



Full wwPDB EM Validation Report ⓘ

Oct 22, 2024 – 08:14 PM EDT

PDB ID : 3JAH
EMDB ID : EMD-3039
Title : Structure of a mammalian ribosomal termination complex with ABCE1, eRF1(AAQ), and the UAG stop codon
Authors : Brown, A.; Shao, S.; Murray, J.; Hegde, R.S.; Ramakrishnan, V.
Deposited on : 2015-06-10
Resolution : 3.45 Å (reported)
Based on initial models : 1DT9, 3J92, 4V51, 3J7P, 3BK7

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

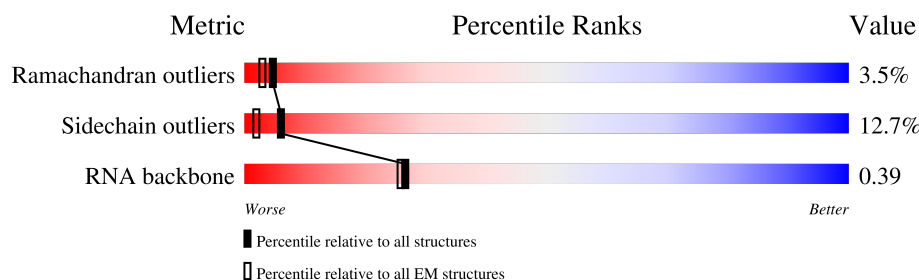
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.45 Å.

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







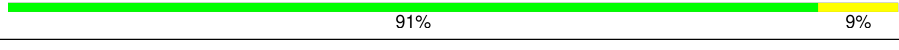

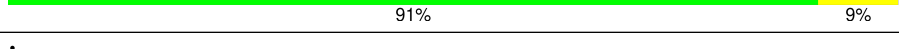
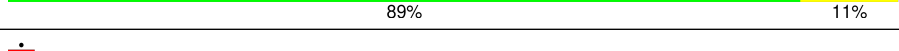
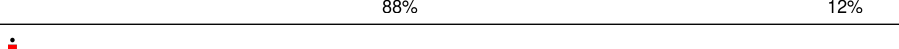
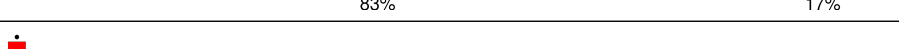
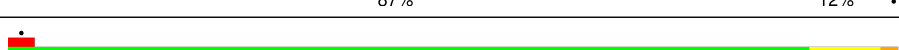

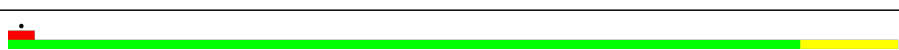

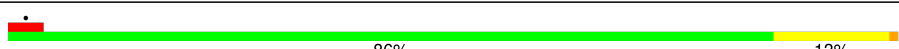


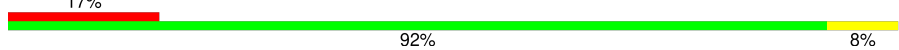


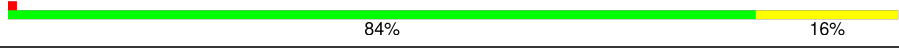
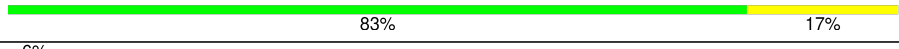



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	244	
2	B	394	
3	C	362	
4	D	292	
5	E	248	
6	F	225	
7	G	241	
8	H	190	



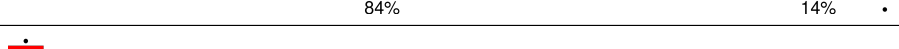
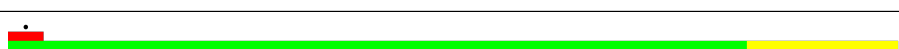


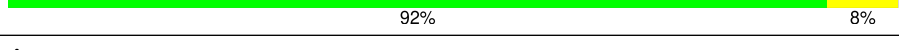






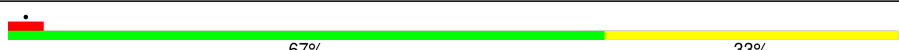


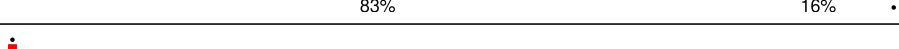







Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	213	
10	J	169	
11	L	210	
12	M	138	
13	N	203	
14	O	199	
15	P	153	
16	Q	187	
17	R	180	
18	S	175	
19	T	159	
20	U	99	
21	V	131	
22	W	63	
23	X	119	
24	Y	134	
25	Z	135	
26	a	147	
27	b	75	
28	c	94	
29	d	107	
30	e	128	
31	f	109	
32	g	114	
33	h	122	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	i	102	
35	j	86	
36	k	69	
37	l	50	
38	m	52	
39	n	23	
40	o	104	
41	p	91	
42	r	125	
43	s	198	
44	t	163	
45	1	15	
46	2	76	
47	3	75	
48	5	3662	
49	7	120	
50	8	156	
51	9	1719	
52	AA	208	
53	BB	213	
54	CC	218	
55	DD	227	
56	EE	262	
57	FF	191	
58	GG	237	

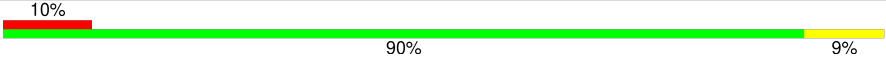
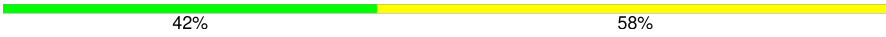

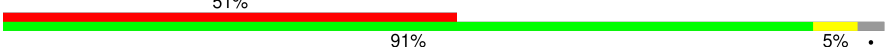
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
59	HH	189	
60	II	206	
61	JJ	185	
62	KK	98	
63	LL	152	
64	MM	124	
65	NN	150	
66	OO	136	
67	PP	127	
68	QQ	141	
69	RR	129	
70	SS	137	
71	TT	141	
72	UU	104	
73	VV	83	
74	WW	129	
75	XX	141	
76	YY	126	
77	ZZ	75	
78	aa	98	
79	bb	83	
80	cc	61	
81	dd	53	
82	ee	57	
83	ff	68	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
84	gg	313	
85	hh	12	
86	ii	416	
87	jj	594	

2 Entry composition [i](#)

There are 91 unique types of molecules in this entry. The entry contains 226454 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	244	Total	C	N	O	S	0	0
			1868	1171	382	309	6		

- Molecule 2 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	394	Total	C	N	O	S	0	0
			3148	2007	591	537	13		

- Molecule 3 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	362	Total	C	N	O	S	0	0
			2884	1814	578	478	14		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	361	LYS	-	expression tag	UNP G1SVW5
C	362	LYS	-	expression tag	UNP G1SVW5
C	363	SER	-	expression tag	UNP G1SVW5

- Molecule 4 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	292	Total	C	N	O	S	0	0
			2386	1509	437	426	14		

- Molecule 5 is a protein called eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	236	Total	C	N	O	S	0	0
			1898	1215	362	318	3		

- Molecule 6 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 7 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	241	Total	C	N	O	S	0	0
			1934	1233	371	326	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	191	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	204	Total	C	N	O	S	0	0
			1655	1051	319	272	13		

- Molecule 10 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	169	Total	C	N	O	S	0	0
			1353	855	252	240	6		

- Molecule 11 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	210	Total	C	N	O	S	0	0
			1703	1065	354	280	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
			1638	1056	321	256	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	776	241	216	9		

- Molecule 16 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	187	Total	C	N	O	S	0	0
			1506	941	311	249	5		

- 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	175	Total	C	N	O	S	0	0
			1454	925	284	235	10		

- 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
			808	518	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	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- Molecule 23 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	119	Total	C	N	O	S	0	0
			976	624	183	168	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		

- Molecule 27 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	75	Total	C	N	O	S	0	0
			609	378	130	98	3		

- Molecule 28 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	94	Total	C	N	O	S	0	0
			732	465	130	131	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
			444	281	98	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	23	Total	C	N	O	S	0	0
			222	134	61	25	2		

- 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	125	Total	C	N	O	S	0	0
			1001	621	206	168	6		

- Molecule 43 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	198	Total	C	N	O	S	0	0
			1523	969	265	280	9		

- Molecule 44 is a protein called uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	163	Total	C	N	O	S	0	0
			1238	773	230	230	5		

- Molecule 45 is a protein called peptide.

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 tRNA(Val).

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 tRNA(Lys).

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	3662	Total	C	N	O	P	0	0
			78486	34947	14363	25515	3661		

- 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	156	Total	C	N	O	P	0	0
			3314	1480	585	1094	155		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	9	1719	Total	C	N	O	P	0	0
			36680	16371	6586	12005	1718		

- Molecule 52 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AA	208	Total	C	N	O	S	0	0
			1642	1045	289	300	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	218	Total	C	N	O	S	0	0
			1692	1102	287	296	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	194	ARG	HIS	conflict	UNP G1TUT9
CC	228	GLY	SER	conflict	UNP G1TUT9

- Molecule 55 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	DD	227	Total	C	N	O	S	0	0
			1764	1124	317	315	8		

- Molecule 56 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	EE	262	Total	C	N	O	S	0	0
			2073	1323	384	357	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EE	25	GLY	SER	conflict	UNP G1TK17

- Molecule 57 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	FF	191	Total	C	N	O	S	0	0
			1509	943	286	273	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	189	Total	C	N	O	S	0	0
			1521	969	280	271	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	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 63 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	LL	152	Total	C	N	O	S	0	0
			1238	788	232	212	6		

- Molecule 64 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	MM	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 65 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	NN	150	Total	C	N	O	S	0	0
			1208	773	229	205	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	127	Total	C	N	O	S	0	0
			1060	673	201	179	7		

- Molecule 68 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	QQ	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 69 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	RR	129	Total	C	N	O	S	0	0
			1047	658	193	191	5		

- Molecule 70 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SS	137	Total	C	N	O	S	0	0
			1139	714	231	193	1		

- Molecule 71 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	TT	141	Total	C	N	O	S	0	0
			1102	692	212	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	104	Total	C	N	O	S	0	0
			821	514	155	148	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	394	118	119	5		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
VV	3	ASN	SER	conflict	UNP G1TM82
VV	4	ASP	ASN	conflict	UNP G1TM82
VV	50	PHE	SER	conflict	UNP G1TM82
VV	75	ALA	SER	conflict	UNP G1TM82

- 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	126	Total	C	N	O	S	0	0
			1023	646	200	172	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	98	Total	C	N	O	S	0	0
			781	486	161	129	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	61	Total	C	N	O	S	0	0
			475	290	92	91	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
cc	18	ILE	LEU	conflict	UNP G1TIB4
cc	20	LYS	ARG	conflict	UNP G1TIB4
cc	40	HIS	ARG	conflict	UNP G1TIB4
cc	42	THR	ILE	conflict	UNP G1TIB4

- Molecule 81 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	dd	53	Total	C	N	O	S	0	0
			445	278	90	72	5		

- Molecule 82 is a protein called eS30.

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

- Molecule 83 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	ff	62	Total	C	N	O	S	0	0
			520	331	98	85	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ff	?	-	VAL	deletion	UNP G1SK22

- 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	hh	12	Total	C	N	O	P	0	0
			257	115	46	84	12		

- Molecule 86 is a protein called eRF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	ii	416	Total	C	N	O	S	0	0
			3280	2087	559	623	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ii	183	ALA	GLY	engineered mutation	UNP P62495
ii	184	ALA	GLY	engineered mutation	UNP P62495

- Molecule 87 is a protein called ABCE1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	jj	576	Total	C	N	O	S	0	0
			4543	2904	779	829	31		

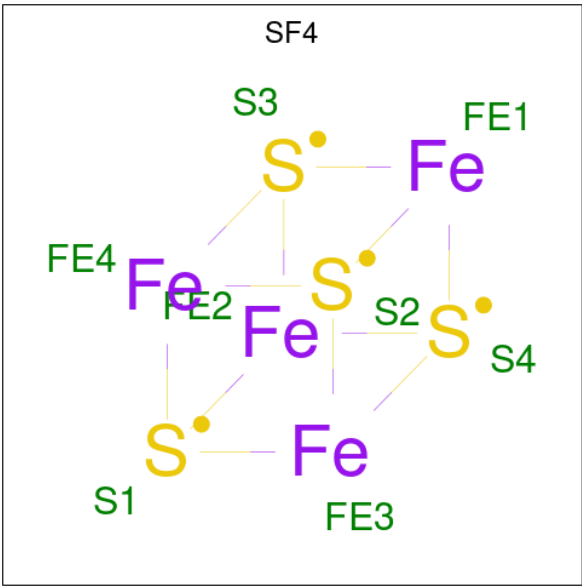
- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	B	1	Total 1	Mg 1	0
88	C	1	Total 1	Mg 1	0
88	I	1	Total 1	Mg 1	0
88	P	1	Total 1	Mg 1	0
88	V	1	Total 1	Mg 1	0
88	g	1	Total 1	Mg 1	0
88	5	146	Total 146	Mg 146	0
88	7	5	Total 5	Mg 5	0
88	8	2	Total 2	Mg 2	0
88	9	34	Total 34	Mg 34	0
88	LL	1	Total 1	Mg 1	0
88	hh	1	Total 1	Mg 1	0

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

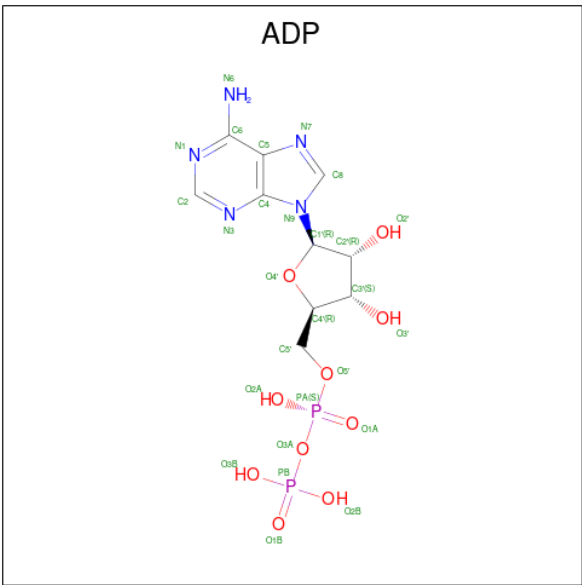
Mol	Chain	Residues	Atoms		AltConf
89	g	1	Total 1	Zn 1	0
89	j	1	Total 1	Zn 1	0
89	m	1	Total 1	Zn 1	0
89	o	1	Total 1	Zn 1	0
89	p	1	Total 1	Zn 1	0
89	aa	1	Total 1	Zn 1	0
89	dd	1	Total 1	Zn 1	0
89	ff	1	Total 1	Zn 1	0

- Molecule 90 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
90	jj	1	Total	Fe	S	0
			8	4	4	
90	jj	1	Total	Fe	S	0
			8	4	4	

- Molecule 91 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

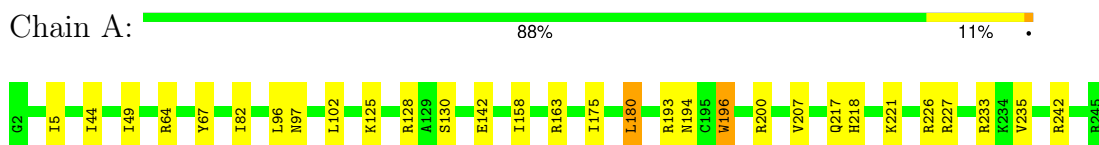


Mol	Chain	Residues	Atoms					AltConf
91	jj	1	Total	C	N	O	P	0
			27	10	5	10	2	
91	jj	1	Total	C	N	O	P	0
			27	10	5	10	2	

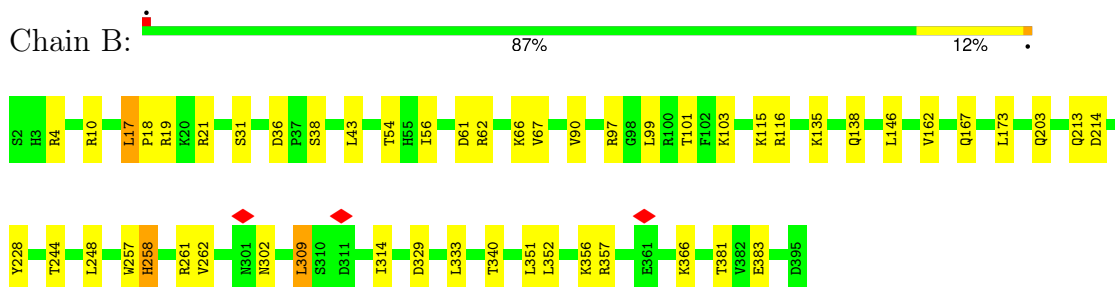
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

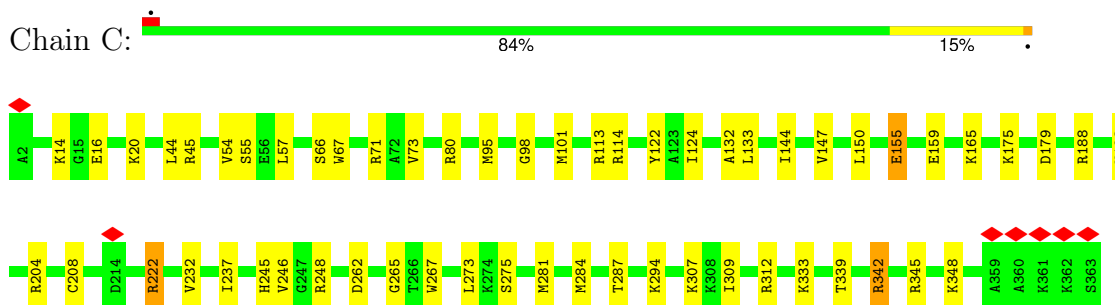
• Molecule 1: uL2



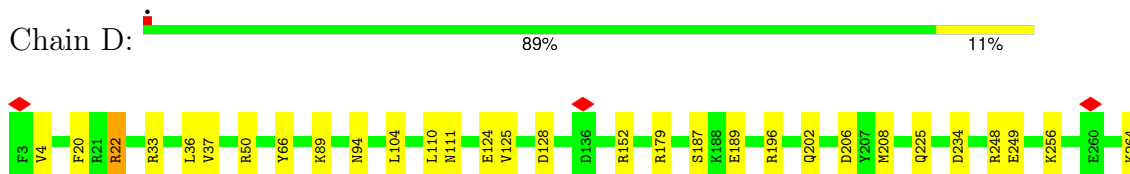
• Molecule 2: uL3



• Molecule 3: uL4

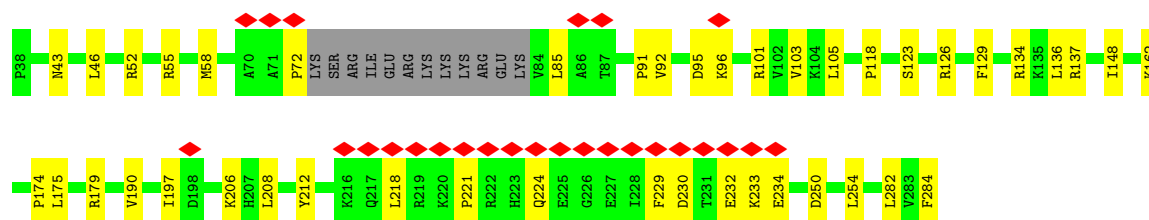
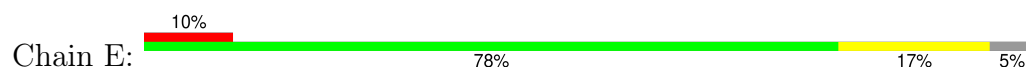


