51	9	160	U
51	9	182	C

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Mol	Chain	Res	Type
51	9	293	C
51	9	312	G
51	9	369	C
51	9	434	G
51	9	465	A
51	9	500	A
51	9	516	A
51	9	532	C
51	9	550	C
51	9	553	U
51	9	555	A
51	9	559	G
51	9	563	G
51	9	591	U
51	9	594	A
51	9	606	G
51	9	607	U
51	9	613	G
51	9	614	C
51	9	615	C
51	9	625	G
51	9	626	G
51	9	627	U
51	9	628	A
51	9	629	A
51	9	642	U
51	9	670	A
51	9	688	U
51	9	752	G
51	9	821	G
51	9	869	A
51	9	870	A
51	9	872	A
51	9	874	G
51	9	932	G
51	9	990	A
51	9	1016	U
51	9	1087	A
51	9	1114	U
51	9	1115	U
51	9	1137	U
51	9	1165	G

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Mol	Chain	Res	Type
51	9	1253	A
51	9	1264	C
51	9	1274	G
51	9	1284	A
51	9	1285	G
51	9	1286	G
51	9	1313	A
51	9	1330	G
51	9	1394	G
51	9	1395	C
51	9	1396	A
51	9	1438	A
51	9	1476	A
51	9	1489	A
51	9	1493	C
51	9	1519	U
51	9	1520	G
51	9	1578	U
51	9	1581	C
51	9	1587	G
51	9	1621	U
51	9	1622	U
51	9	1636	G
51	9	1637	A
51	9	1646	C
51	9	1663	A
51	9	1664	A
51	9	1679	A
51	9	1721	U
51	9	1744	G
51	9	1824	A
51	9	1825	A
51	9	1835	A
51	9	1867	U
51	9	1868	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 291 ligands modelled in this entry, 289 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
90	GCP	9	1972	-	32,34,34	1.39	5 (15%)	49,54,54	1.81	7 (14%)
90	GCP	jj	700	88	32,34,34	1.47	7 (21%)	49,54,54	1.78	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	GCP	9	1972	-	-	5/19/38/38	0/3/3/3
90	GCP	jj	700	88	-	4/19/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	jj	700	GCP	C5-C4	3.31	1.47	1.38
90	9	1972	GCP	C5-C4	2.95	1.46	1.38
90	jj	700	GCP	PG-O3G	2.93	1.61	1.55
90	jj	700	GCP	PG-O2G	2.93	1.61	1.55
90	9	1972	GCP	PG-O2G	2.84	1.61	1.55
90	9	1972	GCP	PG-O3G	2.75	1.61	1.55
90	9	1972	GCP	C6-N1	-2.49	1.34	1.38
90	jj	700	GCP	PB-O3A	2.44	1.61	1.58
90	9	1972	GCP	C5-N7	-2.18	1.34	1.39
90	jj	700	GCP	C5-N7	-2.13	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	jj	700	GCP	C6-N1	-2.11	1.34	1.38
90	jj	700	GCP	PB-O2B	2.09	1.61	1.56

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	jj	700	GCP	C5-C4-N3	-6.16	118.59	128.39
90	9	1972	GCP	C5-C4-N3	-5.81	119.15	128.39
90	jj	700	GCP	C2-N3-C4	5.13	121.14	112.30
90	9	1972	GCP	C2-N3-C4	5.02	120.94	112.30
90	9	1972	GCP	PB-O3A-PA	-4.66	117.17	132.37
90	jj	700	GCP	N9-C4-N3	4.51	134.98	125.95
90	9	1972	GCP	N9-C4-N3	4.22	134.38	125.95
90	9	1972	GCP	C6-C5-N7	3.42	136.51	130.29
90	jj	700	GCP	C6-C5-N7	3.32	136.34	130.29
90	jj	700	GCP	C4-C5-N7	-2.69	106.41	110.67
90	jj	700	GCP	PB-O3A-PA	-2.60	123.88	132.37
90	9	1972	GCP	C4-C5-N7	-2.51	106.69	110.67
90	9	1972	GCP	O6-C6-C5	-2.18	120.79	126.53
90	jj	700	GCP	O6-C6-C5	-2.13	120.90	126.53

There are no chirality outliers.

All (9) torsion outliers are listed below:

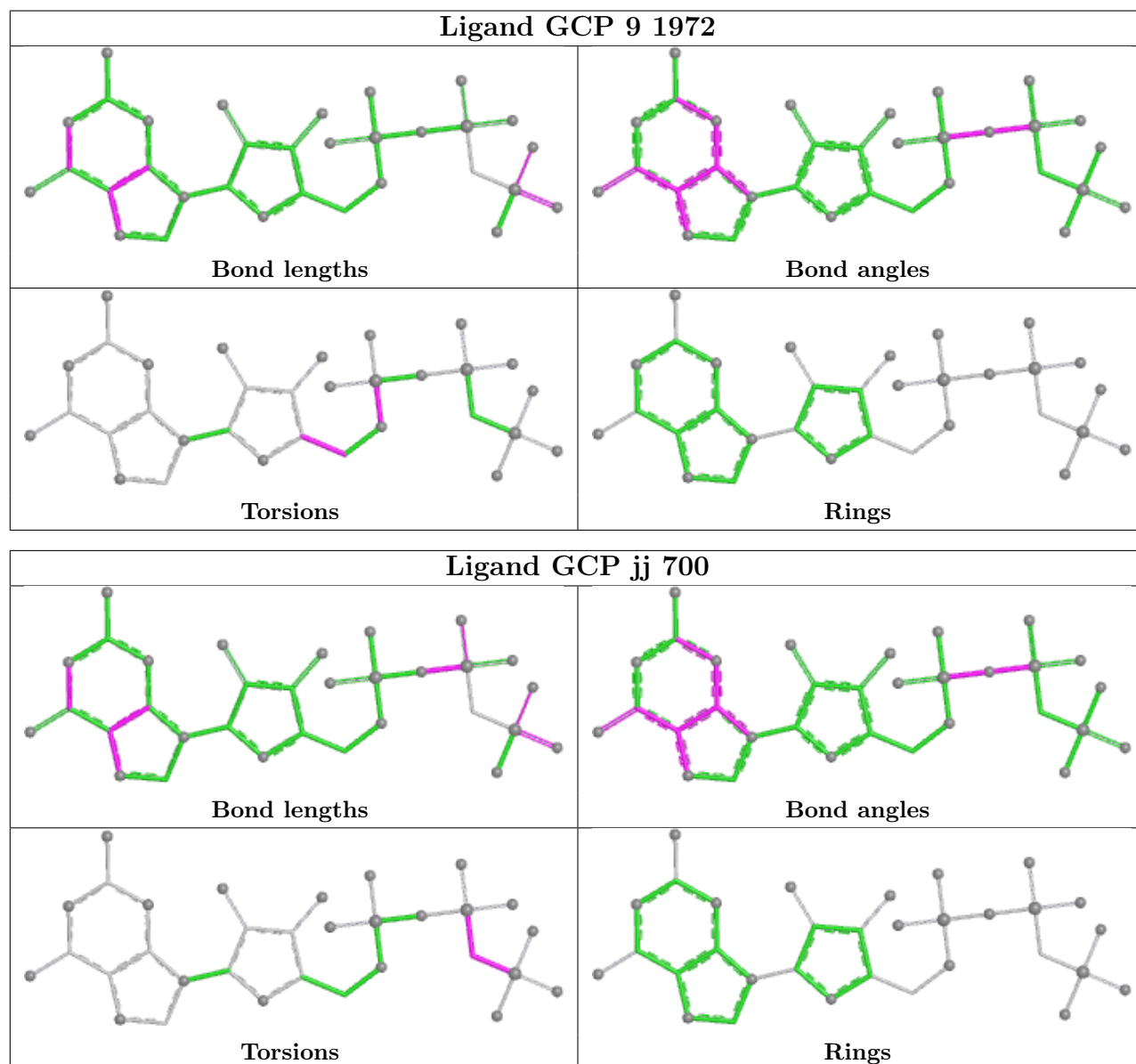
Mol	Chain	Res	Type	Atoms
90	9	1972	GCP	C5'-O5'-PA-O3A
90	9	1972	GCP	C5'-O5'-PA-O1A
90	9	1972	GCP	C5'-O5'-PA-O2A
90	jj	700	GCP	PG-C3B-PB-O1B
90	jj	700	GCP	PG-C3B-PB-O2B
90	jj	700	GCP	PG-C3B-PB-O3A
90	9	1972	GCP	C3'-C4'-C5'-O5'
90	9	1972	GCP	O4'-C4'-C5'-O5'
90	jj	700	GCP	PB-C3B-PG-O1G