• Molecule 4: uL18

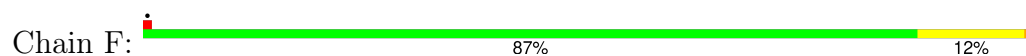




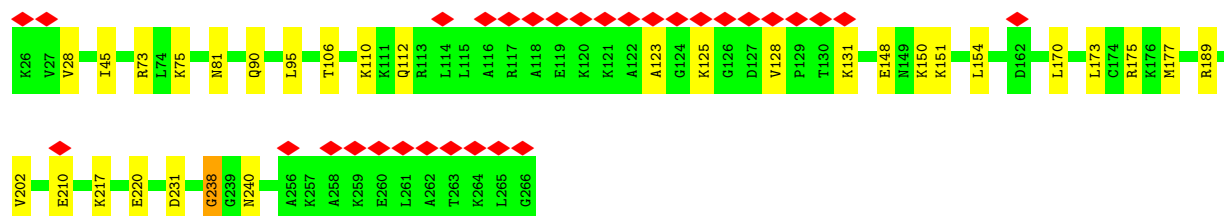
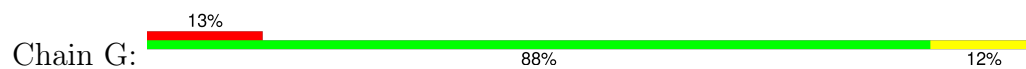
• Molecule 5: eL6



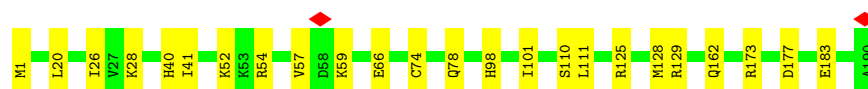
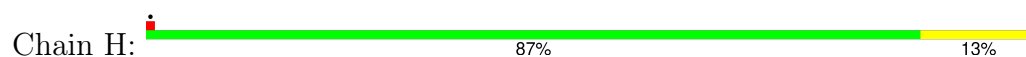
• Molecule 6: uL30



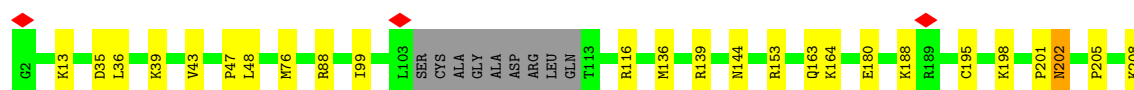
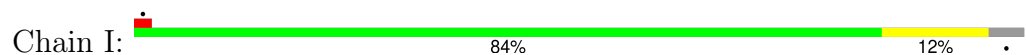
• Molecule 7: eL8



• Molecule 8: uL6

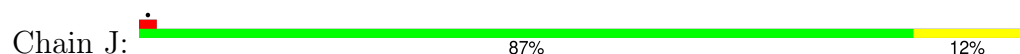


• Molecule 9: uL16

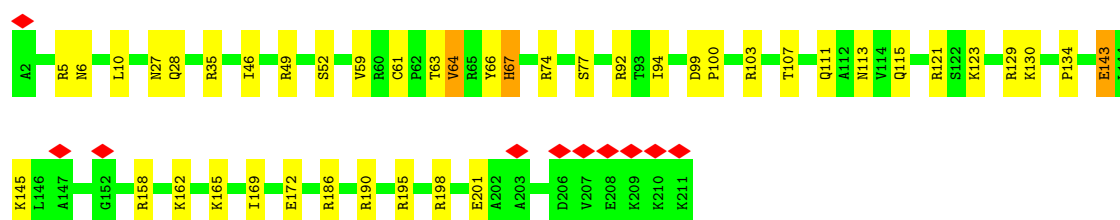
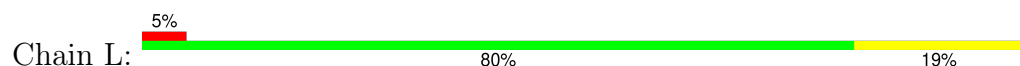




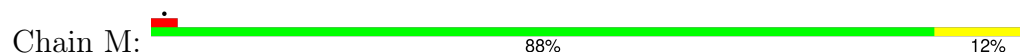
- Molecule 10: uL5



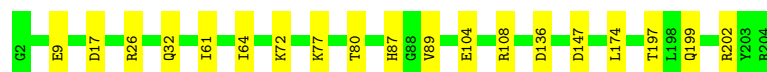
- Molecule 11: eL13



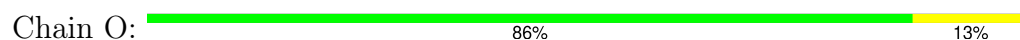
- Molecule 12: eL14



- Molecule 13: eL15




- Molecule 14: uL13




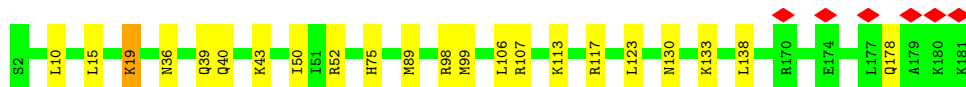
- Molecule 15: uL22




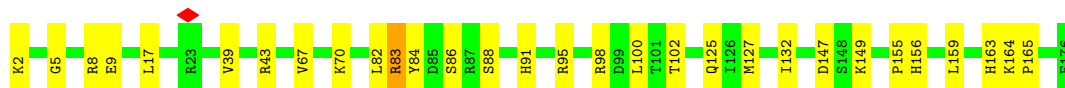
• Molecule 16: uL14

Chain Q:  89% 11%


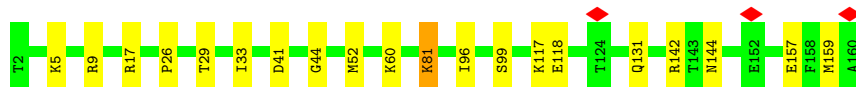
• Molecule 17: eL19

Chain R:  88% 12%


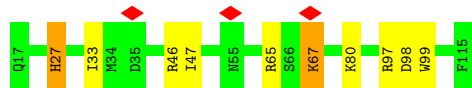
• Molecule 18: eL20

Chain S:  83% 17%


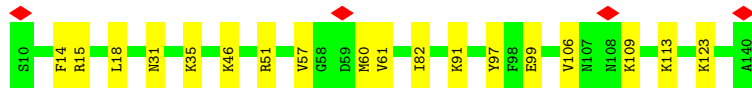
• Molecule 19: eL21

Chain T:  87% 12%


• Molecule 20: eL22

Chain U:  90% 8%

• Molecule 21: uL14

Chain V:  86% 14%

• Molecule 22: eL24

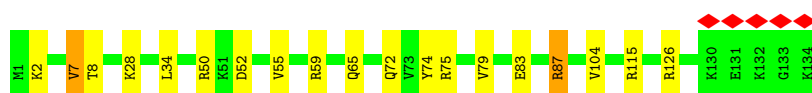
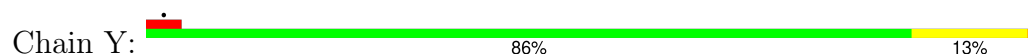
Chain W:  89% 11%



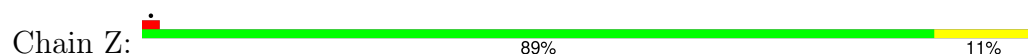
• Molecule 23: uL23



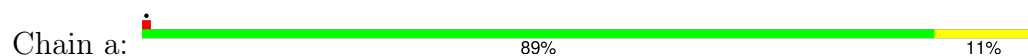
• Molecule 24: uL24



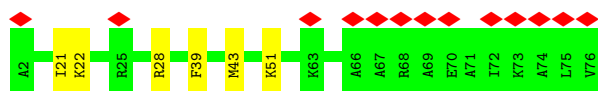
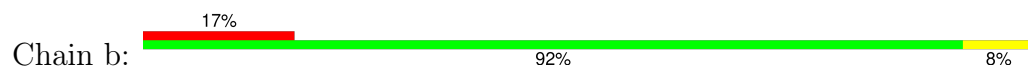
• Molecule 25: eL27



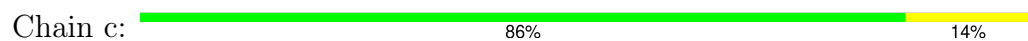
• Molecule 26: uL15



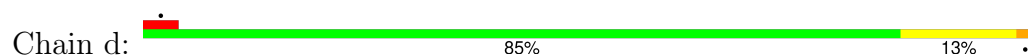
• Molecule 27: eL29

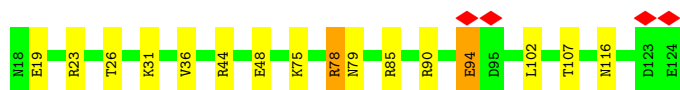


• Molecule 28: eL30

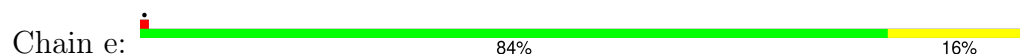


• Molecule 29: eL31

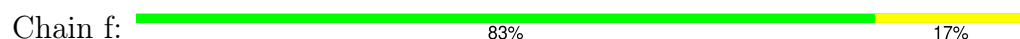




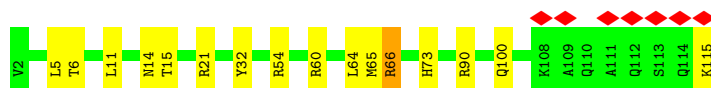
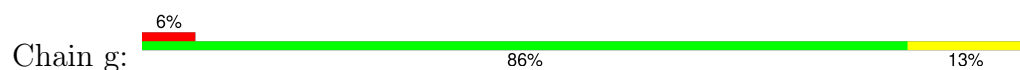
• Molecule 30: eL32



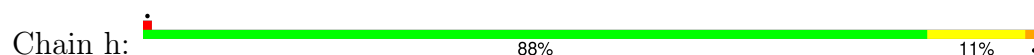
• Molecule 31: eL33



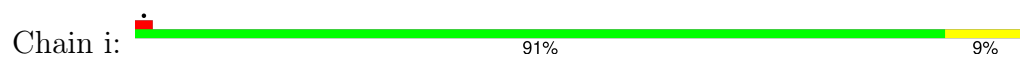
• Molecule 32: eL34



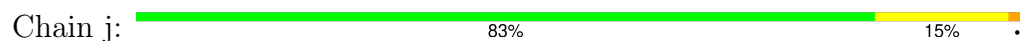
• Molecule 33: uL29



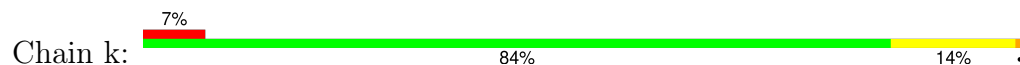
• Molecule 34: eL36

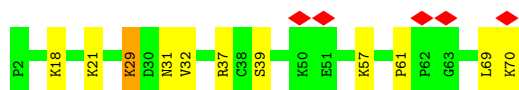


• Molecule 35: eL37

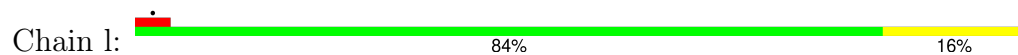


• Molecule 36: eL38

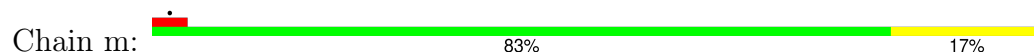




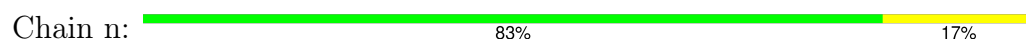
• Molecule 37: eL39



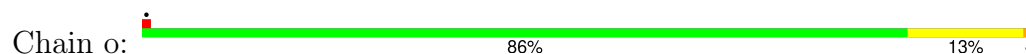
• Molecule 38: eL40



• Molecule 39: eL41



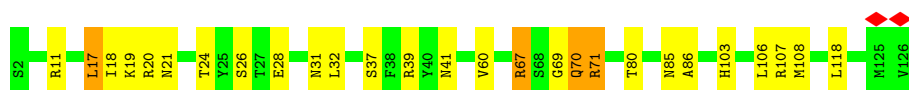
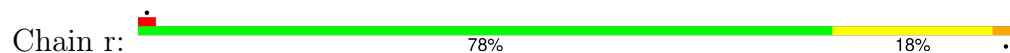
• Molecule 40: eL42



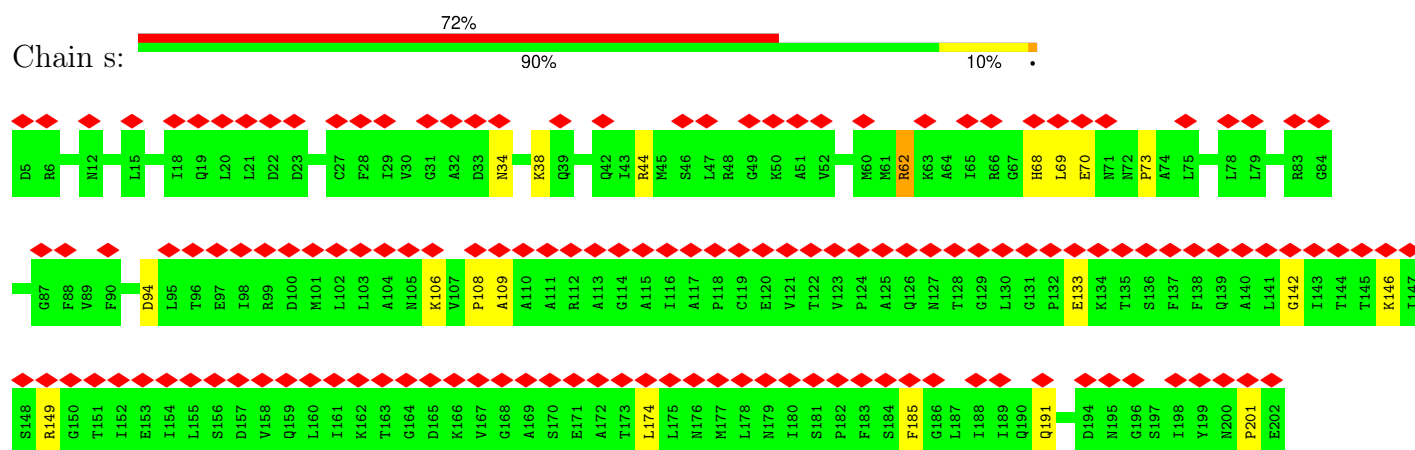
• Molecule 41: eL43



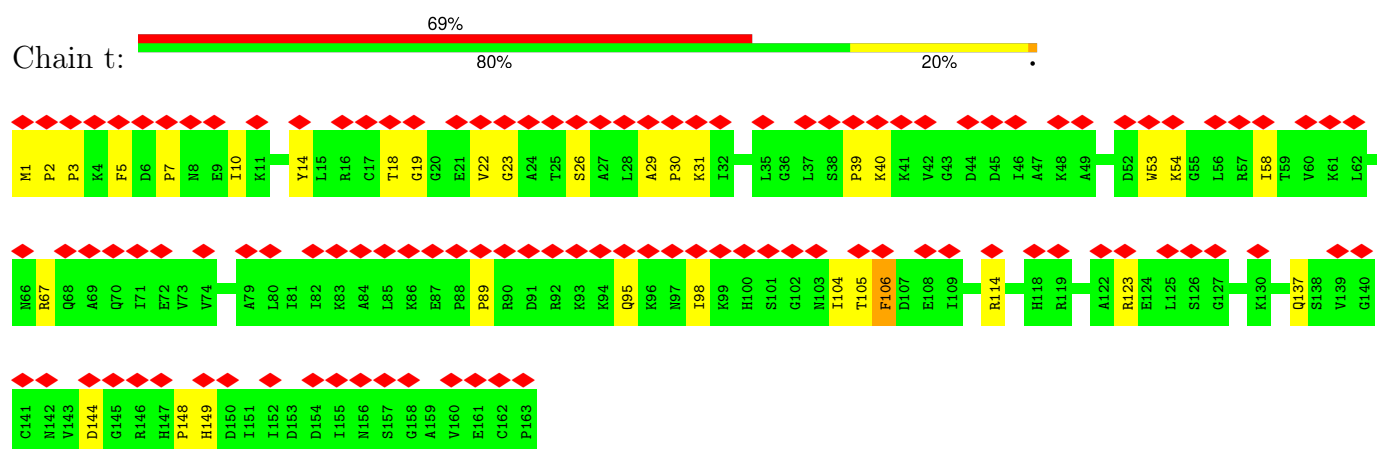
• Molecule 42: eL28



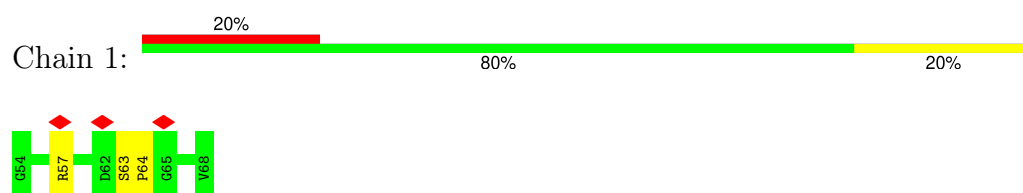
• Molecule 43: uL10



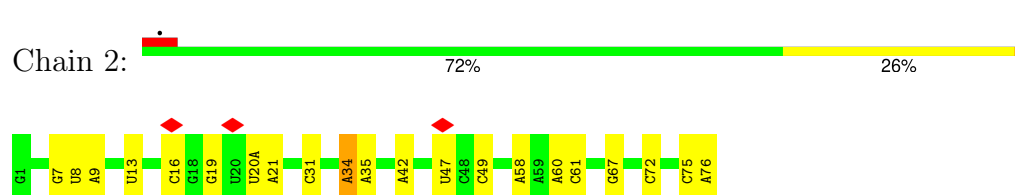
• Molecule 44: uL11



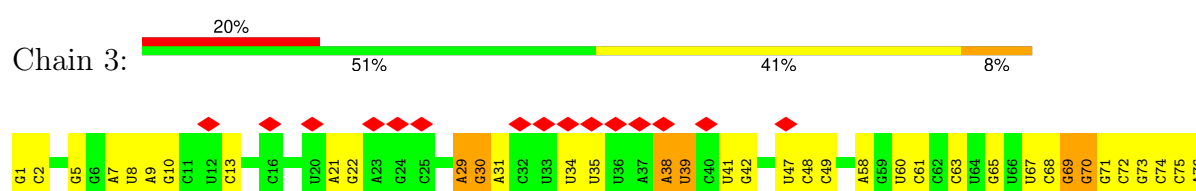
• Molecule 45: peptide



• Molecule 46: tRNA(Val)

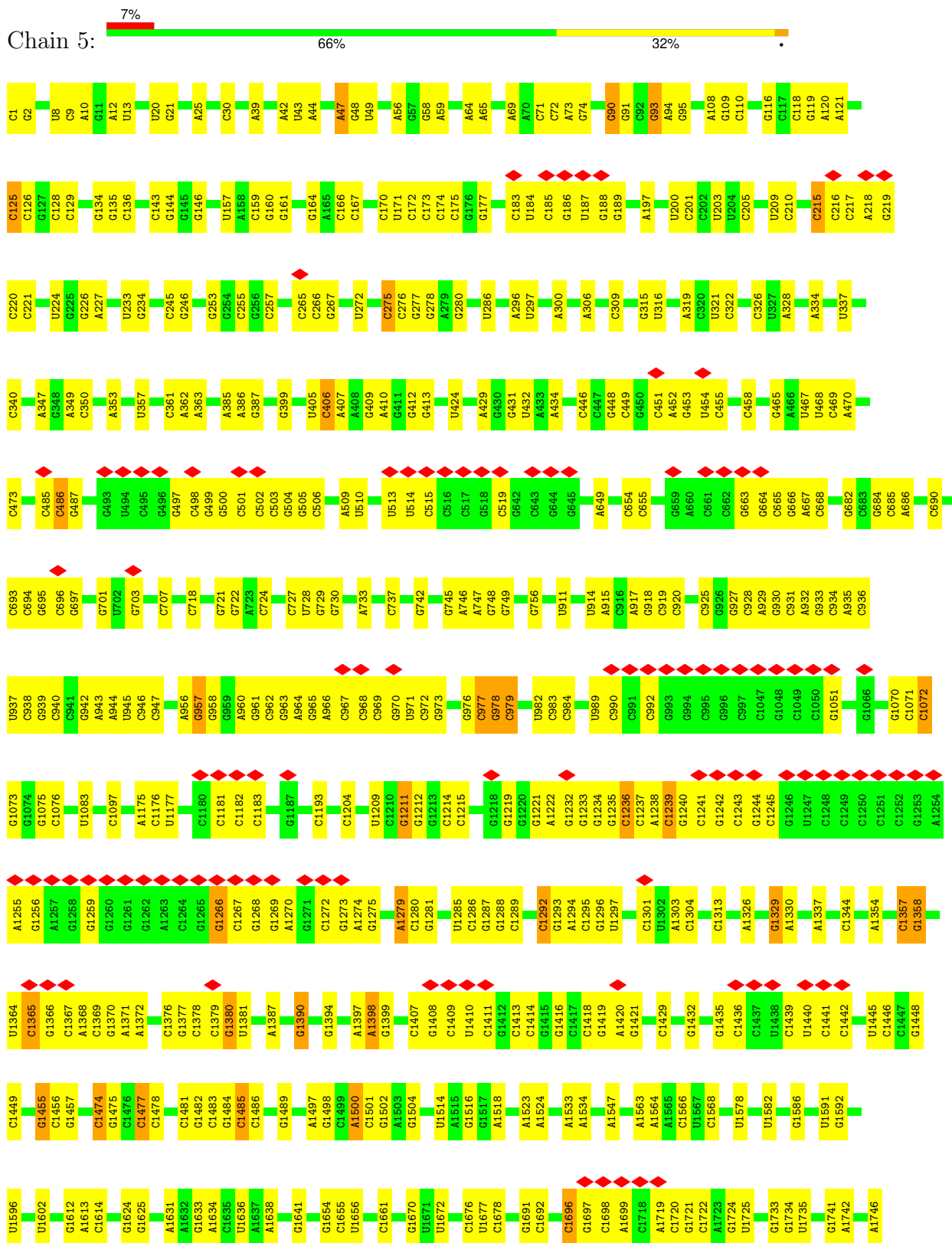


• Molecule 47: tRNA(Lys)

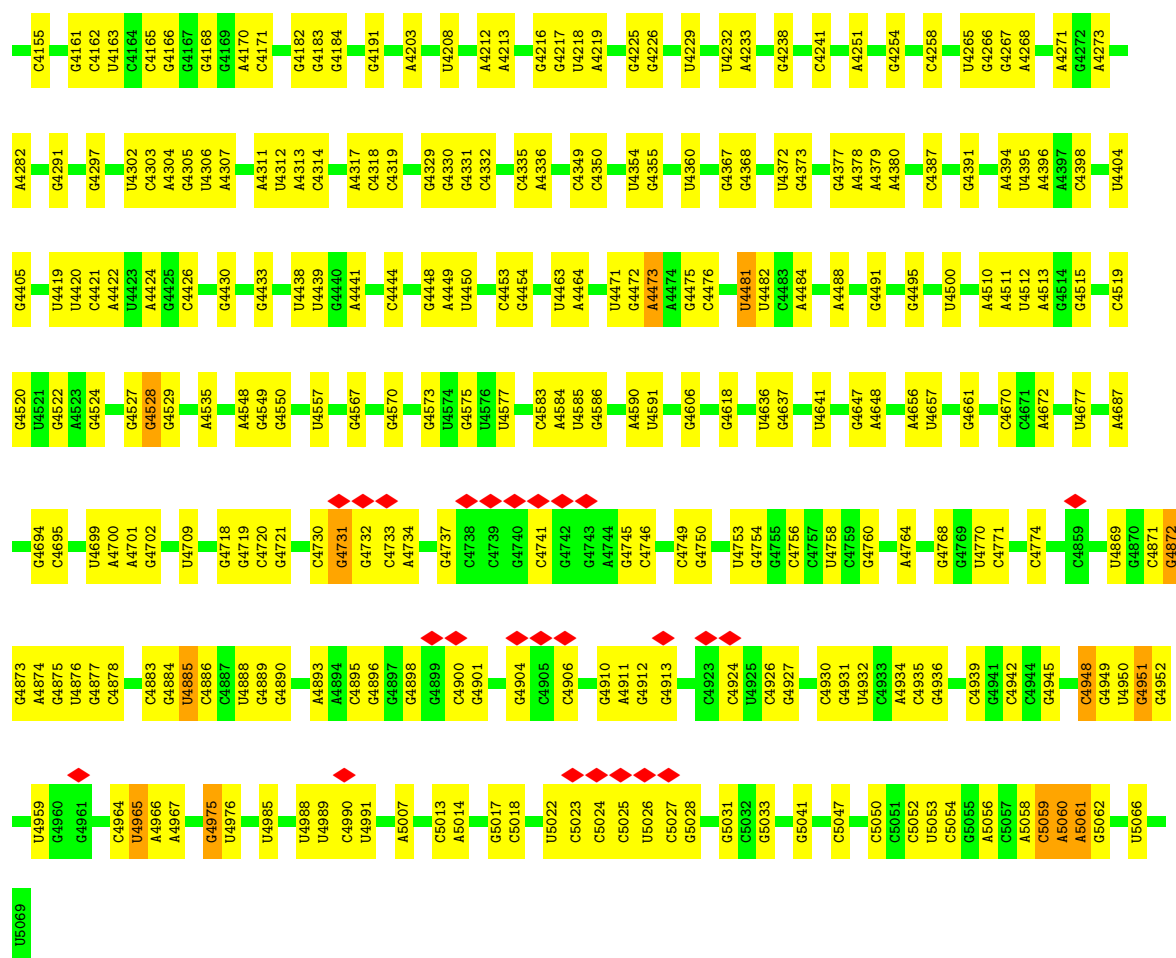


• Molecule 48: 28S ribosomal RNA

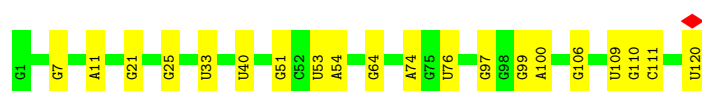
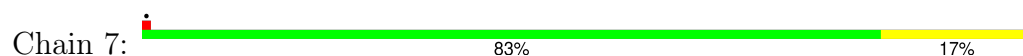
Chain 5:



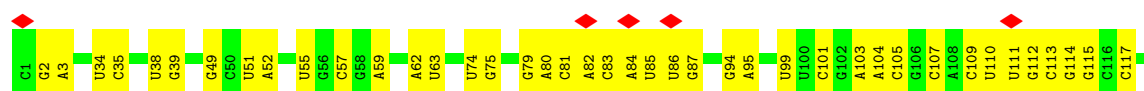




• Molecule 49: 5S ribosomal RNA

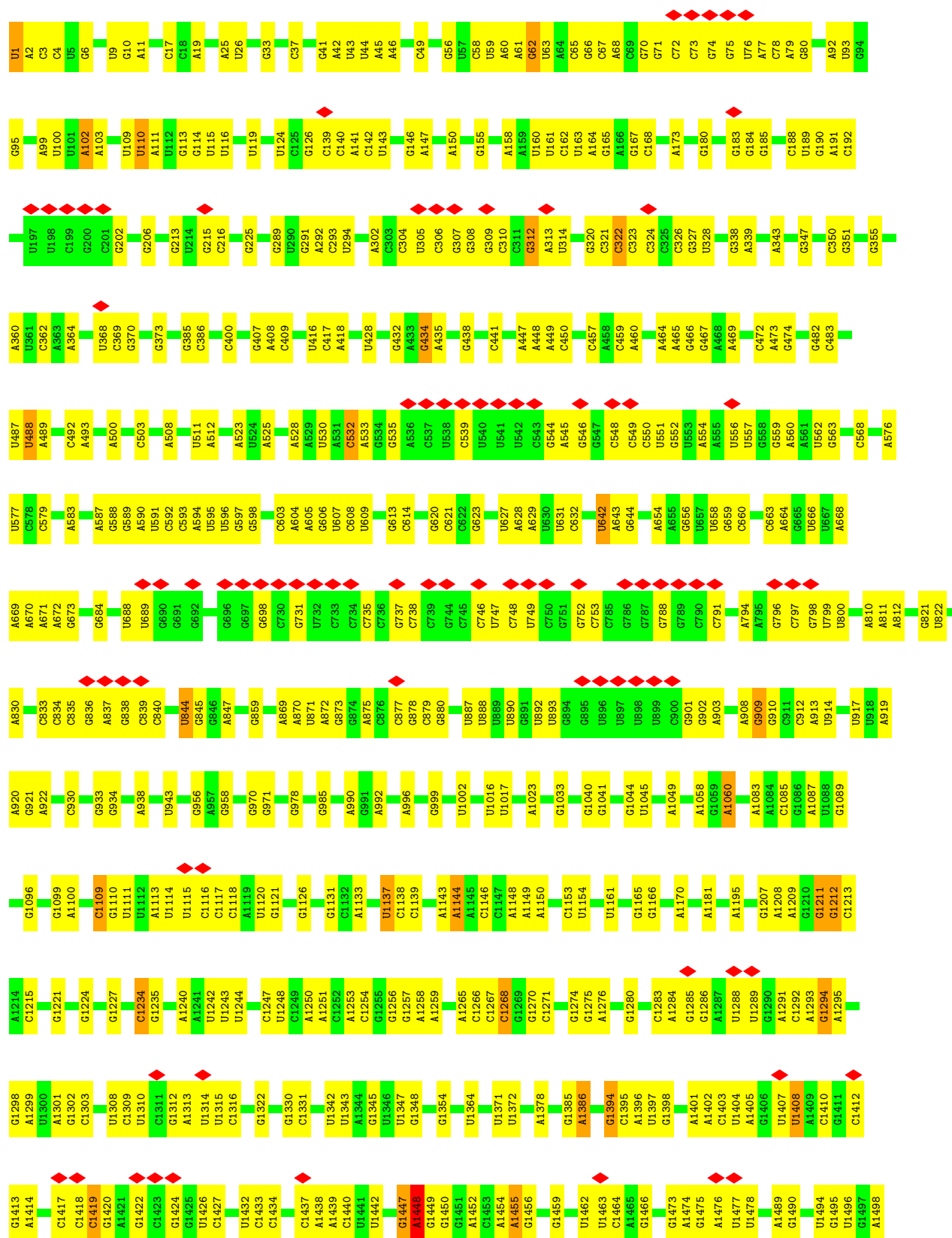


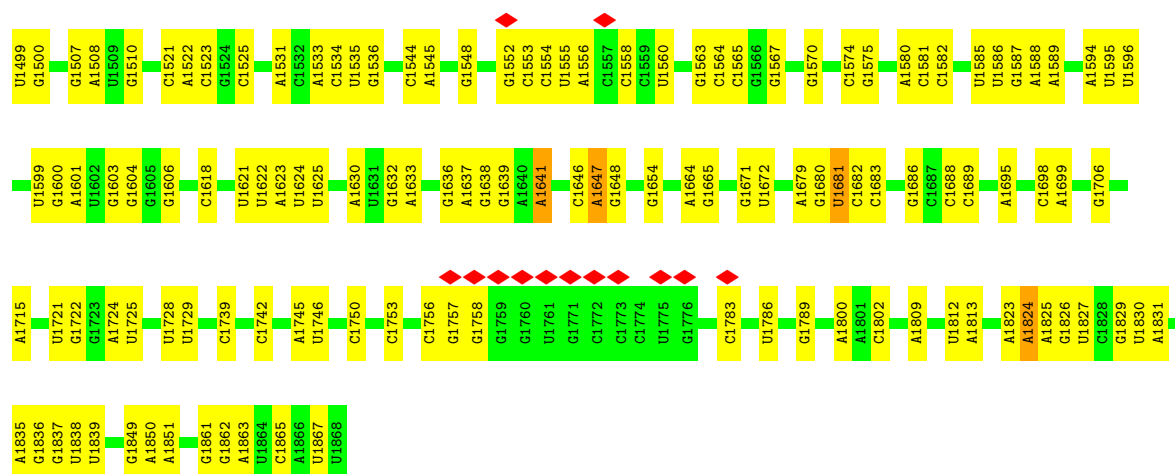
• Molecule 50: 5.8S ribosomal RNA



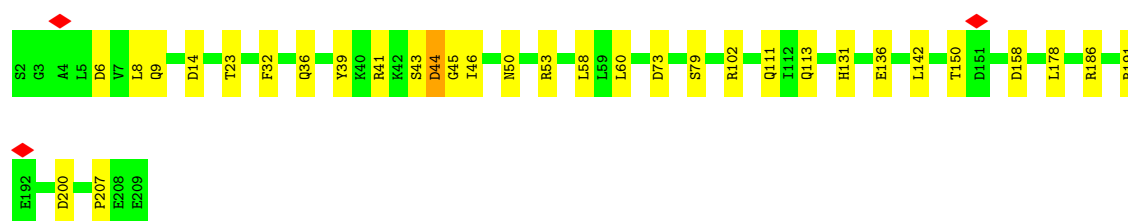
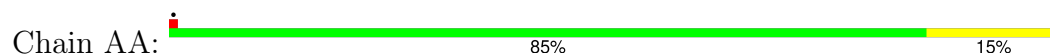
• Molecule 51: 18S ribosomal RNA



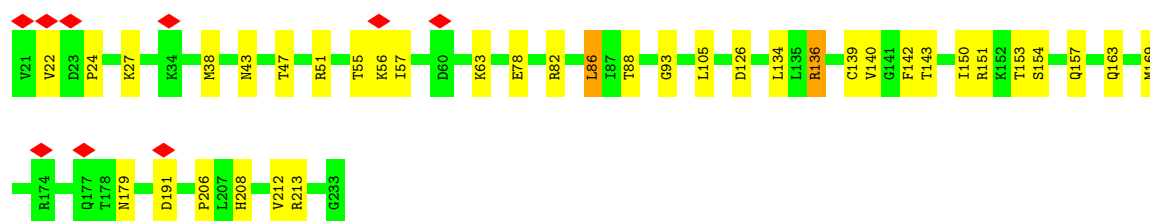
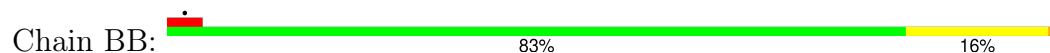




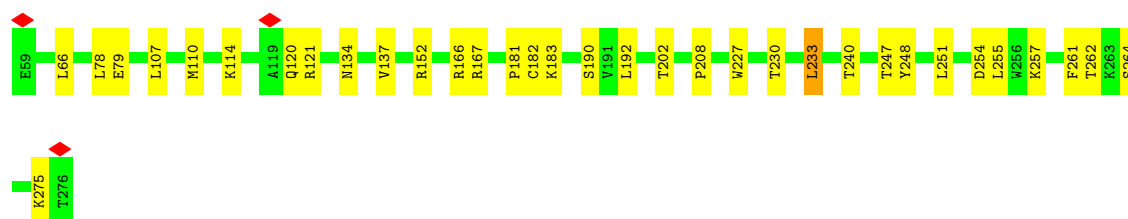
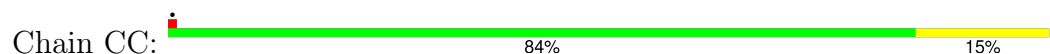
• Molecule 52: uS2



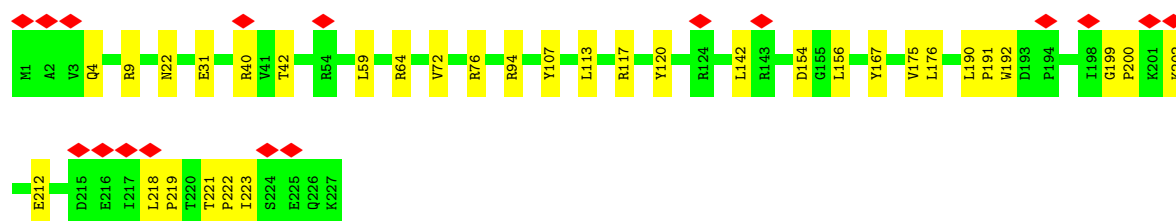
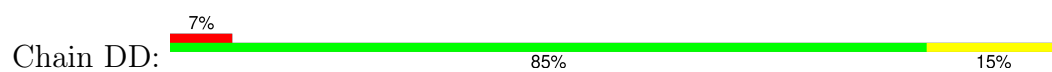
• Molecule 53: eS1