There are no ring outliers.

1 monomer is involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	9	1972	GCP	28	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	5	44
51	9	8
47	3	2
46	2	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	40.78
1	5	1252:C	O3'	1271:G	P	35.85
1	5	1219:G	O3'	1233:G	P	22.84
1	5	1405:C	O3'	1406:G	P	22.78
1	5	3948:C	O3'	4065:G	P	19.74
1	5	1406:G	O3'	1406(A):G	P	19.63
1	5	4138:C	O3'	4146:G	P	18.06
1	5	990:C	O3'	1064:G	P	18.05
1	5	523:C	O3'	638:G	P	17.99
1	5	4101:C	O3'	4107:G	P	17.46
1	5	1406(C):G	O3'	1411:C	P	17.15
1	5	4777:C	O3'	4859:C	P	16.56
1	5	760:G	O3'	904:C	P	14.90
1	5	5022:U	O3'	5028:G	P	14.80
1	5	1696:C	O3'	1720:C	P	14.57
1	5	1364:U	O3'	1368:A	P	14.45
1	5	1411:C	O3'	1411(A):G	P	14.41
1	5	182:G	O3'	189:G	P	14.04
1	5	921:C	O3'	922:C	P	13.49
1	5	2901:G	O3'	3597:G	P	13.37
1	5	970:G	O3'	971:U	P	10.82
1	5	512:U	O3'	515:C	P	9.81
1	5	4729:A	O3'	4735:G	P	9.78
1	5	971:U	O3'	971(A):G	P	9.74
1	5	934:C	O3'	935:A	P	9.42
1	5	737:C	O3'	738:C	P	9.01
1	5	1180:C	O3'	1183:C	P	9.01

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	481:G	O3'	481(A):C	P	8.81
1	5	500:G	O3'	504:G	P	6.68
1	5	480:C	O3'	481:G	P	5.80
1	5	1100:U	O3'	1168:G	P	5.73
1	3	19:G	O3'	20:U	P	5.67
1	5	1239:C	O3'	1244:G	P	5.22
1	9	322:C	O3'	323:C	P	5.10
1	5	4740:G	O3'	4743:G	P	4.93
1	3	16:C	O3'	18:U	P	4.79
1	9	309:G	O3'	310:C	P	4.68
1	9	798:G	O3'	799:U	P	4.57
1	5	935:A	O3'	935(A):G	P	4.49
1	9	304:C	O3'	305:U	P	4.39
1	2	16:C	O3'	18:G	P	4.25
1	5	738:C	O3'	738(A):C	P	4.14
1	5	170:C	O3'	171:U	P	3.93
1	5	4899:G	O3'	4902:C	P	3.39
1	9	902:G	O3'	903:A	P	3.39
1	9	903:A	O3'	904:A	P	3.34
1	9	1295:A	O3'	1296:U	P	3.34
1	5	1438:U	O3'	1440:U	P	3.33
1	5	5020:G	O3'	5021:C	P	3.21
1	5	267:G	O3'	268:G	P	3.16
1	5	751:G	O3'	752:G	P	3.13
1	9	593:C	O3'	594:A	P	3.06
1	5	2031:C	O3'	2032:U	P	2.65
1	5	922(A):G	O3'	922(B):C	P	1.81
1	5	922:C	O3'	922(A):G	P	1.76

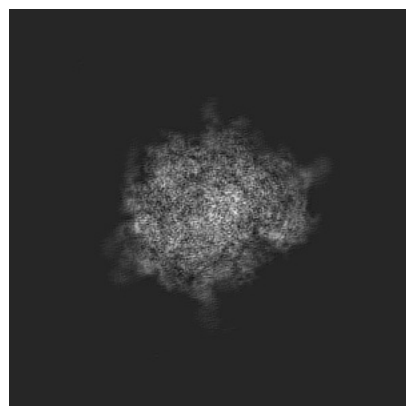
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4134. These allow visual inspection of the internal detail of the map and identification of artifacts.

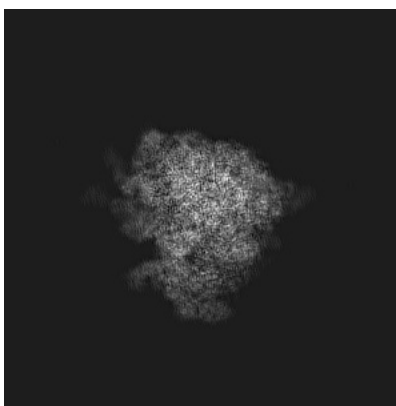
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

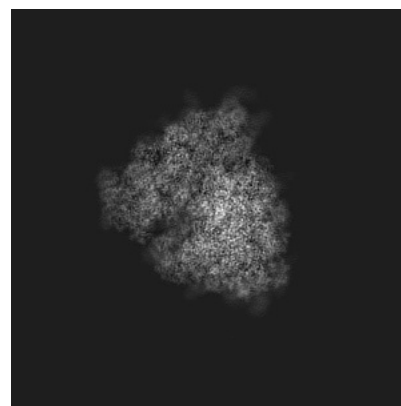
6.1.1 Primary map



X

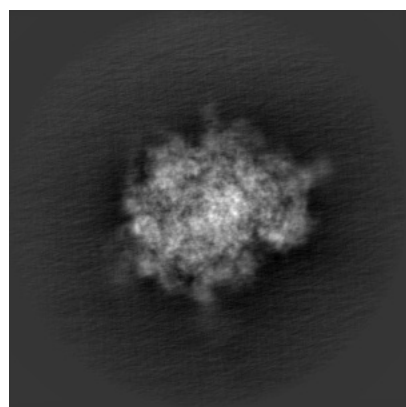


Y

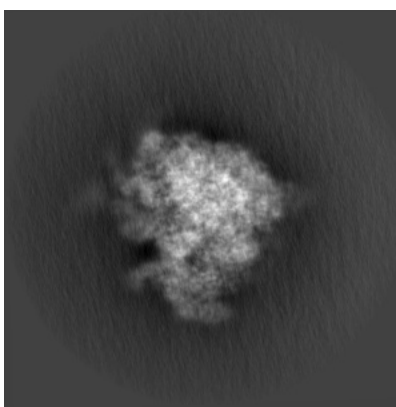


Z

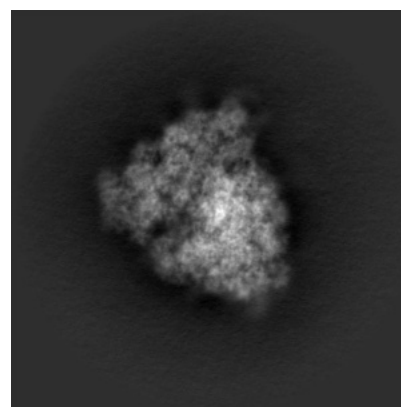
6.1.2 Raw map



X



Y

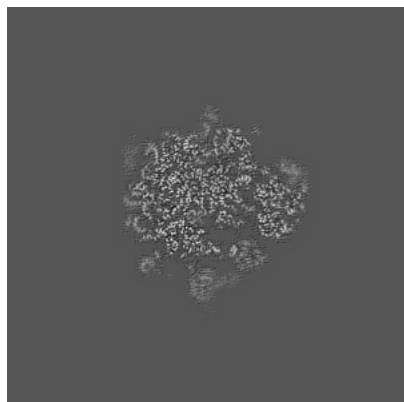


Z

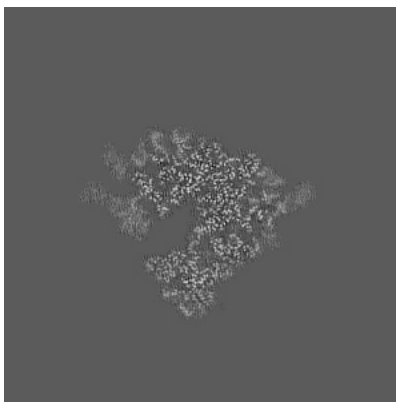
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

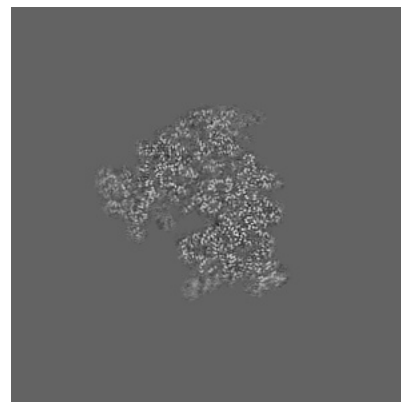
6.2.1 Primary map



X Index: 210

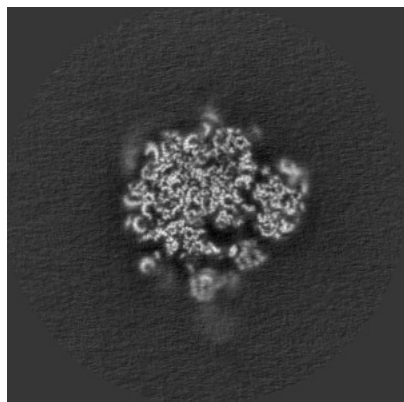


Y Index: 210

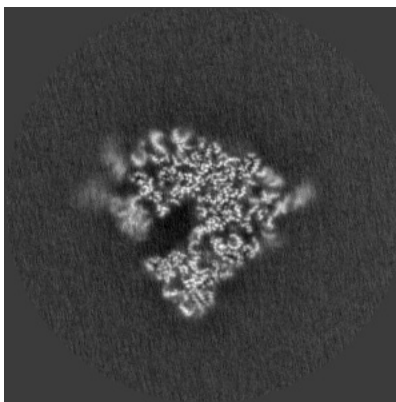


Z Index: 210

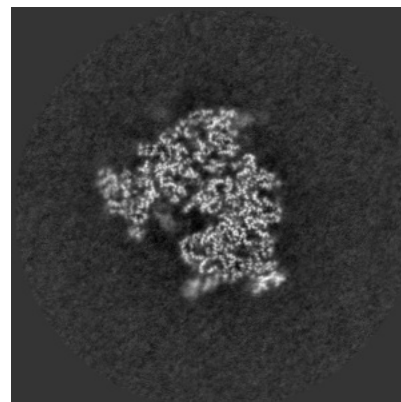
6.2.2 Raw map



X Index: 210



Y Index: 210

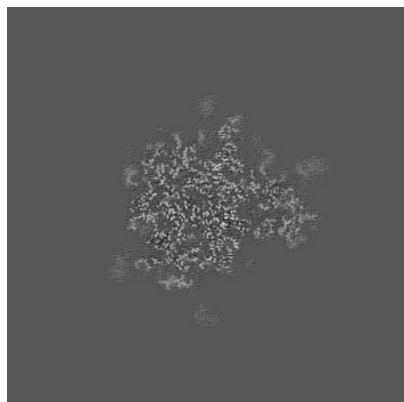


Z Index: 210

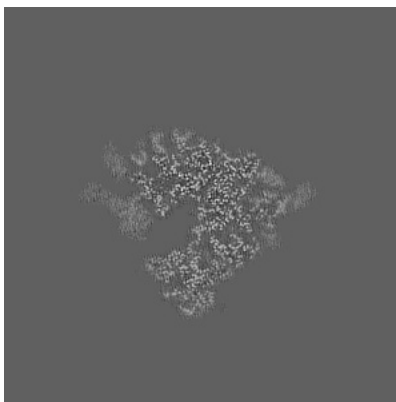
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