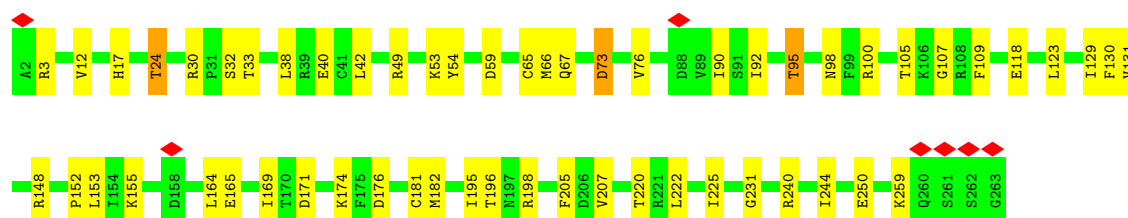
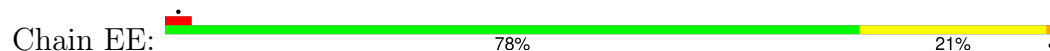
• Molecule 54: uS5



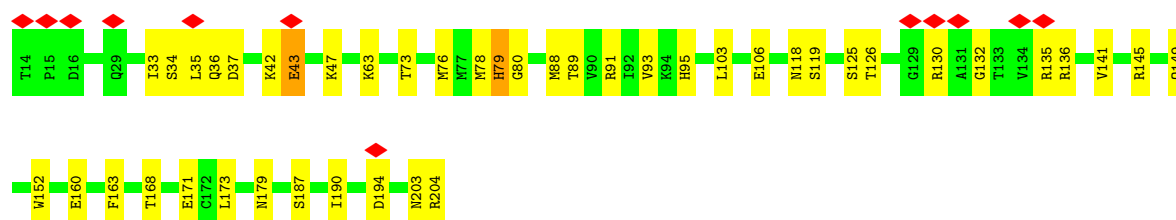
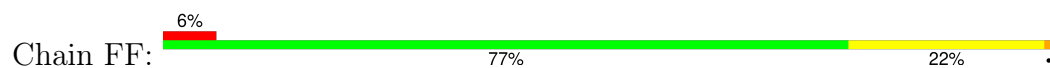
• Molecule 55: uS3



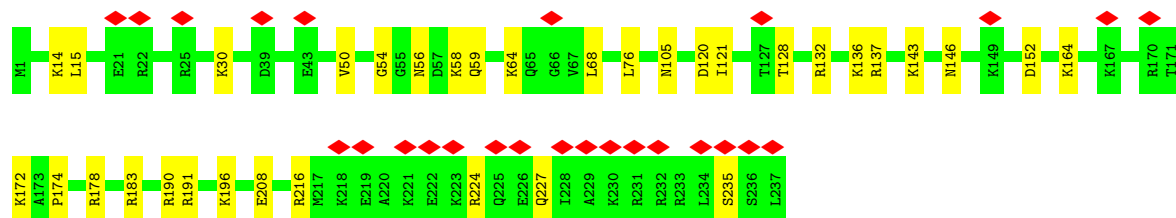
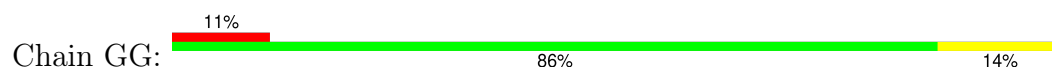
• Molecule 56: eS4



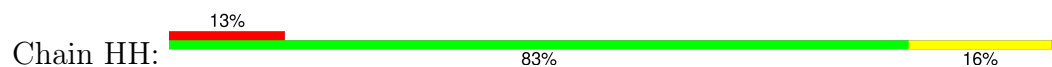
• Molecule 57: uS7

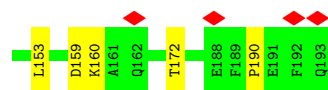


• Molecule 58: eS6

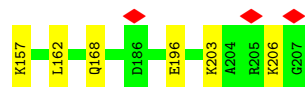
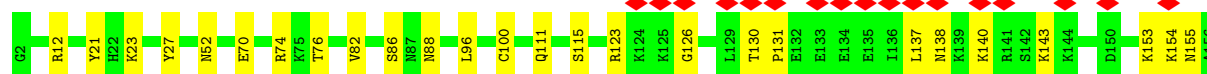
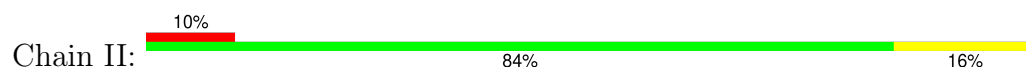


• Molecule 59: eS7

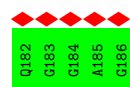
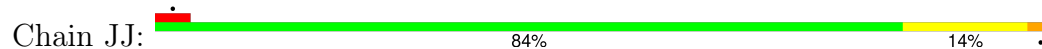




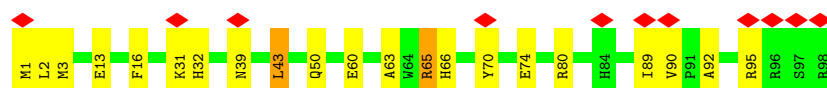
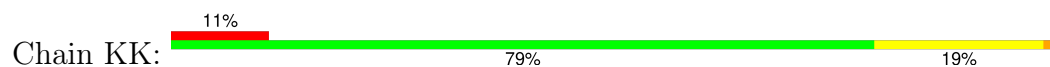
- Molecule 60: eS8



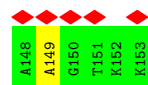
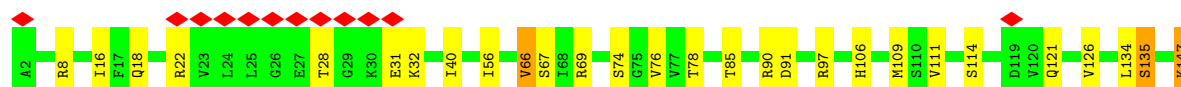
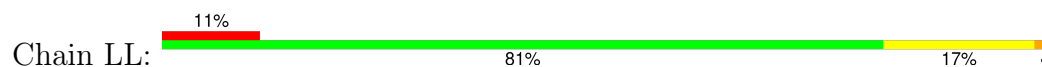
- Molecule 61: uS4



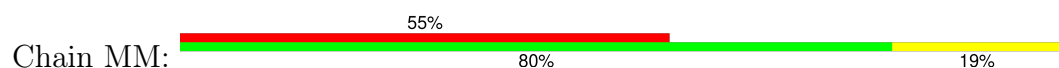
- Molecule 62: eS10

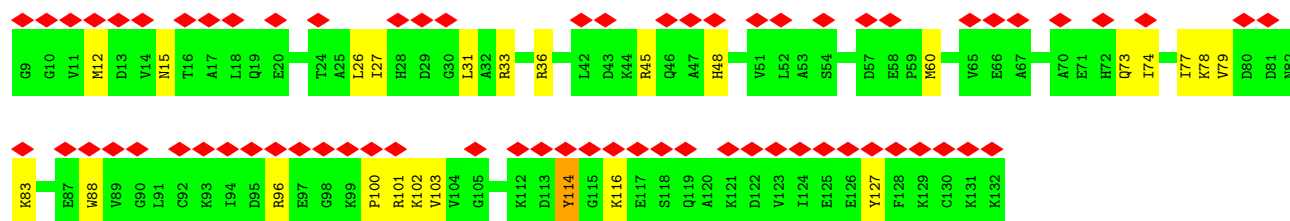


- Molecule 63: uS17

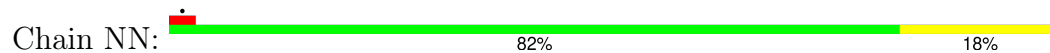


- Molecule 64: eS12

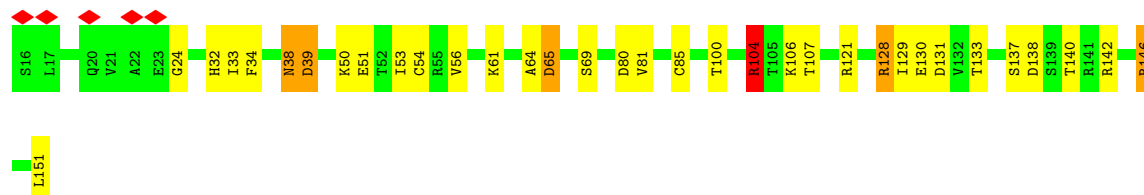
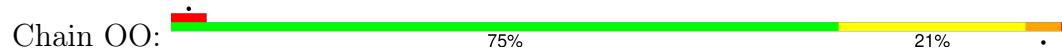




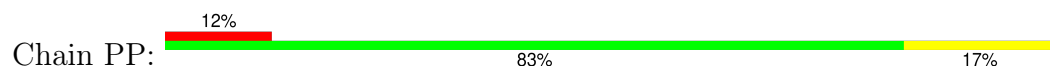
• Molecule 65: uS15



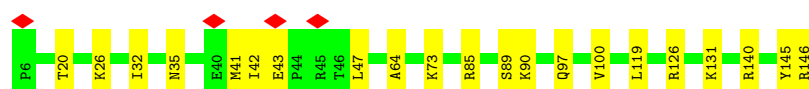
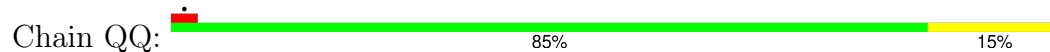
• Molecule 66: uS11



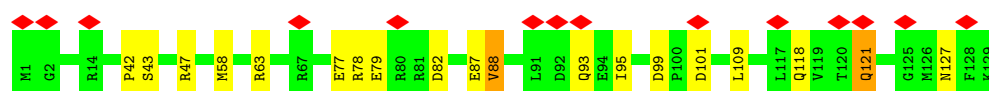
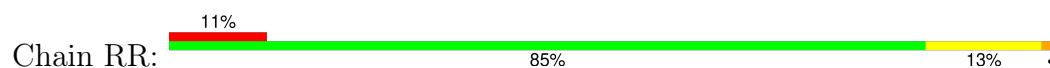
• Molecule 67: uS19



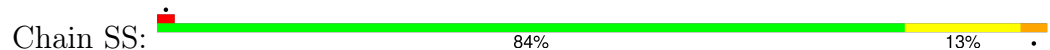
• Molecule 68: uS9

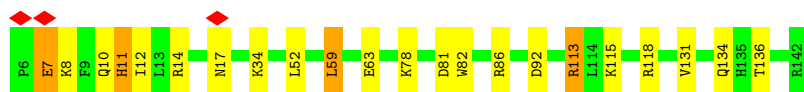


• Molecule 69: eS17

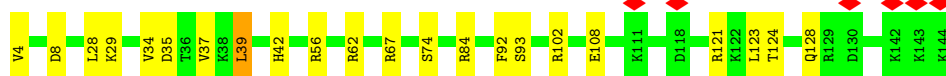
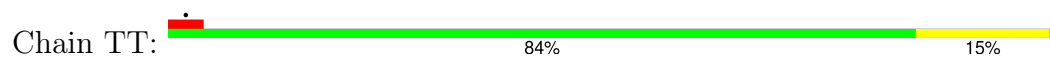


• Molecule 70: uS13

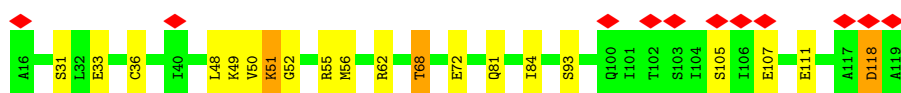
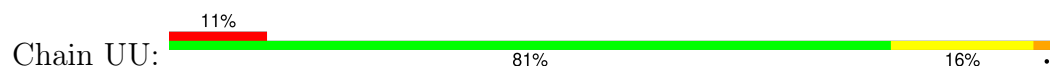




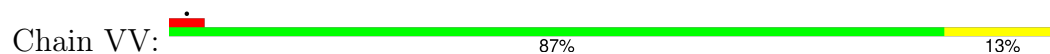
• Molecule 71: eS19



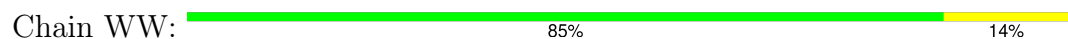
• Molecule 72: uS10



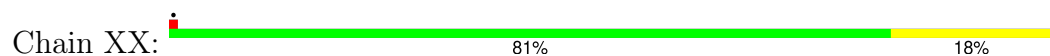
• Molecule 73: eS21



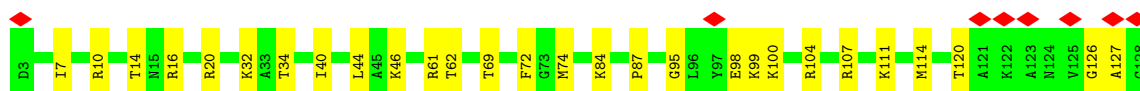
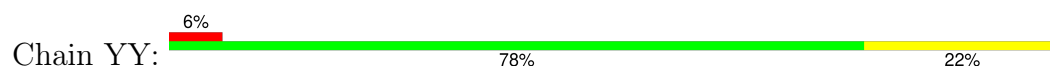
• Molecule 74: uS8



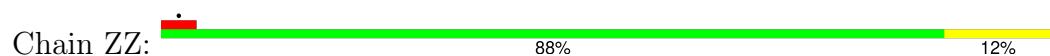
• Molecule 75: uS12



• Molecule 76: eS24

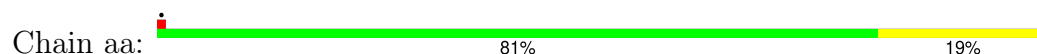


• Molecule 77: eS25

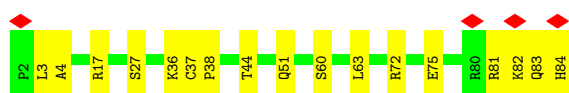
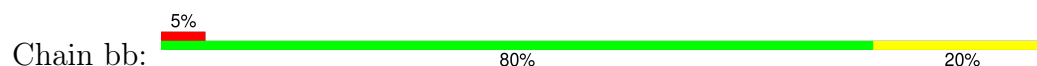




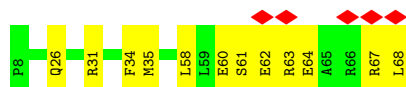
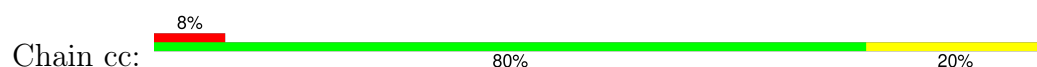
• Molecule 78: eS26



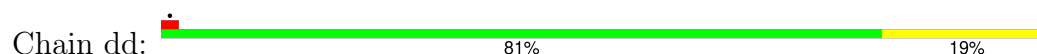
• Molecule 79: eS27



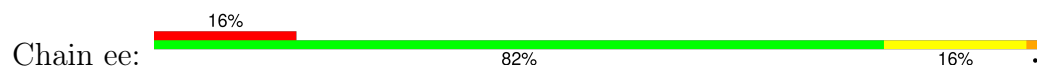
• Molecule 80: eS28



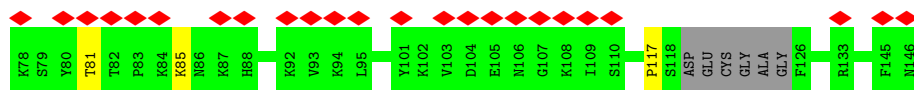
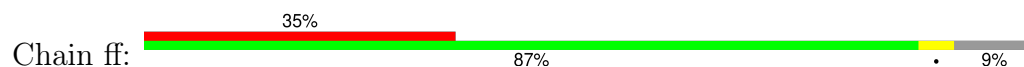
• Molecule 81: uS14



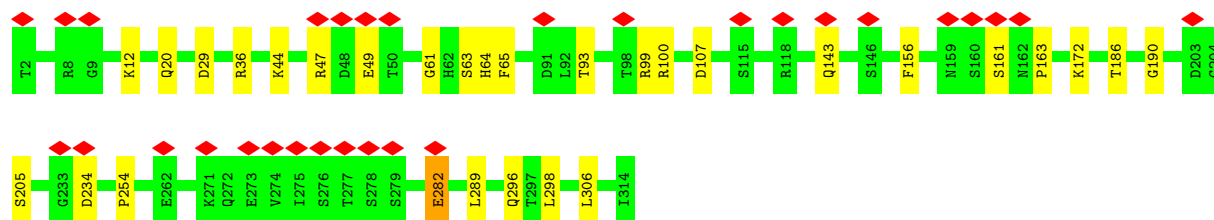
• Molecule 82: eS30



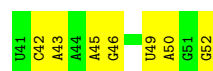
• Molecule 83: eS31



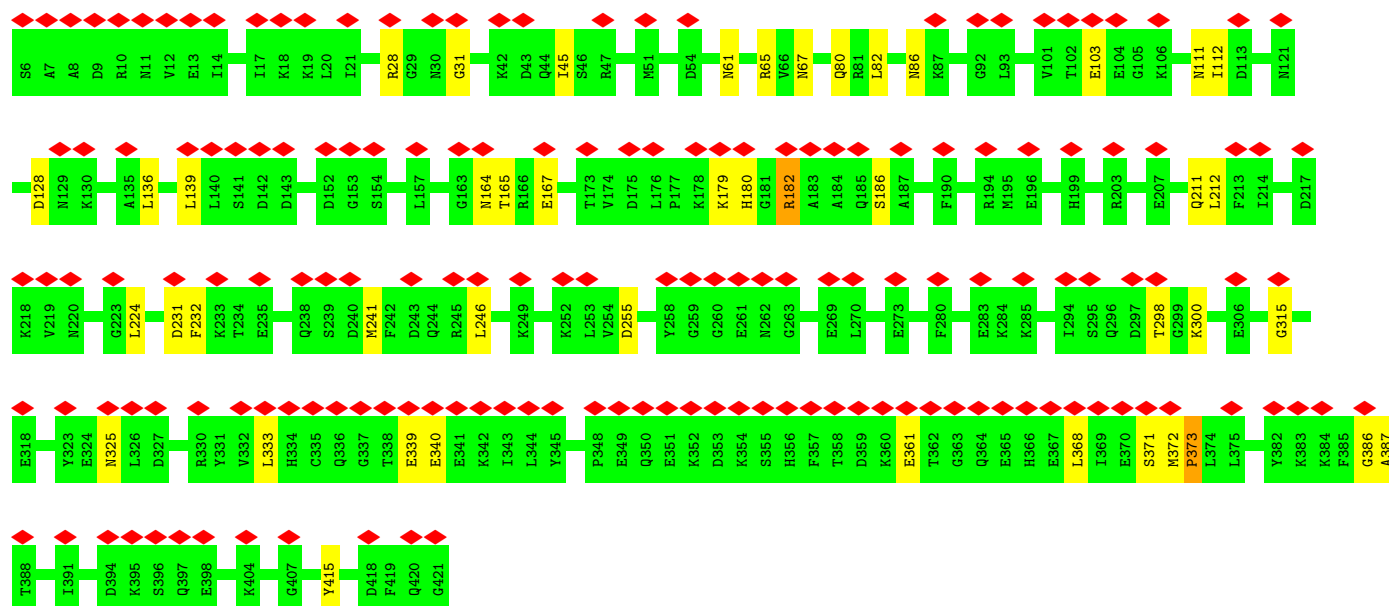
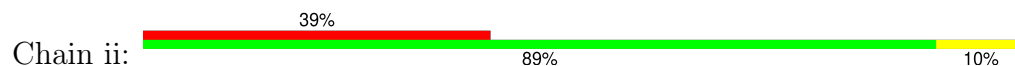
• Molecule 84: RACK1



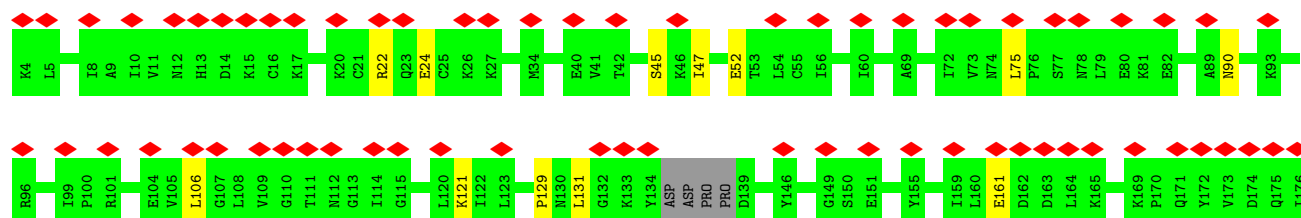
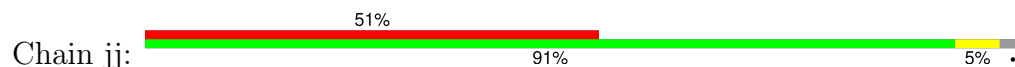
• Molecule 85: mRNA

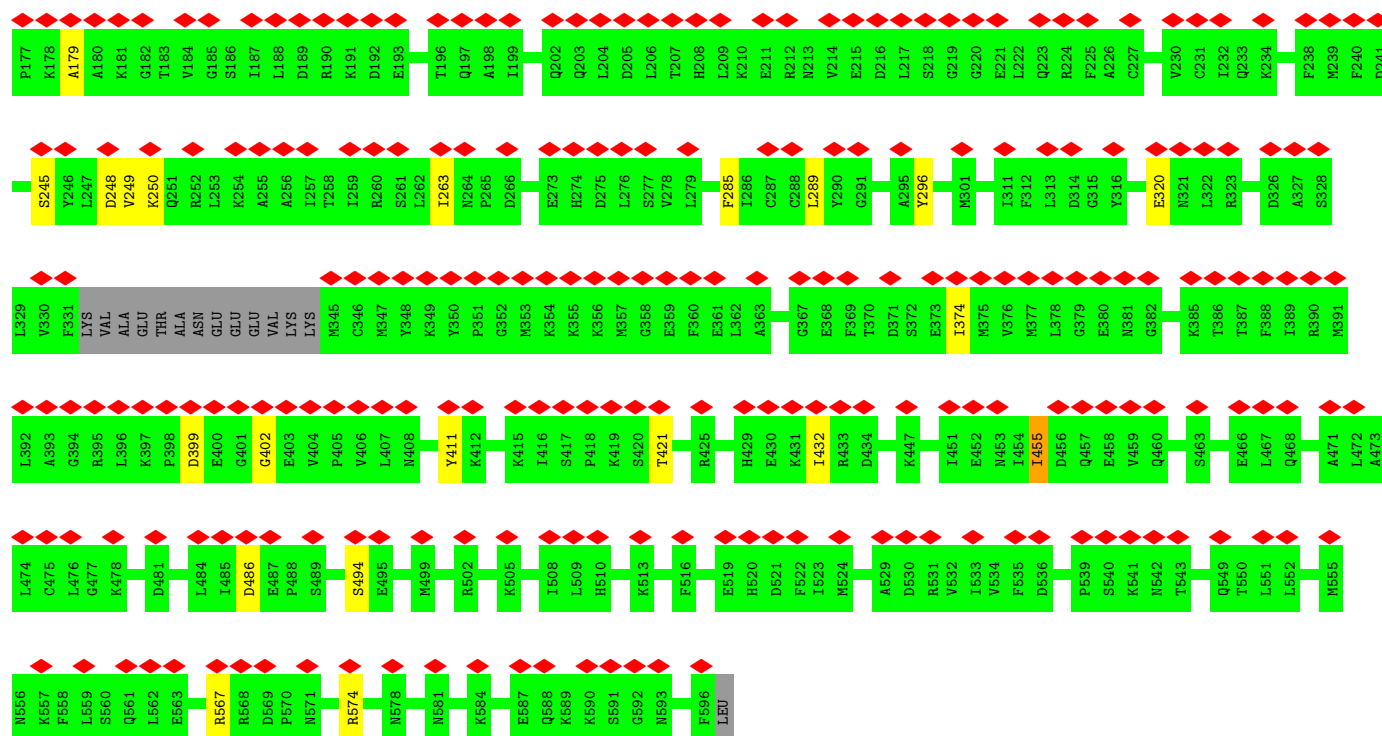


• Molecule 86: eRF1



• Molecule 87: ABCE1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	20515	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.528	Depositor
Minimum map value	-0.315	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.07	Depositor
Map size (\AA)	562.8, 562.8, 562.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: SF4, MG, ADP, 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	0.46	0/1906	0.79	0/2556
2	B	0.40	0/3216	0.78	1/4311 (0.0%)
3	C	0.43	0/2938	0.80	5/3946 (0.1%)
4	D	0.37	0/2432	0.70	2/3257 (0.1%)
5	E	0.46	0/1936	0.82	2/2600 (0.1%)
6	F	0.40	0/1905	0.75	1/2539 (0.0%)
7	G	0.38	0/1967	0.73	1/2647 (0.0%)
8	H	0.37	0/1535	0.71	0/2063
9	I	0.41	0/1693	0.69	0/2260
10	J	0.38	0/1376	0.73	0/1841
11	L	0.41	0/1734	0.79	0/2317
12	M	0.37	0/1158	0.74	0/1547
13	N	0.43	0/1746	0.83	0/2338
14	O	0.40	0/1671	0.77	0/2234
15	P	0.42	0/1268	0.75	0/1701
16	Q	0.41	0/1530	0.81	1/2041 (0.0%)
17	R	0.41	0/1524	0.79	0/2013
18	S	0.40	0/1493	0.85	3/2002 (0.1%)
19	T	0.41	0/1326	0.72	0/1770
20	U	0.41	0/822	0.68	0/1103
21	V	0.40	0/993	0.73	0/1332
22	W	0.48	0/541	0.83	1/720 (0.1%)
23	X	0.42	0/993	0.74	0/1334
24	Y	0.37	0/1132	0.80	2/1504 (0.1%)
25	Z	0.39	0/1130	0.72	0/1507
26	a	0.40	0/1191	0.79	0/1590
27	b	0.44	0/619	0.73	0/818
28	c	0.36	0/742	0.69	0/996
29	d	0.38	0/903	0.81	1/1216 (0.1%)
30	e	0.47	0/1071	0.85	0/1429
31	f	0.52	0/895	0.87	0/1198
32	g	0.42	0/916	0.81	1/1220 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.36	0/1021	0.77	1/1348 (0.1%)
34	i	0.40	0/841	0.82	2/1112 (0.2%)
35	j	0.45	0/720	0.93	1/952 (0.1%)
36	k	0.37	0/575	0.68	0/761
37	l	0.50	0/454	0.84	0/599
38	m	0.37	0/435	0.76	0/575
39	n	0.41	0/223	0.91	0/284
40	o	0.39	0/864	0.75	0/1140
41	p	0.42	0/718	0.71	0/953
42	r	0.48	0/1017	0.80	1/1364 (0.1%)
43	s	0.38	0/1547	0.58	0/2088
44	t	0.41	0/1257	0.69	0/1697
45	1	0.45	0/129	0.72	0/173
46	2	0.26	0/1805	0.72	1/2809 (0.0%)
47	3	0.36	0/1777	0.97	10/2763 (0.4%)
48	5	0.37	4/87790 (0.0%)	0.79	75/136937 (0.1%)
49	7	0.30	0/2858	0.69	0/4455
50	8	0.36	0/3701	0.74	0/5766
51	9	0.32	1/41013 (0.0%)	0.79	45/63919 (0.1%)
52	AA	0.36	0/1679	0.70	0/2283
53	BB	0.38	0/1756	0.77	4/2350 (0.2%)
54	CC	0.41	0/1730	0.76	1/2344 (0.0%)
55	DD	0.37	0/1792	0.72	0/2412
56	EE	0.39	0/2115	0.78	0/2843
57	FF	0.49	0/1531	0.78	1/2059 (0.0%)
58	GG	0.37	0/1946	0.78	0/2590
59	HH	0.44	0/1544	0.72	1/2068 (0.0%)
60	II	0.41	0/1715	0.78	0/2287
61	JJ	0.41	0/1550	0.88	4/2069 (0.2%)
62	KK	0.47	0/851	0.73	0/1147
63	LL	0.40	0/1259	0.78	0/1684
64	MM	0.42	0/968	0.64	0/1296
65	NN	0.39	0/1232	0.77	0/1656
66	OO	0.42	0/1029	0.88	1/1380 (0.1%)
67	PP	0.39	0/1079	0.76	0/1437
68	QQ	0.37	0/1142	0.70	0/1528
69	RR	0.42	0/1060	0.71	0/1421
70	SS	0.38	0/1157	0.84	1/1548 (0.1%)
71	TT	0.43	0/1120	0.78	2/1499 (0.1%)
72	UU	0.36	0/831	0.71	0/1115
73	VV	0.39	0/645	0.75	0/865
74	WW	0.38	0/1051	0.79	0/1406
75	XX	0.38	0/1116	0.80	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	YY	0.39	0/1040	0.74	0/1382
77	ZZ	0.37	0/604	0.75	0/810
78	aa	0.39	0/794	0.83	0/1065
79	bb	0.37	0/665	0.67	0/891
80	cc	0.36	0/478	0.78	0/640
81	dd	0.40	0/455	0.80	0/603
82	ee	0.46	0/462	0.75	0/607
83	ff	0.39	0/531	0.62	0/703
84	gg	0.37	0/2493	0.65	0/3394
85	hh	0.29	0/287	0.76	0/445
86	ii	0.39	0/3333	0.63	2/4483 (0.0%)
87	jj	0.47	1/4625 (0.0%)	0.58	0/6238
All	All	0.38	6/242712 (0.0%)	0.78	174/355683 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	4
3	C	0	2
4	D	0	1
5	E	0	1
7	G	0	1
9	I	0	2
11	L	0	3
17	R	0	1
18	S	0	2
19	T	0	1
20	U	0	1
24	Y	0	1
31	f	0	1
42	r	0	2
48	5	0	1
51	9	0	1
52	AA	0	1
56	EE	0	2
57	FF	0	2
59	HH	0	1
60	II	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
61	JJ	0	2
66	OO	0	1
68	QQ	0	1
70	SS	0	1
71	TT	0	1
72	UU	0	2
73	VV	0	1
74	WW	0	2
75	XX	0	1
78	aa	0	1
86	ii	0	3
All	All	0	49

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	1965	G	O3'-P	-23.01	1.33	1.61
87	jj	121	LYS	CE-NZ	19.94	1.99	1.49
51	9	908	A	O3'-P	8.98	1.72	1.61
48	5	1847	C	O3'-P	-6.16	1.53	1.61
48	5	957	G	O3'-P	5.62	1.67	1.61
48	5	1358	G	O3'-P	5.10	1.67	1.61