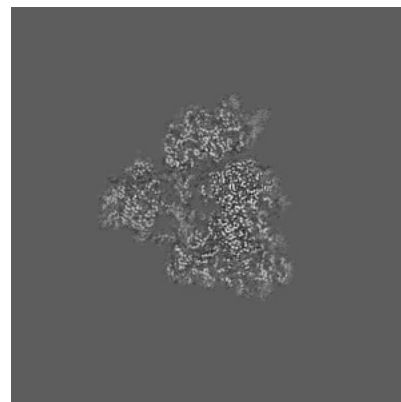
6.3.1 Primary map



X Index: 228

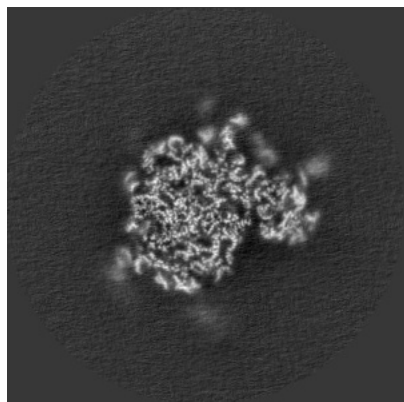


Y Index: 211

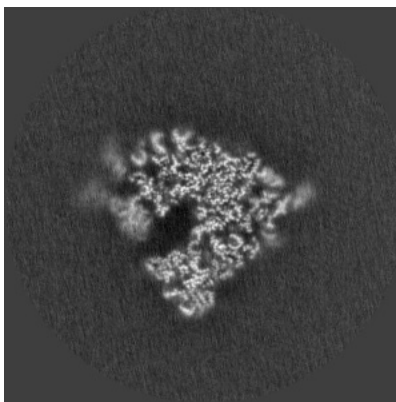


Z Index: 195

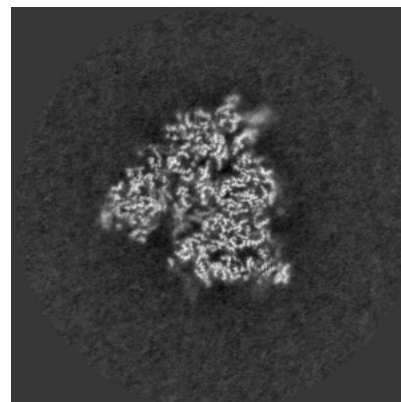
6.3.2 Raw map



X Index: 233



Y Index: 211

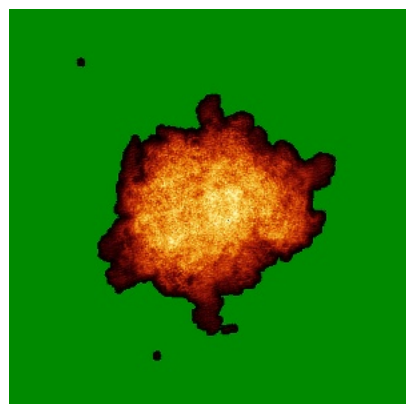


Z Index: 201

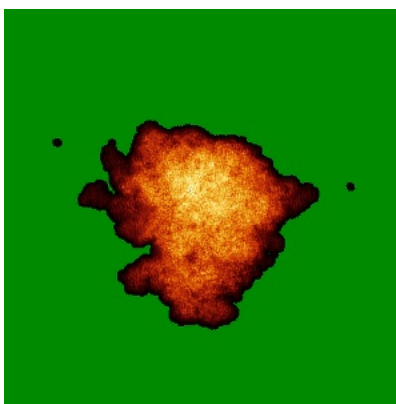
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