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	909	G	O5'-P-OP2	-16.21	91.11	105.70
47	3	70	G	N9-C1'-C2'	-13.18	96.87	114.00
48	5	3753	G	N9-C1'-C2'	-11.91	98.52	114.00
51	9	1235	G	N9-C1'-C2'	-11.46	99.11	114.00
48	5	3718	A	N9-C1'-C2'	-10.30	100.61	114.00
48	5	1358	G	C4'-C3'-O3'	10.21	133.41	113.00
51	9	1386	A	N9-C1'-C2'	-10.19	100.76	114.00
51	9	1212	G	N9-C1'-C2'	-10.02	100.98	114.00
48	5	1357	C	C4'-C3'-O3'	9.68	132.37	113.00
24	Y	87	ARG	NE-CZ-NH2	9.17	124.89	120.30
48	5	4975	G	C2'-C3'-O3'	8.96	129.21	109.50
51	9	1294	G	N9-C1'-C2'	-8.95	102.15	112.00
47	3	38	A	N9-C1'-C2'	-8.89	102.22	112.00
47	3	30	G	N9-C1'-C2'	-8.83	102.28	112.00
53	BB	136	ARG	NE-CZ-NH2	8.82	124.71	120.30
22	W	44	ARG	NE-CZ-NH1	8.56	124.58	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	90	G	C2'-C3'-O3'	8.38	127.95	109.50
48	5	4528	G	C2'-C3'-O3'	8.37	127.90	109.50
48	5	3888	G	C2'-C3'-O3'	8.31	127.79	109.50
47	3	70	G	C4'-C3'-O3'	8.30	129.60	113.00
51	9	1394	G	C2'-C3'-O3'	8.28	127.71	109.50
48	5	1969	G	N9-C1'-C2'	-8.26	102.91	112.00
70	SS	113	ARG	NE-CZ-NH1	8.20	124.40	120.30
61	JJ	127	ARG	NE-CZ-NH1	8.12	124.36	120.30
48	5	4948	C	C2'-C3'-O3'	8.04	127.19	109.50
51	9	1385	G	N9-C1'-C2'	-8.01	103.19	112.00
18	S	83	ARG	NE-CZ-NH2	7.99	124.29	120.30
48	5	1211	G	C2'-C3'-O3'	7.95	126.98	109.50
48	5	3697	U	C2'-C3'-O3'	7.90	126.87	109.50
35	j	63	ARG	NE-CZ-NH1	7.84	124.22	120.30
48	5	1455	G	C2'-C3'-O3'	7.78	126.60	109.50
51	9	1235	G	C4'-C3'-O3'	7.73	128.47	113.00
61	JJ	131	ARG	NE-CZ-NH1	7.71	124.15	120.30
48	5	2858	A	N9-C1'-C2'	-7.65	103.59	112.00
48	5	2858	A	C4'-C3'-O3'	7.62	128.23	113.00
47	3	39	U	N1-C1'-C2'	-7.58	103.66	112.00
51	9	1681	U	N1-C1'-C2'	-7.56	103.68	112.00
48	5	1292	C	C2'-C3'-O3'	7.52	126.05	109.50
3	C	342	ARG	NE-CZ-NH1	7.51	124.05	120.30
48	5	3718	A	C4'-C3'-O3'	7.50	128.00	113.00
51	9	322	C	N1-C1'-C2'	-7.45	103.80	112.00
51	9	1448	A	N9-C1'-C2'	-7.42	103.84	112.00
51	9	1641	A	O5'-P-OP1	-7.38	99.06	105.70
48	5	275	C	C2'-C3'-O3'	7.36	125.68	109.50
48	5	5060	A	C2'-C3'-O3'	7.33	125.62	109.50
48	5	125	C	C2'-C3'-O3'	7.32	125.61	109.50
48	5	1477	C	C2'-C3'-O3'	7.27	125.50	109.50
48	5	2797	C	N1-C1'-C2'	-7.26	104.02	112.00
71	TT	56	ARG	NE-CZ-NH1	7.26	123.93	120.30
61	JJ	24	ARG	NE-CZ-NH1	7.24	123.92	120.30
48	5	5061	A	C2'-C3'-O3'	7.19	125.33	109.50
51	9	1144	A	N9-C1'-C2'	7.18	123.34	114.00
48	5	47	A	C4'-C3'-O3'	7.18	127.36	113.00
48	5	2695	A	C2'-C3'-O3'	7.14	125.21	109.50
51	9	1268	C	N1-C1'-C2'	-7.13	104.15	112.00
48	5	406	C	C2'-C3'-O3'	7.13	125.19	109.50
48	5	2027	U	N1-C1'-C2'	-7.13	104.16	112.00
48	5	5059	C	C2'-C3'-O3'	7.13	125.18	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	ii	182	ARG	NE-CZ-NH1	7.12	123.86	120.30
47	3	1	G	C5'-C4'-O4'	7.08	117.59	109.10
51	9	1455	A	N9-C1'-C2'	-7.07	104.22	112.00
51	9	102	A	C2'-C3'-O3'	7.04	124.99	109.50
48	5	1485	C	C2'-C3'-O3'	6.93	124.80	113.70
61	JJ	131	ARG	NE-CZ-NH2	-6.91	116.85	120.30
51	9	642	U	C4'-C3'-O3'	6.88	126.76	113.00
51	9	666	U	N1-C1'-C2'	6.84	122.89	114.00
48	5	1279	A	C2'-C3'-O3'	6.80	124.58	113.70
48	5	2046	G	C2'-C3'-O3'	6.76	124.52	113.70
48	5	1236	C	C2'-C3'-O3'	6.71	124.43	113.70
48	5	977	C	C2'-C3'-O3'	6.68	124.39	113.70
48	5	4885	U	C2'-C3'-O3'	6.66	124.35	113.70
48	5	93	G	C4'-C3'-O3'	6.64	126.29	113.00
34	i	25	ARG	NE-CZ-NH1	6.54	123.57	120.30
51	9	312	G	C2'-C3'-O3'	6.53	124.15	113.70
48	5	1818	G	C2'-C3'-O3'	6.51	124.12	113.70
51	9	1447	G	N9-C1'-C2'	-6.49	104.86	112.00
48	5	2083	C	C4'-C3'-O3'	6.44	125.87	113.00
51	9	1386	A	C4'-C3'-O3'	6.44	125.88	113.00
51	9	1060	A	N9-C1'-C2'	6.42	122.34	114.00
48	5	93	G	N9-C1'-C2'	-6.39	104.97	112.00
47	3	69	G	O4'-C1'-N9	6.39	113.31	108.20
48	5	3657	U	C2'-C3'-O3'	6.36	123.87	113.70
4	D	22	ARG	NE-CZ-NH1	6.34	123.47	120.30
48	5	1474	C	C2'-C3'-O3'	6.32	123.82	113.70
5	E	208	LEU	CA-CB-CG	6.32	129.84	115.30
48	5	1500	A	C2'-C3'-O3'	6.29	123.76	113.70
51	9	1	U	C5'-C4'-O4'	6.29	116.64	109.10
48	5	1398	A	C2'-C3'-O3'	6.28	123.74	113.70
51	9	110	U	C2'-C3'-O3'	6.28	123.74	113.70
48	5	2123	C	C2'-C3'-O3'	6.23	123.67	113.70
48	5	1380	G	N9-C1'-C2'	6.22	122.09	114.00
48	5	1969	G	C4'-C3'-O3'	6.22	125.45	113.00
48	5	1239	C	C2'-C3'-O3'	6.21	123.64	113.70
48	5	2632	U	N1-C1'-C2'	6.17	122.02	114.00
51	9	322	C	C2'-C3'-O3'	-6.15	95.97	109.50
51	9	1211	G	N9-C1'-C2'	-6.12	105.27	112.00
51	9	62	G	C2'-C3'-O3'	6.09	123.45	113.70
51	9	434	G	C2'-C3'-O3'	6.05	123.38	113.70
48	5	1072	C	N1-C1'-C2'	6.03	121.84	114.00
48	5	1672	U	N1-C1'-C2'	6.02	121.83	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	1848	C	C2'-C3'-O3'	6.01	123.31	113.70
29	d	78	ARG	NE-CZ-NH1	5.98	123.29	120.30
48	5	1390	G	C2'-C3'-O3'	5.93	123.19	113.70
34	i	85	ARG	NE-CZ-NH1	5.93	123.26	120.30
48	5	1965	G	P-O3'-C3'	5.90	126.78	119.70
48	5	1696	C	C2'-C3'-O3'	5.90	123.13	113.70
51	9	1419	C	C2'-C3'-O3'	5.89	123.12	113.70
16	Q	104	ARG	NE-CZ-NH1	5.87	123.23	120.30
48	5	978	G	C2'-C3'-O3'	5.81	123.00	113.70
48	5	4872	G	C2'-C3'-O3'	5.78	122.95	113.70
5	E	72	PRO	N-CA-CB	5.78	110.24	103.30
48	5	4951	G	C2'-C3'-O3'	5.77	122.93	113.70
48	5	1329	G	C2'-C3'-O3'	5.76	122.91	113.70
48	5	4975	G	C4'-C3'-O3'	-5.72	97.39	109.40
48	5	215	C	C2'-C3'-O3'	5.69	122.80	113.70
51	9	1824	A	C2'-C3'-O3'	5.67	122.77	113.70
3	C	98	GLY	N-CA-C	-5.65	98.97	113.10
47	3	1	G	C5'-C4'-C3'	5.63	125.00	116.00
51	9	1	U	C5'-C4'-C3'	5.62	124.99	116.00
51	9	1234	C	N1-C1'-C2'	-5.60	105.83	112.00
6	F	91	LEU	CA-CB-CG	5.54	128.05	115.30
18	S	83	ARG	NE-CZ-NH1	-5.51	117.55	120.30
2	B	36	ASP	C-N-CD	5.50	139.96	128.40
51	9	1137	U	C2'-C3'-O3'	5.49	122.48	113.70
57	FF	135	ARG	NE-CZ-NH2	-5.48	117.56	120.30
47	3	29	A	N9-C1'-C2'	-5.46	105.99	112.00
48	5	979	C	C2'-C3'-O3'	5.46	122.44	113.70
48	5	4473	A	N9-C1'-C2'	5.46	121.09	114.00
48	5	2054	U	N1-C1'-C2'	5.45	121.08	114.00
53	BB	136	ARG	CG-CD-NE	5.45	123.23	111.80
71	TT	56	ARG	NE-CZ-NH2	-5.42	117.59	120.30
47	3	30	G	C4'-C3'-O3'	5.41	123.82	113.00
48	5	2028	C	N1-C1'-C2'	-5.41	106.05	112.00
48	5	957	G	P-O3'-C3'	5.40	126.19	119.70
51	9	1385	G	C4'-C3'-O3'	5.38	123.77	113.00
59	HH	118	ARG	NE-CZ-NH1	5.38	122.99	120.30
24	Y	75	ARG	NE-CZ-NH1	5.38	122.99	120.30
48	5	1365	C	C4'-C3'-O3'	5.37	123.75	113.00
51	9	1144	A	C8-N9-C1'	-5.35	118.07	127.70
51	9	844	U	C5'-C4'-O4'	5.34	115.51	109.10
86	ii	372	MET	C-N-CD	5.33	139.60	128.40
66	OO	146	ARG	NE-CZ-NH2	-5.31	117.64	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1212	G	C4'-C3'-O3'	5.29	123.59	113.00
53	BB	136	ARG	NE-CZ-NH1	-5.29	117.65	120.30
48	5	486	C	C2'-C3'-O3'	5.29	122.16	113.70
51	9	909	G	O5'-P-OP1	5.29	117.05	110.70
48	5	1266	G	C2'-C3'-O3'	5.28	122.15	113.70
48	5	3715	U	N1-C1'-C2'	-5.27	106.20	112.00
48	5	2586	G	N9-C1'-C2'	5.25	120.82	114.00
3	C	262	ASP	CB-CG-OD2	5.23	123.00	118.30
18	S	83	ARG	CG-CD-NE	5.22	122.76	111.80
33	h	22	ASP	CB-CG-OD2	5.21	122.98	118.30
51	9	1647	A	C2'-C3'-O3'	5.18	122.00	113.70
51	9	1144	A	C4-N9-C1'	5.16	135.58	126.30
7	G	231	ASP	CB-CG-OD2	5.15	122.94	118.30
51	9	1408	U	O5'-P-OP1	-5.13	101.09	105.70
48	5	4731	G	N9-C1'-C2'	5.11	120.65	114.00
42	r	17	LEU	CA-CB-CG	5.11	127.05	115.30
48	5	2661	U	C2'-C3'-O3'	5.11	121.88	113.70
53	BB	136	ARG	CD-NE-CZ	5.10	130.74	123.60
48	5	4481	U	C5'-C4'-O4'	5.09	115.21	109.10
48	5	4965	U	C2'-C3'-O3'	5.07	121.81	113.70
51	9	532	C	C2'-C3'-O3'	5.06	121.79	113.70
51	9	1109	C	N1-C1'-C2'	5.05	120.57	114.00
3	C	67	TRP	N-CA-C	-5.04	97.39	111.00
48	5	1755	C	C2'-C3'-O3'	5.04	121.77	113.70
51	9	488	U	N1-C1'-C2'	5.04	120.55	114.00
3	C	45	ARG	NE-CZ-NH1	5.04	122.82	120.30
32	g	66	ARG	NE-CZ-NH1	5.04	122.82	120.30
46	2	34	A	N9-C1'-C2'	-5.03	106.46	112.00
54	CC	233	LEU	CA-CB-CG	5.03	126.87	115.30
51	9	1354	G	C2'-C3'-O3'	5.03	121.75	113.70
4	D	22	ARG	CG-CD-NE	5.02	122.33	111.80
48	5	2246	C	C2'-C3'-O3'	5.01	121.72	113.70

There are no chirality outliers.

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	5	2793	G	Sidechain
51	9	1448	A	Sidechain
1	A	196	TRP	Peptide
52	AA	73	ASP	Peptide
2	B	17	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	B	257	TRP	Peptide
2	B	258	HIS	Peptide
2	B	351	LEU	Peptide
3	C	245	HIS	Peptide
3	C	339	THR	Peptide
4	D	36	LEU	Peptide
5	E	123	SER	Peptide
56	EE	129	ILE	Peptide
56	EE	155	LYS	Peptide
57	FF	42	LYS	Peptide
57	FF	43	GLU	Peptide
7	G	238	GLY	Peptide
59	HH	111	LYS	Peptide
9	I	188	LYS	Peptide
9	I	202	ASN	Peptide
60	II	154	LYS	Peptide
61	JJ	38	ARG	Peptide
61	JJ	93	LYS	Peptide
11	L	27	ASN	Peptide
11	L	46	ILE	Peptide
11	L	66	TYR	Peptide
66	OO	104	ARG	Peptide
68	QQ	42	ILE	Peptide
17	R	19	LYS	Peptide
18	S	163	HIS	Peptide
18	S	164	LYS	Peptide
70	SS	11	HIS	Peptide
19	T	26	PRO	Peptide
71	TT	42	HIS	Peptide
20	U	27	HIS	Peptide
72	UU	68	THR	Peptide
72	UU	72	GLU	Peptide
73	VV	32	ILE	Peptide
74	WW	27	ILE	Peptide
74	WW	54	ASP	Peptide
75	XX	98	ASP	Peptide
24	Y	7	VAL	Peptide
78	aa	7	ASN	Peptide
31	f	105	LEU	Peptide
86	ii	325	ASN	Peptide
86	ii	371	SER	Peptide
86	ii	373	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
42	r	106	LEU	Peptide
42	r	70	GLN	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/244 (99%)	209 (86%)	28 (12%)	5 (2%)	5	32
2	B	392/394 (100%)	345 (88%)	42 (11%)	5 (1%)	10	41
3	C	360/362 (99%)	322 (89%)	27 (8%)	11 (3%)	3	26
4	D	290/292 (99%)	262 (90%)	25 (9%)	3 (1%)	13	46
5	E	232/248 (94%)	179 (77%)	36 (16%)	17 (7%)	1	10
6	F	223/225 (99%)	204 (92%)	17 (8%)	2 (1%)	14	48
7	G	239/241 (99%)	203 (85%)	31 (13%)	5 (2%)	5	32
8	H	188/190 (99%)	165 (88%)	20 (11%)	3 (2%)	8	37
9	I	200/213 (94%)	181 (90%)	15 (8%)	4 (2%)	6	33
10	J	167/169 (99%)	147 (88%)	13 (8%)	7 (4%)	2	19
11	L	208/210 (99%)	180 (86%)	16 (8%)	12 (6%)	1	13
12	M	136/138 (99%)	123 (90%)	12 (9%)	1 (1%)	19	53
13	N	201/203 (99%)	181 (90%)	20 (10%)	0	100	100
14	O	197/199 (99%)	184 (93%)	12 (6%)	1 (0%)	25	59
15	P	151/153 (99%)	135 (89%)	16 (11%)	0	100	100
16	Q	185/187 (99%)	169 (91%)	14 (8%)	2 (1%)	12	44
17	R	178/180 (99%)	166 (93%)	9 (5%)	3 (2%)	7	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	S	173/175 (99%)	157 (91%)	12 (7%)	4 (2%)	5	31
19	T	157/159 (99%)	139 (88%)	15 (10%)	3 (2%)	6	34
20	U	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	2	20
21	V	129/131 (98%)	115 (89%)	13 (10%)	1 (1%)	16	50
22	W	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	8	37
23	X	117/119 (98%)	109 (93%)	6 (5%)	2 (2%)	7	36
24	Y	132/134 (98%)	114 (86%)	17 (13%)	1 (1%)	16	50
25	Z	133/135 (98%)	113 (85%)	13 (10%)	7 (5%)	1	15
26	a	145/147 (99%)	122 (84%)	19 (13%)	4 (3%)	4	27
27	b	73/75 (97%)	67 (92%)	5 (7%)	1 (1%)	9	40
28	c	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
29	d	105/107 (98%)	91 (87%)	13 (12%)	1 (1%)	13	46
30	e	126/128 (98%)	115 (91%)	6 (5%)	5 (4%)	2	20
31	f	107/109 (98%)	94 (88%)	8 (8%)	5 (5%)	2	17
32	g	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	14	48
33	h	120/122 (98%)	107 (89%)	9 (8%)	4 (3%)	3	25
34	i	100/102 (98%)	92 (92%)	6 (6%)	2 (2%)	6	33
35	j	84/86 (98%)	70 (83%)	9 (11%)	5 (6%)	1	13
36	k	67/69 (97%)	56 (84%)	7 (10%)	4 (6%)	1	13
37	l	48/50 (96%)	40 (83%)	7 (15%)	1 (2%)	5	32
38	m	50/52 (96%)	44 (88%)	6 (12%)	0	100	100
39	n	21/23 (91%)	21 (100%)	0	0	100	100
40	o	102/104 (98%)	92 (90%)	7 (7%)	3 (3%)	3	27
41	p	89/91 (98%)	80 (90%)	8 (9%)	1 (1%)	12	44
42	r	123/125 (98%)	102 (83%)	14 (11%)	7 (6%)	1	14
43	s	196/198 (99%)	164 (84%)	22 (11%)	10 (5%)	1	16
44	t	161/163 (99%)	102 (63%)	33 (20%)	26 (16%)	0	2
45	1	13/15 (87%)	11 (85%)	0	2 (15%)	0	2
52	AA	206/208 (99%)	173 (84%)	23 (11%)	10 (5%)	2	16
53	BB	211/213 (99%)	165 (78%)	33 (16%)	13 (6%)	1	12
54	CC	216/218 (99%)	184 (85%)	26 (12%)	6 (3%)	4	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	DD	225/227 (99%)	181 (80%)	33 (15%)	11 (5%)	2	16
56	EE	260/262 (99%)	200 (77%)	42 (16%)	18 (7%)	1	10
57	FF	189/191 (99%)	160 (85%)	21 (11%)	8 (4%)	2	19
58	GG	235/237 (99%)	198 (84%)	31 (13%)	6 (3%)	4	29
59	HH	187/189 (99%)	148 (79%)	25 (13%)	14 (8%)	1	9
60	II	204/206 (99%)	168 (82%)	28 (14%)	8 (4%)	2	21
61	JJ	183/185 (99%)	153 (84%)	20 (11%)	10 (6%)	1	14
62	KK	96/98 (98%)	65 (68%)	21 (22%)	10 (10%)	0	6
63	LL	150/152 (99%)	125 (83%)	19 (13%)	6 (4%)	2	20
64	MM	122/124 (98%)	87 (71%)	28 (23%)	7 (6%)	1	14
65	NN	148/150 (99%)	126 (85%)	17 (12%)	5 (3%)	3	24
66	OO	134/136 (98%)	99 (74%)	21 (16%)	14 (10%)	0	6
67	PP	125/127 (98%)	107 (86%)	15 (12%)	3 (2%)	5	30
68	QQ	139/141 (99%)	116 (84%)	18 (13%)	5 (4%)	3	23
69	RR	127/129 (98%)	106 (84%)	15 (12%)	6 (5%)	2	17
70	SS	135/137 (98%)	114 (84%)	16 (12%)	5 (4%)	2	22
71	TT	139/141 (99%)	126 (91%)	10 (7%)	3 (2%)	5	32
72	UU	102/104 (98%)	87 (85%)	9 (9%)	6 (6%)	1	13
73	VV	81/83 (98%)	67 (83%)	10 (12%)	4 (5%)	2	16
74	WW	127/129 (98%)	106 (84%)	16 (13%)	5 (4%)	2	21
75	XX	139/141 (99%)	118 (85%)	13 (9%)	8 (6%)	1	13
76	YY	124/126 (98%)	99 (80%)	17 (14%)	8 (6%)	1	12
77	ZZ	73/75 (97%)	59 (81%)	12 (16%)	2 (3%)	4	28
78	aa	96/98 (98%)	73 (76%)	13 (14%)	10 (10%)	0	6
79	bb	81/83 (98%)	61 (75%)	16 (20%)	4 (5%)	2	16
80	cc	59/61 (97%)	47 (80%)	10 (17%)	2 (3%)	3	24
81	dd	51/53 (96%)	45 (88%)	3 (6%)	3 (6%)	1	13
82	ee	55/57 (96%)	40 (73%)	12 (22%)	3 (6%)	1	14
83	ff	58/68 (85%)	50 (86%)	6 (10%)	2 (3%)	3	24
84	gg	311/313 (99%)	269 (86%)	33 (11%)	9 (3%)	3	27
86	ii	414/416 (100%)	380 (92%)	26 (6%)	8 (2%)	6	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
87	jj	568/594 (96%)	513 (90%)	41 (7%)	14 (2%)	4	29
All	All	12492/12709 (98%)	10717 (86%)	1333 (11%)	442 (4%)	5	24

All (442) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	TRP
3	C	273	LEU
5	E	91	PRO
5	E	95	ASP
5	E	118	PRO
5	E	175	LEU
5	E	221	PRO
7	G	45	ILE
7	G	128	VAL
8	H	40	HIS
8	H	110	SER
9	I	47	PRO
11	L	64	VAL
11	L	67	HIS
17	R	36	ASN
18	S	165	PRO
20	U	47	ILE
25	Z	84	ARG
26	a	90	ALA
29	d	94	GLU
30	e	92	ASN
31	f	80	ASN
33	h	7	ARG
36	k	61	PRO
40	o	32	SER
42	r	86	ALA
43	s	62	ARG
43	s	201	PRO
44	t	29	ALA
44	t	30	PRO
44	t	31	LYS
44	t	53	TRP
44	t	89	PRO
44	t	144	ASP
44	t	148	PRO
44	t	149	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	AA	186	ARG
53	BB	57	ILE
53	BB	179	ASN
53	BB	191	ASP
55	DD	192	TRP
55	DD	202	LYS
55	DD	223	ILE
56	EE	24	THR
56	EE	76	VAL
56	EE	118	GLU
56	EE	164	LEU
56	EE	196	THR
57	FF	34	SER
57	FF	163	PHE
58	GG	174	PRO
59	HH	18	GLU
59	HH	66	VAL
59	HH	116	ARG
59	HH	159	ASP
60	II	27	TYR
60	II	155	ASN
60	II	157	LYS
61	JJ	4	ALA
61	JJ	22	LYS
61	JJ	121	LYS
62	KK	95	ARG
64	MM	79	VAL
64	MM	102	LYS
64	MM	114	TYR
65	NN	24	THR
66	OO	56	VAL
66	OO	65	ASP
66	OO	128	ARG
66	OO	140	THR
68	QQ	43	GLU
68	QQ	64	ALA
69	RR	88	VAL
69	RR	93	GLN
71	TT	34	VAL
72	UU	107	GLU
73	VV	41	LYS
73	VV	48	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
75	XX	34	THR
75	XX	42	GLY
76	YY	104	ARG
76	YY	114	MET
76	YY	120	THR
77	ZZ	113	THR
78	aa	10	ARG
82	ee	9	VAL
84	gg	254	PRO
84	gg	282	GLU
86	ii	298	THR
87	jj	245	SER
87	jj	455	ILE
1	A	217	GLN
2	B	38	SER
2	B	302	ASN
3	C	73	VAL
3	C	155	GLU
3	C	275	SER
4	D	187	SER
5	E	85	LEU
5	E	92	VAL
5	E	174	PRO
5	E	234	GLU
10	J	116	GLY
10	J	155	HIS
11	L	63	THR
11	L	143	GLU
11	L	172	GLU
17	R	130	ASN
18	S	88	SER
19	T	81	LYS
20	U	98	ASP
23	X	131	ASP
25	Z	34	SER
26	a	76	ASP
30	e	44	ARG
34	i	11	LEU
35	j	36	LYS
35	j	39	TYR
36	k	32	VAL
42	r	67	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	r	71	ARG
43	s	70	GLU
43	s	106	LYS
43	s	109	ALA
44	t	5	PHE
44	t	26	SER
44	t	39	PRO
44	t	58	ILE
44	t	106	PHE
52	AA	44	ASP
52	AA	45	GLY
53	BB	86	LEU
53	BB	140	VAL
53	BB	153	THR
54	CC	181	PRO
54	CC	190	SER
55	DD	219	PRO
56	EE	40	GLU
56	EE	95	THR
56	EE	153	LEU
56	EE	231	GLY
57	FF	33	ILE
57	FF	80	GLY
58	GG	152	ASP
59	HH	160	LYS
59	HH	190	PRO
60	II	138	ASN
61	JJ	21	GLU
61	JJ	120	ALA
62	KK	3	MET
62	KK	39	ASN
62	KK	63	ALA
63	LL	66	VAL
63	LL	135	SER
64	MM	15	ASN
65	NN	3	ARG
65	NN	28	LEU
65	NN	138	ASN
66	OO	39	ASP
66	OO	104	ARG
66	OO	129	ILE
67	PP	14	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	PP	75	VAL
69	RR	63	ARG
70	SS	12	ILE
70	SS	92	ASP
71	TT	29	LYS
71	TT	39	LEU
72	UU	50	VAL
74	WW	3	ARG
75	XX	10	ALA
75	XX	110	HIS
76	YY	84	LYS
76	YY	95	GLY
76	YY	127	ALA
77	ZZ	112	ASN
78	aa	8	ASN
78	aa	25	ASN
79	bb	4	ALA
79	bb	82	LYS
80	cc	26	GLN
81	dd	47	ALA
82	ee	43	VAL
84	gg	61	GLY
84	gg	161	SER
86	ii	31	GLY
86	ii	224	LEU
86	ii	315	GLY
86	ii	387	ALA
2	B	18	PRO
3	C	16	GLU
3	C	132	ALA
3	C	248	ARG
5	E	96	LYS
5	E	179	ARG
5	E	232	GLU
6	F	239	GLU
9	I	205	PRO
10	J	11	PRO
10	J	146	ARG
16	Q	14	ARG
17	R	19	LYS
21	V	14	PHE
25	Z	55	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	Z	124	THR
26	a	92	LYS
30	e	125	PRO
30	e	126	ASN
31	f	37	ASP
31	f	79	GLY
33	h	97	LYS
34	i	3	LEU
37	l	47	THR
42	r	19	LYS
42	r	85	ASN
43	s	69	LEU
43	s	108	PRO
43	s	142	GLY
44	t	54	LYS
44	t	67	ARG
44	t	105	THR
44	t	137	GLN
52	AA	50	ASN
52	AA	191	ARG
53	BB	88	THR
53	BB	206	PRO
54	CC	255	LEU
55	DD	175	VAL
55	DD	200	PRO
55	DD	222	PRO
56	EE	98	ASN
57	FF	119	SER
58	GG	59	GLN
59	HH	107	LYS
60	II	137	LEU
60	II	143	LYS
61	JJ	39	ASN
62	KK	31	LYS
62	KK	65	ARG
62	KK	92	ALA
63	LL	147	LYS
63	LL	149	ALA
64	MM	100	PRO
66	OO	32	HIS
66	OO	64	ALA
67	PP	15	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
68	QQ	100	VAL
70	SS	11	HIS
73	VV	21	ASN
73	VV	45	ARG
74	WW	93	LEU
75	XX	6	GLY
76	YY	34	THR
78	aa	9	GLY
78	aa	61	ALA
78	aa	62	TYR
78	aa	64	LEU
78	aa	65	PRO
79	bb	75	GLU
86	ii	28	ARG
87	jj	22	ARG
87	jj	179	ALA
87	jj	421	THR
1	A	180	LEU
2	B	54	THR
5	E	129	PHE
5	E	224	GLN
8	H	101	ILE
11	L	5	ARG
11	L	52	SER
19	T	29	THR
24	Y	83	GLU
25	Z	31	ASP
26	a	98	ALA
30	e	89	LEU
32	g	65	MET
33	h	89	ARG
36	k	29	LYS
41	p	41	PHE
44	t	2	PRO
44	t	18	THR
45	1	57	ARG
52	AA	43	SER
52	AA	102	ARG
52	AA	207	PRO
53	BB	154	SER
54	CC	264	SER
55	DD	191	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	EE	30	ARG
56	EE	73	ASP
57	FF	132	GLY
59	HH	16	PRO
59	HH	100	ILE
59	HH	111	LYS
59	HH	119	SER
59	HH	122	LEU
61	JJ	138	ARG
61	JJ	147	PHE
63	LL	28	THR
63	LL	32	LYS
66	OO	138	ASP
69	RR	121	GLN
70	SS	7	GLU
72	UU	51	LYS
72	UU	105	SER
72	UU	118	ASP
74	WW	112	ASP
75	XX	53	GLU
75	XX	129	SER
78	aa	15	ARG
78	aa	35	ALA
82	ee	22	GLN
83	ff	85	LYS
83	ff	117	PRO
84	gg	12	LYS
84	gg	190	GLY
84	gg	205	SER
84	gg	296	GLN
86	ii	373	PRO
86	ii	386	GLY
87	jj	285	PHE
1	A	130	SER
2	B	309	LEU
4	D	20	PHE
5	E	218	LEU
5	E	229	PHE
7	G	123	ALA
7	G	125	LYS
10	J	153	ALA
11	L	6	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	L	103	ARG
16	Q	148	VAL
20	U	27	HIS
25	Z	91	LEU
31	f	107	PRO
33	h	40	ALA
35	j	34	CYS
35	j	61	THR
36	k	21	LYS
40	o	77	CYS
42	r	11	ARG
43	s	34	ASN
44	t	7	PRO
45	l	64	PRO
52	AA	6	ASP
52	AA	36	GLN
53	BB	22	VAL
53	BB	24	PRO
53	BB	208	HIS
54	CC	134	ASN
55	DD	4	GLN
55	DD	199	GLY
56	EE	109	PHE
56	EE	131	VAL
56	EE	152	PRO
57	FF	37	ASP
57	FF	79	HIS
58	GG	54	GLY
58	GG	105	ASN
58	GG	146	ASN
59	HH	6	ALA
60	II	131	PRO
62	KK	90	VAL
64	MM	103	VAL
64	MM	116	LYS
66	OO	54	CYS
68	QQ	35	ASN
69	RR	42	PRO
69	RR	95	ILE
70	SS	59	LEU
74	WW	66	THR
79	bb	38	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	cc	64	GLU
81	dd	11	PRO
87	jj	47	ILE
1	A	67	TYR
3	C	222	ARG
3	C	309	ILE
10	J	124	GLY
11	L	100	PRO
11	L	169	ILE
14	O	49	ARG
18	S	5	GLY
20	U	67	LYS
22	W	15	PRO
31	f	106	TYR
35	j	60	GLY
40	o	33	LEU
44	t	10	ILE
44	t	19	GLY
44	t	22	VAL
54	CC	261	PHE
56	EE	90	ILE
59	HH	57	ARG
61	JJ	102	ILE
62	KK	32	HIS
62	KK	43	LEU
65	NN	60	VAL
66	OO	24	GLY
66	OO	33	ILE
66	OO	38	ASN
68	QQ	32	ILE
87	jj	24	GLU
87	jj	45	SER
87	jj	402	GLY
3	C	133	LEU
9	I	99	ILE
27	b	21	ILE
43	s	73	PRO
76	YY	126	GLY
87	jj	129	PRO
4	D	125	VAL
9	I	201	PRO
11	L	134	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	Z	90	PRO
53	BB	93	GLY
55	DD	218	LEU
56	EE	195	ILE
60	II	126	GLY
61	JJ	18	ARG
87	jj	249	VAL
87	jj	432	ILE
3	C	265	GLY
5	E	103	VAL
6	F	230	VAL
7	G	238	GLY
19	T	44	GLY
75	XX	116	PRO
84	gg	163	PRO
87	jj	263	ILE
10	J	174	ILE
12	M	7	VAL
18	S	155	PRO
44	t	3	PRO
44	t	98	ILE
72	UU	52	GLY
74	WW	29	PRO
81	dd	23	VAL
23	X	119	ILE
42	r	69	GLY
44	t	23	GLY
56	EE	107	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/187 (100%)	161 (86%)	26 (14%)	3	17
2	B	336/342 (98%)	291 (87%)	45 (13%)	3	18
3	C	302/302 (100%)	260 (86%)	42 (14%)	3	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	247/247 (100%)	218 (88%)	29 (12%)	4	22
5	E	208/221 (94%)	185 (89%)	23 (11%)	5	24
6	F	194/195 (100%)	165 (85%)	29 (15%)	2	15
7	G	206/206 (100%)	182 (88%)	24 (12%)	4	22
8	H	169/169 (100%)	148 (88%)	21 (12%)	4	20
9	I	174/180 (97%)	153 (88%)	21 (12%)	4	20
10	J	142/142 (100%)	126 (89%)	16 (11%)	4	23
11	L	176/176 (100%)	145 (82%)	31 (18%)	1	8
12	M	117/117 (100%)	102 (87%)	15 (13%)	3	19
13	N	171/171 (100%)	152 (89%)	19 (11%)	5	24
14	O	171/171 (100%)	144 (84%)	27 (16%)	2	13
15	P	134/134 (100%)	120 (90%)	14 (10%)	5	26
16	Q	163/163 (100%)	145 (89%)	18 (11%)	5	24
17	R	159/159 (100%)	140 (88%)	19 (12%)	4	21
18	S	156/156 (100%)	132 (85%)	24 (15%)	2	14
19	T	139/139 (100%)	122 (88%)	17 (12%)	4	20
20	U	89/89 (100%)	82 (92%)	7 (8%)	10	35
21	V	101/101 (100%)	84 (83%)	17 (17%)	1	10
22	W	55/55 (100%)	50 (91%)	5 (9%)	7	30
23	X	107/107 (100%)	97 (91%)	10 (9%)	7	30
24	Y	124/124 (100%)	107 (86%)	17 (14%)	3	17
25	Z	117/117 (100%)	109 (93%)	8 (7%)	13	41
26	a	119/119 (100%)	107 (90%)	12 (10%)	6	27
27	b	62/62 (100%)	57 (92%)	5 (8%)	9	34
28	c	79/79 (100%)	66 (84%)	13 (16%)	2	11
29	d	98/98 (100%)	82 (84%)	16 (16%)	2	11
30	e	114/114 (100%)	99 (87%)	15 (13%)	3	18
31	f	88/88 (100%)	76 (86%)	12 (14%)	3	18
32	g	98/98 (100%)	83 (85%)	15 (15%)	2	14
33	h	109/109 (100%)	97 (89%)	12 (11%)	5	24
34	i	86/86 (100%)	81 (94%)	5 (6%)	17	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	j	73/73 (100%)	62 (85%)	11 (15%)	2	14
36	k	64/64 (100%)	56 (88%)	8 (12%)	3	20
37	l	47/47 (100%)	40 (85%)	7 (15%)	2	15
38	m	48/48 (100%)	39 (81%)	9 (19%)	1	7
39	n	22/22 (100%)	18 (82%)	4 (18%)	1	7
40	o	92/92 (100%)	79 (86%)	13 (14%)	3	17
41	p	74/74 (100%)	68 (92%)	6 (8%)	9	34
42	r	109/109 (100%)	88 (81%)	21 (19%)	1	6
43	s	166/166 (100%)	155 (93%)	11 (7%)	14	42
44	t	136/136 (100%)	128 (94%)	8 (6%)	16	45
45	1	13/13 (100%)	12 (92%)	1 (8%)	10	36
52	AA	174/174 (100%)	152 (87%)	22 (13%)	3	19
53	BB	194/194 (100%)	169 (87%)	25 (13%)	3	19
54	CC	183/183 (100%)	155 (85%)	28 (15%)	2	14
55	DD	190/190 (100%)	168 (88%)	22 (12%)	4	22
56	EE	223/223 (100%)	183 (82%)	40 (18%)	1	8
57	FF	161/161 (100%)	126 (78%)	35 (22%)	1	4
58	GG	207/207 (100%)	179 (86%)	28 (14%)	3	18
59	HH	169/169 (100%)	151 (89%)	18 (11%)	5	25
60	II	178/178 (100%)	155 (87%)	23 (13%)	3	19
61	JJ	161/161 (100%)	141 (88%)	20 (12%)	4	20
62	KK	89/89 (100%)	76 (85%)	13 (15%)	2	16
63	LL	136/136 (100%)	110 (81%)	26 (19%)	1	6
64	MM	104/104 (100%)	85 (82%)	19 (18%)	1	7
65	NN	130/130 (100%)	108 (83%)	22 (17%)	1	10
66	OO	106/106 (100%)	81 (76%)	25 (24%)	0	3
67	PP	116/116 (100%)	98 (84%)	18 (16%)	2	13
68	QQ	117/117 (100%)	102 (87%)	15 (13%)	3	19
69	RR	117/117 (100%)	102 (87%)	15 (13%)	3	19
70	SS	119/119 (100%)	100 (84%)	19 (16%)	2	12
71	TT	112/112 (100%)	94 (84%)	18 (16%)	2	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	UU	94/94 (100%)	79 (84%)	15 (16%)	2	12
73	VV	67/67 (100%)	61 (91%)	6 (9%)	8	31
74	WW	112/112 (100%)	99 (88%)	13 (12%)	4	22
75	XX	113/113 (100%)	94 (83%)	19 (17%)	1	10
76	YY	108/108 (100%)	88 (82%)	20 (18%)	1	7
77	ZZ	66/66 (100%)	59 (89%)	7 (11%)	5	25
78	aa	85/85 (100%)	77 (91%)	8 (9%)	7	29
79	bb	75/75 (100%)	62 (83%)	13 (17%)	1	9
80	cc	54/54 (100%)	44 (82%)	10 (18%)	1	7
81	dd	47/47 (100%)	40 (85%)	7 (15%)	2	15
82	ee	47/47 (100%)	39 (83%)	8 (17%)	1	10
83	ff	58/61 (95%)	57 (98%)	1 (2%)	56	75
84	gg	272/272 (100%)	250 (92%)	22 (8%)	9	34
86	ii	358/358 (100%)	324 (90%)	34 (10%)	7	29
87	jj	506/522 (97%)	487 (96%)	19 (4%)	28	58
All	All	10889/10934 (100%)	9508 (87%)	1381 (13%)	6	19