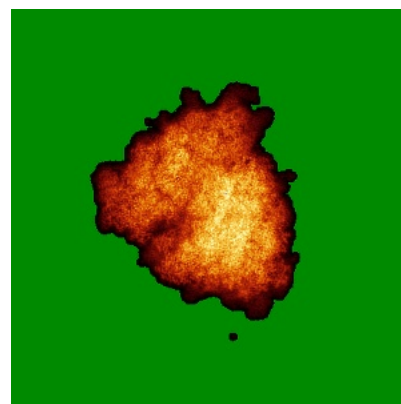
6.4.1 Primary map



X

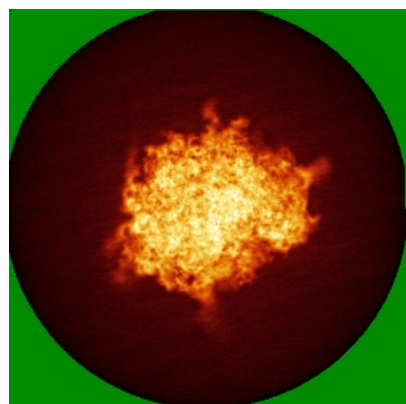


Y

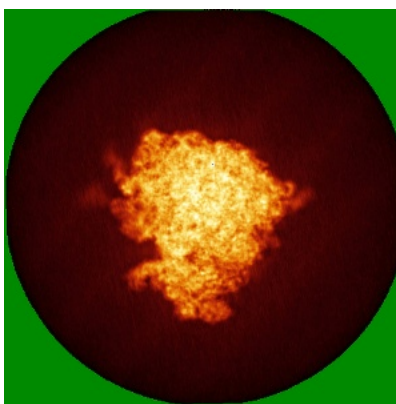


Z

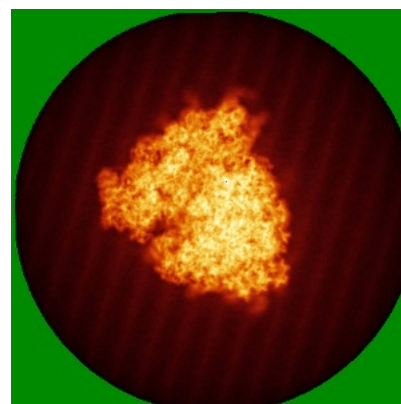
6.4.2 Raw map



X



Y

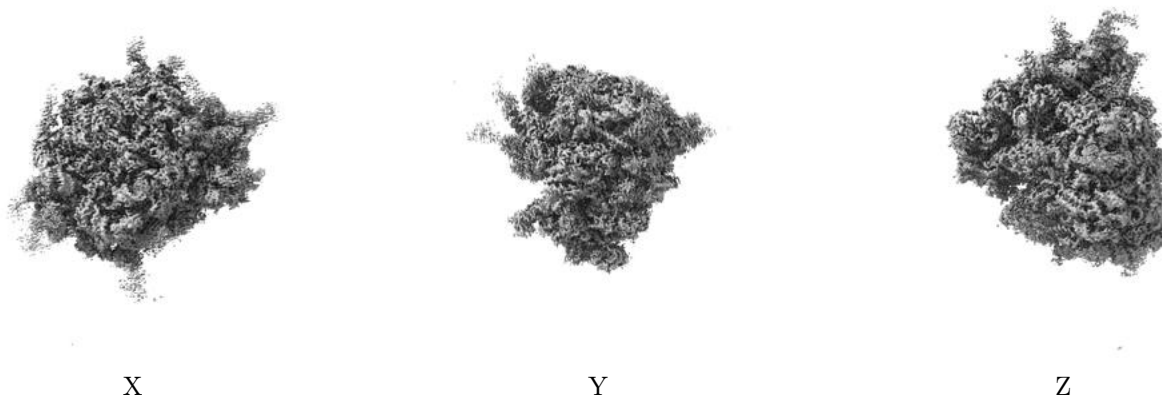


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

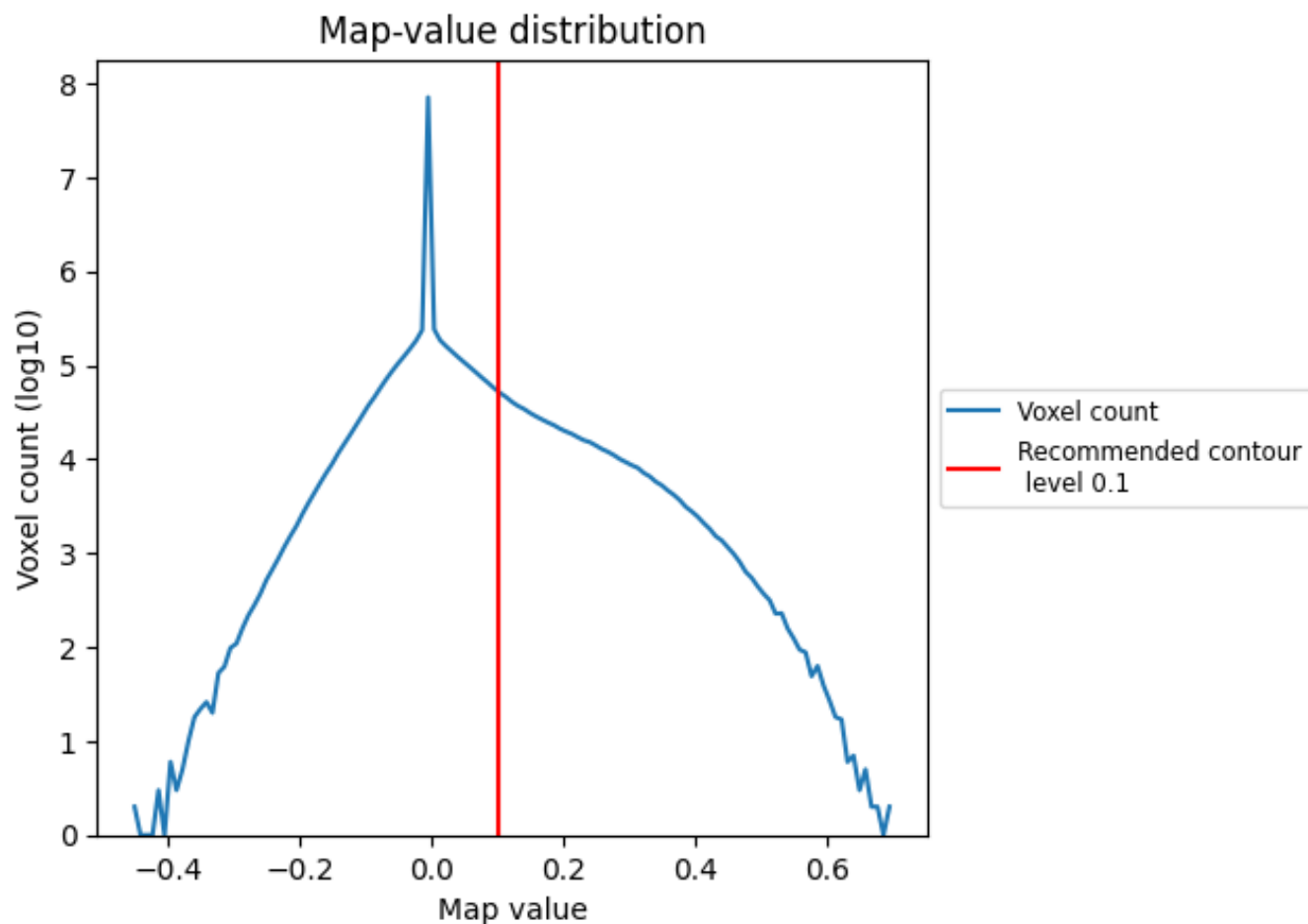
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

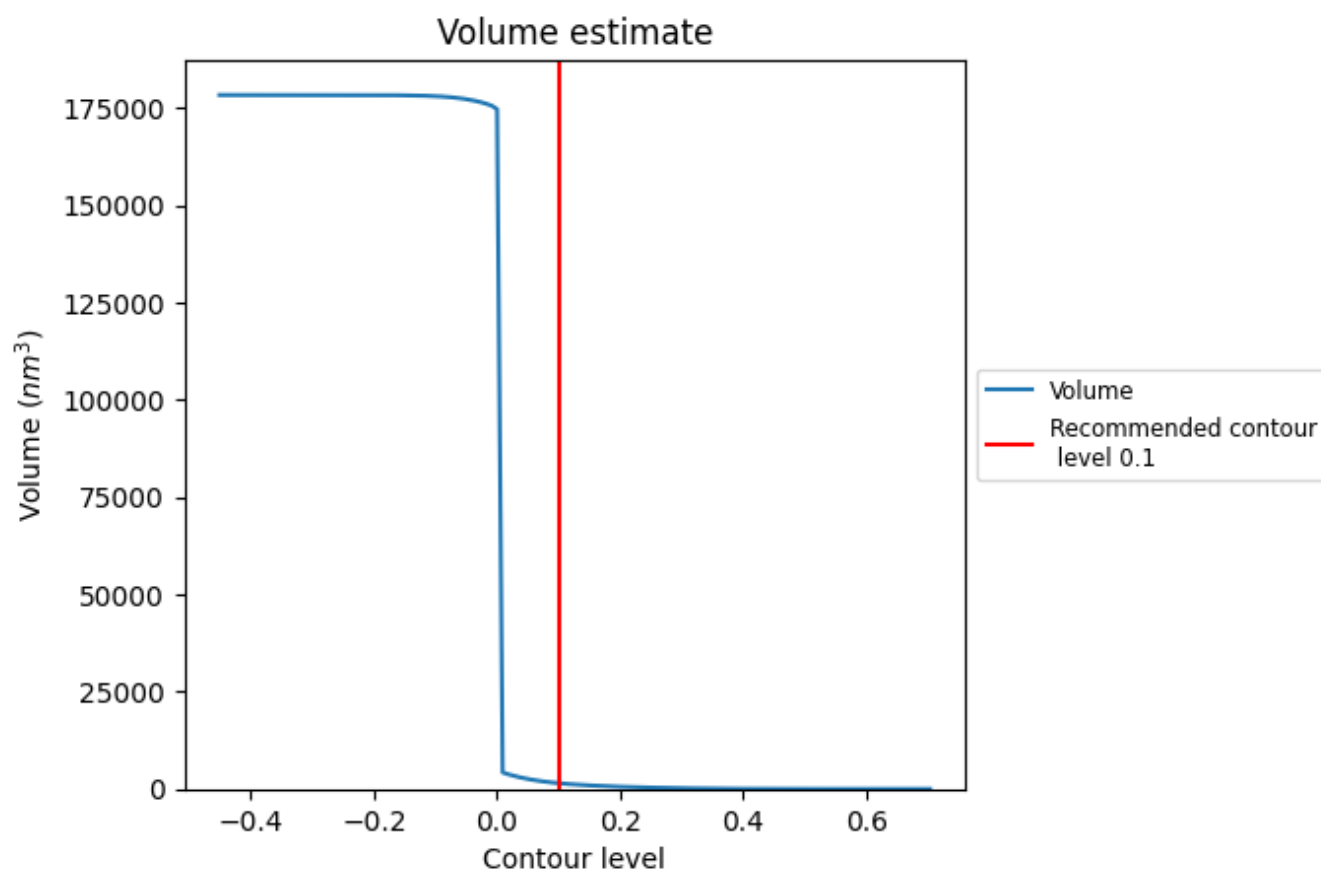
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

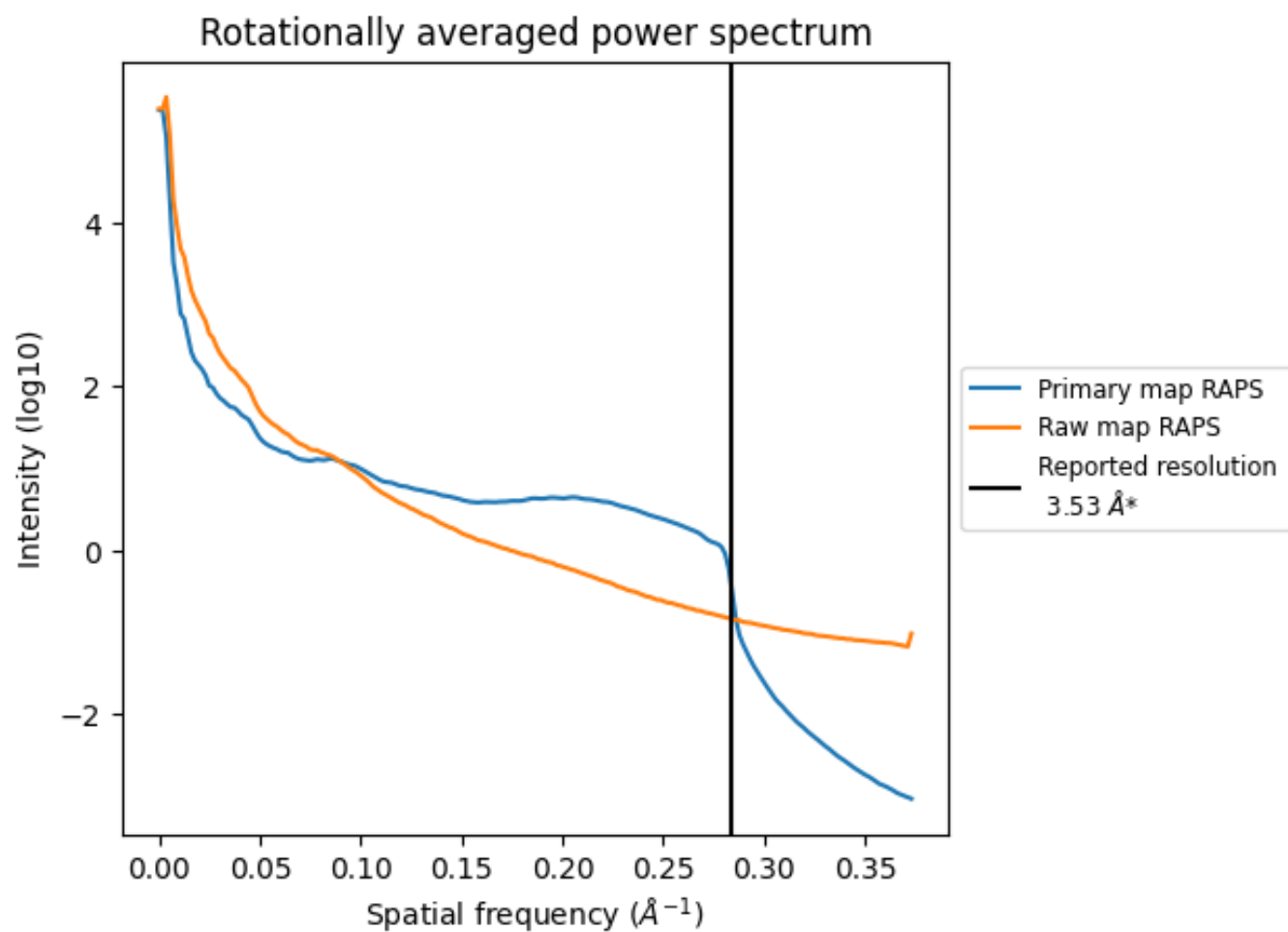
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1479 nm³; this corresponds to an approximate mass of 1336 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

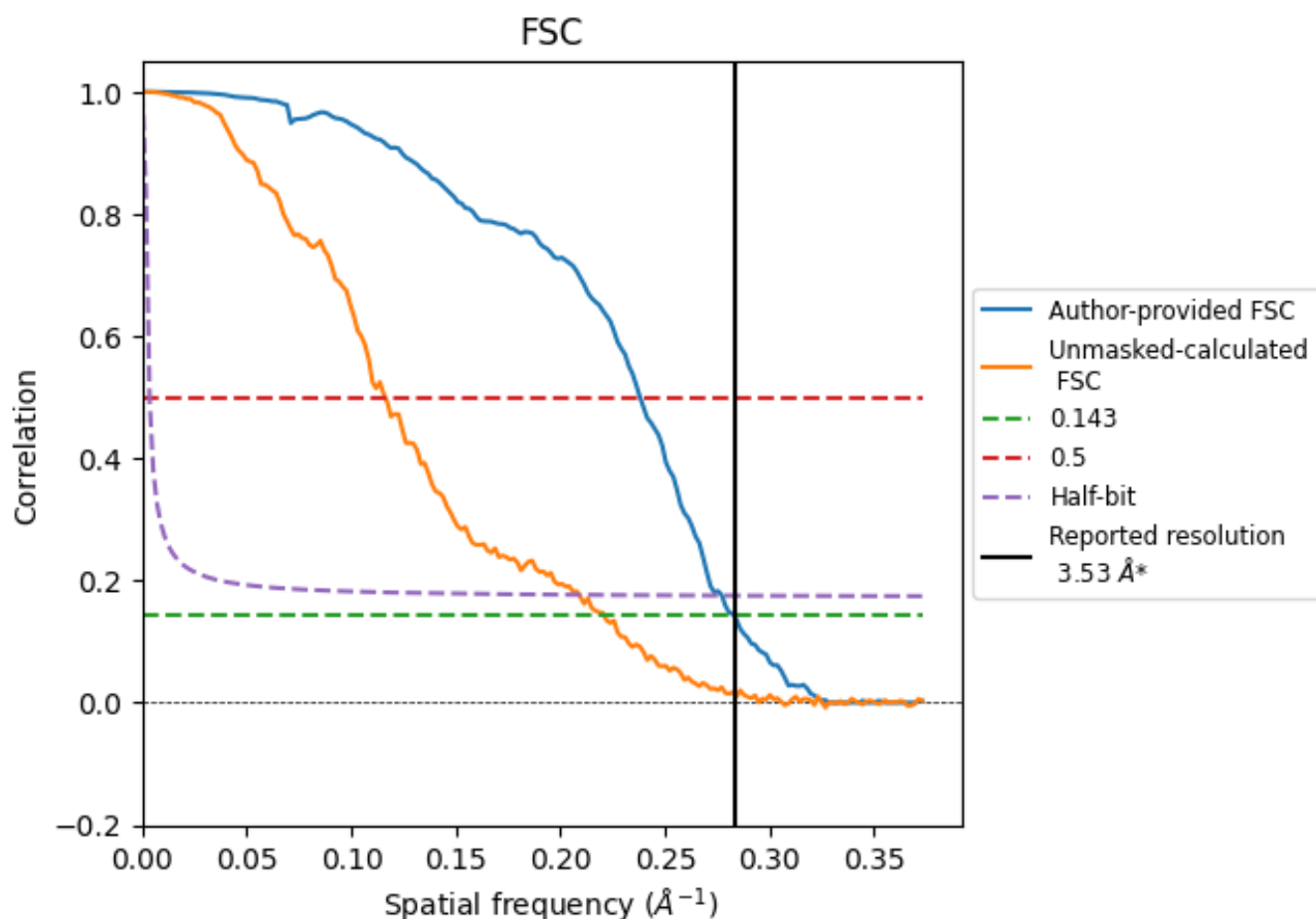


*Reported resolution corresponds to spatial frequency of 0.283 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.283 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

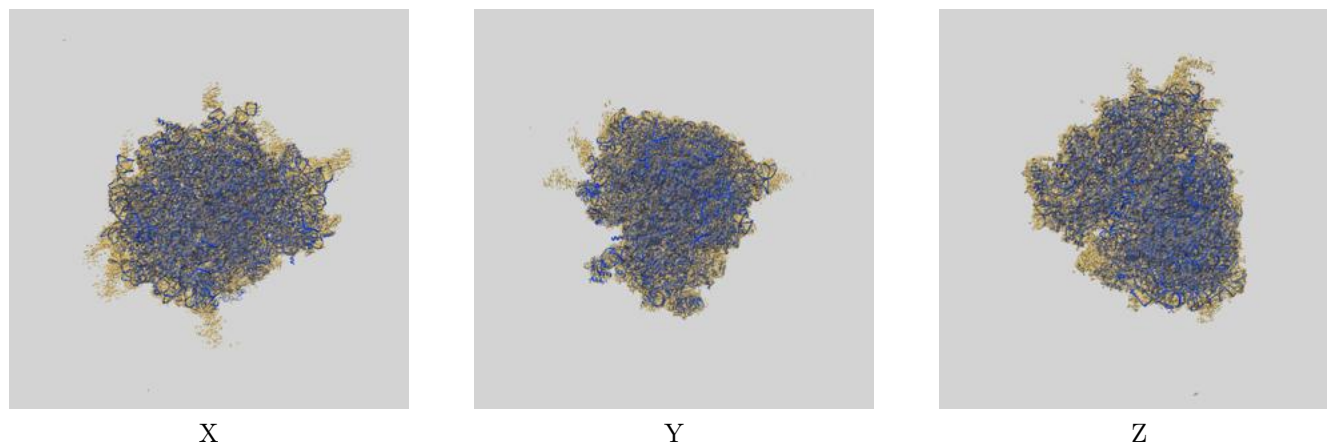
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.53	-	-
Author-provided FSC curve	3.53	4.20	3.61
Unmasked-calculated*	4.53	8.61	4.79

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.53 differs from the reported value 3.53 by more than 10 %

9 Map-model fit [i](#)

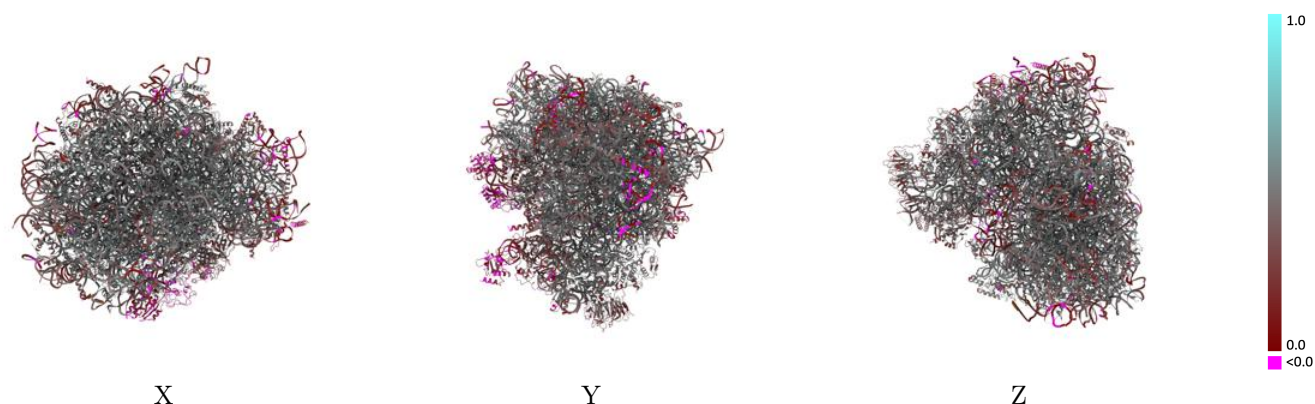
This section contains information regarding the fit between EMDB map EMD-4134 and PDB model 5LZW. Per-residue inclusion information can be found in section [3](#) on page [24](#).

9.1 Map-model overlay [i](#)



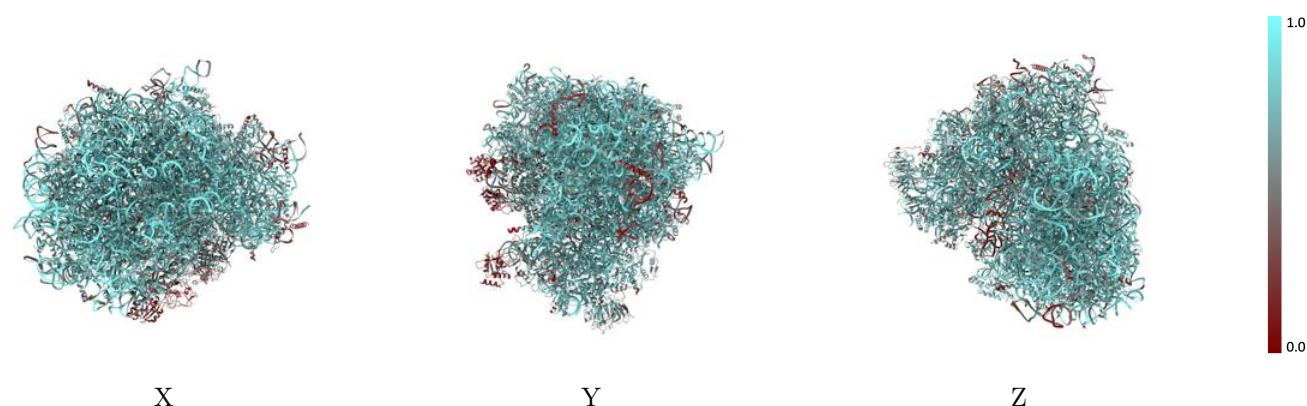
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



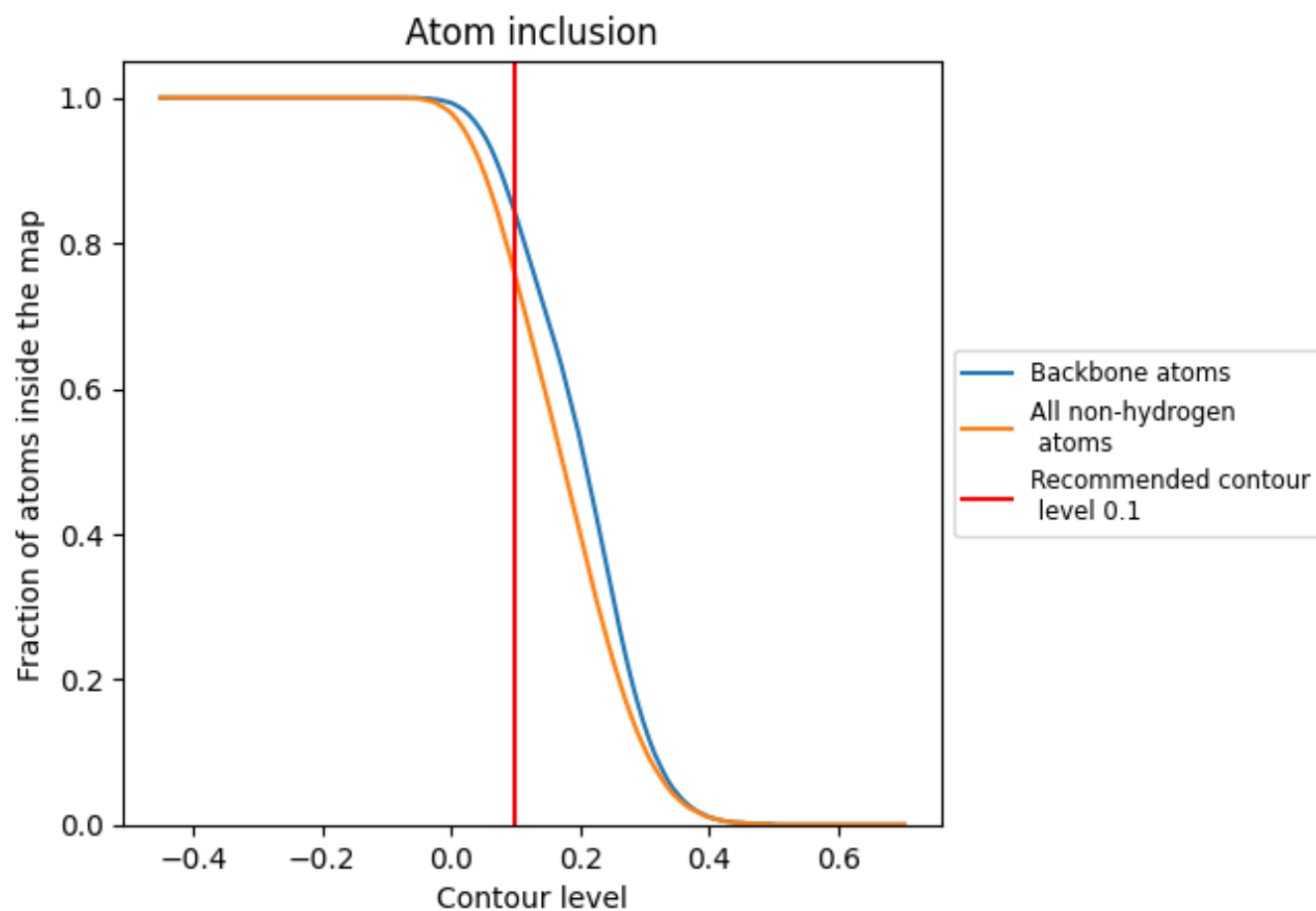
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7530	 0.4220
1	 0.2070	 0.3400
2	 0.5580	 0.3580
3	 0.2080	 0.1650
5	 0.8370	 0.4320
7	 0.9070	 0.4740
8	 0.8460	 0.4320
9	 0.8140	 0.4080
A	 0.7570	 0.4930
AA	 0.7200	 0.4500
B	 0.7540	 0.4910
BB	 0.7030	 0.4540
C	 0.7530	 0.4830
CC	 0.7220	 0.4740
D	 0.7550	 0.4540
DD	 0.6240	 0.3920
E	 0.7610	 0.4670
EE	 0.6990	 0.4370
F	 0.7670	 0.4890
FF	 0.6700	 0.4260
G	 0.6370	 0.3990
GG	 0.6110	 0.3420
H	 0.7130	 0.4660
HH	 0.6110	 0.3890
I	 0.7500	 0.4900
II	 0.6880	 0.4330
J	 0.6930	 0.4320
JJ	 0.6890	 0.4280
KK	 0.5870	 0.3100
L	 0.7000	 0.4430
LL	 0.6970	 0.4600
M	 0.7720	 0.4730
MM	 0.2370	 0.0820
N	 0.7730	 0.4950
NN	 0.7250	 0.4650



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Chain	Atom inclusion	Q-score
O	 0.7680	 0.4870
OO	 0.7040	 0.4540
P	 0.7620	 0.4920
PP	 0.5310	 0.2700
Q	 0.7570	 0.4850
QQ	 0.6960	 0.4240
R	 0.6930	 0.4440
RR	 0.6370	 0.4140
S	 0.7720	 0.4950
SS	 0.6090	 0.3300
T	 0.7240	 0.4660
TT	 0.6950	 0.3830
U	 0.6730	 0.4010
UU	 0.6550	 0.4060
V	 0.7410	 0.4980
VV	 0.7110	 0.4550
W	 0.5760	 0.3400
WW	 0.7500	 0.4910
X	 0.7090	 0.4530
XX	 0.7020	 0.4730
Y	 0.7400	 0.4600
YY	 0.7140	 0.4130
Z	 0.7600	 0.4540
ZZ	 0.5780	 0.3210
a	 0.7710	 0.4950
aa	 0.7300	 0.4730
b	 0.6660	 0.3820
bb	 0.6760	 0.4240
c	 0.7230	 0.4430
cc	 0.6430	 0.4160
d	 0.7320	 0.4750
dd	 0.7560	 0.4520
e	 0.7590	 0.4890
ee	 0.6430	 0.4030
f	 0.7870	 0.5090
ff	 0.2680	 0.1100
g	 0.7270	 0.4690
gg	 0.5890	 0.3540
h	 0.6940	 0.4400
hh	 0.0710	 0.0650
i	 0.7010	 0.4260
ii	 0.4890	 0.3670

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Chain	Atom inclusion	Q-score
j	 0.7800	 0.4900
jj	 0.5240	 0.3550
k	 0.6390	 0.3900
l	 0.7190	 0.4620
m	 0.7360	 0.4750
n	 0.5600	 0.4330
o	 0.7130	 0.4720
p	 0.7230	 0.4760
r	 0.7760	 0.4940
s	 0.1640	 0.0900
t	 0.1060	 0.0190