All (1381) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	44	ILE
1	A	49	ILE
1	A	64	ARG
1	A	82	ILE
1	A	96	LEU
1	A	97	ASN
1	A	102	LEU
1	A	125	LYS
1	A	128	ARG
1	A	142	GLU
1	A	158	ILE
1	A	163	ARG
1	A	175	ILE
1	A	180	LEU
1	A	193	ARG
1	A	194	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	200	ARG
1	A	207	VAL
1	A	218	HIS
1	A	221	LYS
1	A	226	ARG
1	A	227	ARG
1	A	233	ARG
1	A	235	VAL
1	A	242	ARG
2	B	4	ARG
2	B	10	ARG
2	B	17	LEU
2	B	19	ARG
2	B	21	ARG
2	B	31	SER
2	B	43	LEU
2	B	56	ILE
2	B	61	ASP
2	B	62	ARG
2	B	66	LYS
2	B	67	VAL
2	B	90	VAL
2	B	97	ARG
2	B	99	LEU
2	B	101	THR
2	B	103	LYS
2	B	115	LYS
2	B	116	ARG
2	B	135	LYS
2	B	138	GLN
2	B	146	LEU
2	B	162	VAL
2	B	167	GLN
2	B	173	LEU
2	B	203	GLN
2	B	213	GLN
2	B	214	ASP
2	B	228	TYR
2	B	244	THR
2	B	248	LEU
2	B	258	HIS
2	B	261	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	262	VAL
2	B	309	LEU
2	B	314	ILE
2	B	329	ASP
2	B	333	LEU
2	B	340	THR
2	B	352	LEU
2	B	356	LYS
2	B	357	ARG
2	B	366	LYS
2	B	381	THR
2	B	383	GLU
3	C	14	LYS
3	C	20	LYS
3	C	44	LEU
3	C	54	VAL
3	C	55	SER
3	C	57	LEU
3	C	66	SER
3	C	71	ARG
3	C	80	ARG
3	C	95	MET
3	C	101	MET
3	C	113	ARG
3	C	114	ARG
3	C	122	TYR
3	C	124	ILE
3	C	144	ILE
3	C	147	VAL
3	C	150	LEU
3	C	155	GLU
3	C	159	GLU
3	C	165	LYS
3	C	175	LYS
3	C	179	ASP
3	C	188	ARG
3	C	193	LYS
3	C	204	ARG
3	C	208	CYS
3	C	222	ARG
3	C	232	VAL
3	C	237	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	246	VAL
3	C	267	TRP
3	C	281	MET
3	C	284	MET
3	C	287	THR
3	C	294	LYS
3	C	307	LYS
3	C	312	ARG
3	C	333	LYS
3	C	342	ARG
3	C	345	ARG
3	C	348	LYS
4	D	4	VAL
4	D	22	ARG
4	D	33	ARG
4	D	37	VAL
4	D	50	ARG
4	D	66	TYR
4	D	89	LYS
4	D	94	ASN
4	D	104	LEU
4	D	110	LEU
4	D	111	ASN
4	D	124	GLU
4	D	128	ASP
4	D	152	ARG
4	D	179	ARG
4	D	189	GLU
4	D	196	ARG
4	D	202	GLN
4	D	206	ASP
4	D	208	MET
4	D	225	GLN
4	D	234	ASP
4	D	248	ARG
4	D	249	GLU
4	D	256	LYS
4	D	264	LYS
4	D	268	ARG
4	D	279	ARG
4	D	293	ARG
5	E	43	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	46	LEU
5	E	52	ARG
5	E	55	ARG
5	E	58	MET
5	E	101	ARG
5	E	105	LEU
5	E	126	ARG
5	E	134	ARG
5	E	136	LEU
5	E	137	ARG
5	E	148	ILE
5	E	162	LYS
5	E	190	VAL
5	E	197	ILE
5	E	206	LYS
5	E	212	TYR
5	E	230	ASP
5	E	233	LYS
5	E	250	ASP
5	E	254	LEU
5	E	282	LEU
5	E	284	PHE
6	F	33	LYS
6	F	41	GLN
6	F	44	LEU
6	F	49	ARG
6	F	68	ARG
6	F	70	GLU
6	F	72	ARG
6	F	76	MET
6	F	82	ASN
6	F	90	LYS
6	F	91	LEU
6	F	100	ILE
6	F	101	ASN
6	F	127	LEU
6	F	137	ILE
6	F	154	GLU
6	F	179	ARG
6	F	181	LEU
6	F	189	MET
6	F	190	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	192	LEU
6	F	201	LYS
6	F	202	ARG
6	F	214	LYS
6	F	216	SER
6	F	234	ASP
6	F	239	GLU
6	F	248	ARG
6	F	249	MET
7	G	28	VAL
7	G	73	ARG
7	G	75	LYS
7	G	81	ASN
7	G	90	GLN
7	G	95	LEU
7	G	106	THR
7	G	110	LYS
7	G	112	GLN
7	G	131	LYS
7	G	148	GLU
7	G	150	LYS
7	G	151	LYS
7	G	154	LEU
7	G	170	LEU
7	G	173	LEU
7	G	175	ARG
7	G	177	MET
7	G	189	ARG
7	G	202	VAL
7	G	210	GLU
7	G	217	LYS
7	G	220	GLU
7	G	240	ASN
8	H	1	MET
8	H	20	LEU
8	H	26	ILE
8	H	28	LYS
8	H	41	ILE
8	H	52	LYS
8	H	54	ARG
8	H	57	VAL
8	H	59	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	66	GLU
8	H	74	CYS
8	H	78	GLN
8	H	98	HIS
8	H	111	LEU
8	H	125	ARG
8	H	128	MET
8	H	129	ARG
8	H	162	GLN
8	H	173	ARG
8	H	177	ASP
8	H	183	GLU
9	I	13	LYS
9	I	35	ASP
9	I	36	LEU
9	I	39	LYS
9	I	43	VAL
9	I	48	LEU
9	I	76	MET
9	I	88	ARG
9	I	116	ARG
9	I	136	MET
9	I	139	ARG
9	I	144	ASN
9	I	153	ARG
9	I	163	GLN
9	I	164	LYS
9	I	180	GLU
9	I	195	CYS
9	I	198	LYS
9	I	202	ASN
9	I	208	LYS
9	I	212	LEU
10	J	15	LEU
10	J	16	ARG
10	J	33	LEU
10	J	34	THR
10	J	49	VAL
10	J	55	TYR
10	J	72	CYS
10	J	90	ARG
10	J	91	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	110	GLN
10	J	111	GLU
10	J	113	ILE
10	J	146	ARG
10	J	151	ILE
10	J	167	GLN
10	J	168	GLN
11	L	10	LEU
11	L	28	GLN
11	L	35	ARG
11	L	49	ARG
11	L	59	VAL
11	L	61	CYS
11	L	64	VAL
11	L	67	HIS
11	L	74	ARG
11	L	77	SER
11	L	92	ARG
11	L	94	ILE
11	L	99	ASP
11	L	107	THR
11	L	111	GLN
11	L	113	ASN
11	L	115	GLN
11	L	121	ARG
11	L	123	LYS
11	L	129	ARG
11	L	130	LYS
11	L	143	GLU
11	L	145	LYS
11	L	158	ARG
11	L	162	LYS
11	L	165	LYS
11	L	186	ARG
11	L	190	ARG
11	L	195	ARG
11	L	198	ARG
11	L	201	GLU
12	M	5	ARG
12	M	8	GLU
12	M	25	VAL
12	M	33	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	M	38	VAL
12	M	48	GLN
12	M	53	LYS
12	M	57	LEU
12	M	61	ILE
12	M	70	GLN
12	M	96	GLU
12	M	105	THR
12	M	118	MET
12	M	119	ARG
12	M	130	LEU
13	N	9	GLU
13	N	17	ASP
13	N	26	ARG
13	N	32	GLN
13	N	61	ILE
13	N	64	ILE
13	N	72	LYS
13	N	77	LYS
13	N	80	THR
13	N	87	HIS
13	N	89	VAL
13	N	104	GLU
13	N	108	ARG
13	N	136	ASP
13	N	147	ASP
13	N	174	LEU
13	N	197	THR
13	N	199	GLN
13	N	202	ARG
14	O	5	GLN
14	O	18	ARG
14	O	31	ARG
14	O	36	VAL
14	O	37	ARG
14	O	38	CYS
14	O	42	ASN
14	O	49	ARG
14	O	60	LYS
14	O	61	ARG
14	O	62	MET
14	O	67	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	O	74	ARG
14	O	82	ARG
14	O	85	ARG
14	O	103	LYS
14	O	117	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	187	LYS
14	O	195	VAL
14	O	201	PHE
14	O	202	LEU
15	P	5	SER
15	P	7	ASP
15	P	25	HIS
15	P	57	CYS
15	P	69	ARG
15	P	86	LYS
15	P	91	LEU
15	P	92	LEU
15	P	99	GLU
15	P	100	SER
15	P	105	LYS
15	P	127	ARG
15	P	128	ARG
15	P	147	GLU
16	Q	13	VAL
16	Q	31	LEU
16	Q	37	ARG
16	Q	54	SER
16	Q	63	LEU
16	Q	75	ARG
16	Q	78	LYS
16	Q	85	THR
16	Q	89	ASP
16	Q	91	ARG
16	Q	93	GLN
16	Q	95	VAL
16	Q	97	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	Q	108	ARG
16	Q	112	ARG
16	Q	140	SER
16	Q	143	ARG
16	Q	187	LYS
17	R	10	LEU
17	R	15	LEU
17	R	39	GLN
17	R	40	GLN
17	R	43	LYS
17	R	50	ILE
17	R	52	ARG
17	R	75	HIS
17	R	89	MET
17	R	98	ARG
17	R	99	MET
17	R	106	LEU
17	R	107	ARG
17	R	113	LYS
17	R	117	ARG
17	R	123	LEU
17	R	133	LYS
17	R	138	LEU
17	R	178	GLN
18	S	2	LYS
18	S	8	ARG
18	S	9	GLU
18	S	17	LEU
18	S	39	VAL
18	S	43	ARG
18	S	67	VAL
18	S	70	LYS
18	S	82	LEU
18	S	83	ARG
18	S	84	TYR
18	S	86	SER
18	S	91	HIS
18	S	95	ARG
18	S	98	ARG
18	S	100	LEU
18	S	102	THR
18	S	125	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	S	127	MET
18	S	132	ILE
18	S	147	ASP
18	S	149	LYS
18	S	156	HIS
18	S	159	LEU
19	T	5	LYS
19	T	9	ARG
19	T	17	ARG
19	T	33	ILE
19	T	41	ASP
19	T	52	MET
19	T	60	LYS
19	T	81	LYS
19	T	96	ILE
19	T	99	SER
19	T	117	LYS
19	T	118	GLU
19	T	131	GLN
19	T	142	ARG
19	T	144	ASN
19	T	157	GLU
19	T	159	MET
20	U	33	ILE
20	U	46	ARG
20	U	65	ARG
20	U	67	LYS
20	U	80	LYS
20	U	97	ARG
20	U	99	TRP
21	V	15	ARG
21	V	18	LEU
21	V	31	ASN
21	V	35	LYS
21	V	46	LYS
21	V	51	ARG
21	V	57	VAL
21	V	60	MET
21	V	61	VAL
21	V	82	ILE
21	V	91	LYS
21	V	97	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	V	99	GLU
21	V	106	VAL
21	V	109	LYS
21	V	113	LYS
21	V	123	LYS
22	W	4	GLU
22	W	27	LYS
22	W	41	LEU
22	W	43	LYS
22	W	57	ARG
23	X	39	LYS
23	X	41	ARG
23	X	50	LYS
23	X	52	LEU
23	X	59	LYS
23	X	94	ASN
23	X	111	GLN
23	X	129	ARG
23	X	145	ASP
23	X	152	LYS
24	Y	2	LYS
24	Y	7	VAL
24	Y	8	THR
24	Y	28	LYS
24	Y	34	LEU
24	Y	50	ARG
24	Y	52	ASP
24	Y	55	VAL
24	Y	59	ARG
24	Y	65	GLN
24	Y	72	GLN
24	Y	74	TYR
24	Y	79	VAL
24	Y	87	ARG
24	Y	104	VAL
24	Y	115	ARG
24	Y	126	ARG
25	Z	11	VAL
25	Z	17	ARG
25	Z	57	MET
25	Z	59	LYS
25	Z	67	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	Z	93	LYS
25	Z	108	ARG
25	Z	112	ARG
26	a	10	LYS
26	a	12	ARG
26	a	39	HIS
26	a	40	HIS
26	a	46	ASP
26	a	47	LYS
26	a	52	TYR
26	a	59	ARG
26	a	63	LEU
26	a	84	GLU
26	a	122	VAL
26	a	132	ARG
27	b	22	LYS
27	b	28	ARG
27	b	39	PHE
27	b	43	MET
27	b	51	LYS
28	c	28	VAL
28	c	37	MET
28	c	40	GLN
28	c	50	ASN
28	c	59	GLU
28	c	61	GLU
28	c	77	ASN
28	c	78	ASN
28	c	81	LEU
28	c	87	LYS
28	c	91	VAL
28	c	94	LEU
28	c	98	ASP
29	d	19	GLU
29	d	23	ARG
29	d	26	THR
29	d	31	LYS
29	d	36	VAL
29	d	44	ARG
29	d	48	GLU
29	d	75	LYS
29	d	78	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	d	79	ASN
29	d	85	ARG
29	d	90	ARG
29	d	94	GLU
29	d	102	LEU
29	d	107	THR
29	d	116	ASN
30	e	11	LYS
30	e	21	ILE
30	e	22	ARG
30	e	24	GLN
30	e	30	LYS
30	e	32	LYS
30	e	46	ARG
30	e	48	ARG
30	e	64	LYS
30	e	78	LEU
30	e	91	CYS
30	e	104	SER
30	e	106	LYS
30	e	107	ASN
30	e	113	GLU
31	f	16	ARG
31	f	33	VAL
31	f	36	ARG
31	f	38	GLU
31	f	40	GLU
31	f	46	ARG
31	f	52	LYS
31	f	56	ASN
31	f	69	VAL
31	f	84	VAL
31	f	100	ARG
31	f	101	ILE
32	g	5	LEU
32	g	6	THR
32	g	11	LEU
32	g	14	ASN
32	g	15	THR
32	g	21	ARG
32	g	32	TYR
32	g	54	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	g	60	ARG
32	g	64	LEU
32	g	66	ARG
32	g	73	HIS
32	g	90	ARG
32	g	100	GLN
32	g	115	LYS
33	h	10	ARG
33	h	28	LEU
33	h	46	LYS
33	h	65	GLN
33	h	67	GLU
33	h	88	THR
33	h	89	ARG
33	h	97	LYS
33	h	104	THR
33	h	117	ARG
33	h	121	VAL
33	h	122	LYS
34	i	33	LEU
34	i	86	LYS
34	i	87	ARG
34	i	89	GLU
34	i	103	LYS
35	j	2	THR
35	j	3	LYS
35	j	15	THR
35	j	20	ARG
35	j	25	LYS
35	j	29	LEU
35	j	33	THR
35	j	61	THR
35	j	63	ARG
35	j	68	LYS
35	j	79	ARG
36	k	18	LYS
36	k	29	LYS
36	k	31	ASN
36	k	37	ARG
36	k	39	SER
36	k	57	LYS
36	k	69	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	k	70	LYS
37	l	8	ARG
37	l	16	LYS
37	l	17	GLN
37	l	21	ARG
37	l	36	ARG
37	l	46	ARG
37	l	49	LEU
38	m	79	GLU
38	m	82	LEU
38	m	85	LEU
38	m	88	LYS
38	m	97	ARG
38	m	98	LYS
38	m	106	ARG
38	m	111	ARG
38	m	119	ASN
39	n	2	ARG
39	n	9	ARG
39	n	13	LEU
39	n	21	ARG
40	o	17	LYS
40	o	24	THR
40	o	26	TYR
40	o	31	ASP
40	o	33	LEU
40	o	36	GLN
40	o	55	ILE
40	o	61	LYS
40	o	69	ARG
40	o	82	MET
40	o	89	LYS
40	o	96	ASP
40	o	102	GLN
41	p	16	THR
41	p	24	LYS
41	p	49	ARG
41	p	54	ILE
41	p	60	CYS
41	p	84	ARG
42	r	17	LEU
42	r	18	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	r	20	ARG
42	r	21	ASN
42	r	24	THR
42	r	26	SER
42	r	28	GLU
42	r	31	ASN
42	r	32	LEU
42	r	37	SER
42	r	39	ARG
42	r	41	ASN
42	r	60	VAL
42	r	67	ARG
42	r	70	GLN
42	r	71	ARG
42	r	80	THR
42	r	103	HIS
42	r	107	ARG
42	r	108	MET
42	r	118	LEU
43	s	38	LYS
43	s	44	ARG
43	s	62	ARG
43	s	68	HIS
43	s	94	ASP
43	s	133	GLU
43	s	146	LYS
43	s	149	ARG
43	s	174	LEU
43	s	185	PHE
43	s	191	GLN
44	t	1	MET
44	t	14	TYR
44	t	40	LYS
44	t	95	GLN
44	t	104	ILE
44	t	106	PHE
44	t	114	ARG
44	t	123	ARG
45	1	63	SER
52	AA	8	LEU
52	AA	9	GLN
52	AA	14	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	AA	23	THR
52	AA	32	PHE
52	AA	39	TYR
52	AA	41	ARG
52	AA	44	ASP
52	AA	46	ILE
52	AA	53	ARG
52	AA	58	LEU
52	AA	60	LEU
52	AA	79	SER
52	AA	111	GLN
52	AA	113	GLN
52	AA	131	HIS
52	AA	136	GLU
52	AA	142	LEU
52	AA	150	THR
52	AA	158	ASP
52	AA	178	LEU
52	AA	200	ASP
53	BB	27	LYS
53	BB	38	MET
53	BB	43	ASN
53	BB	47	THR
53	BB	51	ARG
53	BB	55	THR
53	BB	56	LYS
53	BB	63	LYS
53	BB	78	GLU
53	BB	82	ARG
53	BB	86	LEU
53	BB	105	LEU
53	BB	126	ASP
53	BB	134	LEU
53	BB	136	ARG
53	BB	139	CYS
53	BB	142	PHE
53	BB	143	THR
53	BB	150	ILE
53	BB	151	ARG
53	BB	157	GLN
53	BB	163	GLN
53	BB	169	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	BB	212	VAL
53	BB	213	ARG
54	CC	66	LEU
54	CC	78	LEU
54	CC	79	GLU
54	CC	107	LEU
54	CC	110	MET
54	CC	114	LYS
54	CC	120	GLN
54	CC	121	ARG
54	CC	137	VAL
54	CC	152	ARG
54	CC	166	ARG
54	CC	167	ARG
54	CC	182	CYS
54	CC	183	LYS
54	CC	192	LEU
54	CC	202	THR
54	CC	208	PRO
54	CC	227	TRP
54	CC	230	THR
54	CC	233	LEU
54	CC	240	THR
54	CC	247	THR
54	CC	248	TYR
54	CC	251	LEU
54	CC	254	ASP
54	CC	257	LYS
54	CC	262	THR
54	CC	275	LYS
55	DD	9	ARG
55	DD	22	ASN
55	DD	31	GLU
55	DD	40	ARG
55	DD	42	THR
55	DD	59	LEU
55	DD	64	ARG
55	DD	72	VAL
55	DD	76	ARG
55	DD	94	ARG
55	DD	107	TYR
55	DD	113	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	DD	117	ARG
55	DD	120	TYR
55	DD	142	LEU
55	DD	154	ASP
55	DD	156	LEU
55	DD	167	TYR
55	DD	176	LEU
55	DD	190	LEU
55	DD	212	GLU
55	DD	221	THR
56	EE	3	ARG
56	EE	12	VAL
56	EE	17	HIS
56	EE	24	THR
56	EE	32	SER
56	EE	33	THR
56	EE	38	LEU
56	EE	42	LEU
56	EE	49	ARG
56	EE	53	LYS
56	EE	54	TYR
56	EE	59	ASP
56	EE	65	CYS
56	EE	66	MET
56	EE	67	GLN
56	EE	73	ASP
56	EE	92	ILE
56	EE	95	THR
56	EE	100	ARG
56	EE	105	THR
56	EE	123	LEU
56	EE	130	PHE
56	EE	148	ARG
56	EE	165	GLU
56	EE	169	ILE
56	EE	171	ASP
56	EE	174	LYS
56	EE	176	ASP
56	EE	181	CYS
56	EE	182	MET
56	EE	198	ARG
56	EE	205	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	EE	207	VAL
56	EE	220	THR
56	EE	222	LEU
56	EE	225	ILE
56	EE	240	ARG
56	EE	244	ILE
56	EE	250	GLU
56	EE	259	LYS
57	FF	35	LEU
57	FF	36	GLN
57	FF	43	GLU
57	FF	47	LYS
57	FF	63	LYS
57	FF	73	THR
57	FF	76	MET
57	FF	78	MET
57	FF	79	HIS
57	FF	88	MET
57	FF	89	THR
57	FF	91	ARG
57	FF	93	VAL
57	FF	95	HIS
57	FF	103	LEU
57	FF	106	GLU
57	FF	118	ASN
57	FF	125	SER
57	FF	126	THR
57	FF	130	ARG
57	FF	136	ARG
57	FF	141	VAL
57	FF	145	ARG
57	FF	149	GLN
57	FF	152	TRP
57	FF	160	GLU
57	FF	168	THR
57	FF	171	GLU
57	FF	173	LEU
57	FF	179	ASN
57	FF	187	SER
57	FF	190	ILE
57	FF	194	ASP
57	FF	203	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	FF	204	ARG
58	GG	14	LYS
58	GG	15	LEU
58	GG	30	LYS
58	GG	50	VAL
58	GG	56	ASN
58	GG	58	LYS
58	GG	64	LYS
58	GG	68	LEU
58	GG	76	LEU
58	GG	120	ASP
58	GG	121	ILE
58	GG	128	THR
58	GG	132	ARG
58	GG	136	LYS
58	GG	137	ARG
58	GG	143	LYS
58	GG	164	LYS
58	GG	172	LYS
58	GG	178	ARG
58	GG	183	ARG
58	GG	190	ARG
58	GG	191	ARG
58	GG	196	LYS
58	GG	208	GLU
58	GG	216	ARG
58	GG	224	ARG
58	GG	227	GLN
58	GG	235	SER
59	HH	7	LYS
59	HH	34	SER
59	HH	35	ASP
59	HH	36	LEU
59	HH	72	PHE
59	HH	74	LYS
59	HH	82	GLU
59	HH	87	PHE
59	HH	95	ILE
59	HH	106	ARG
59	HH	109	ARG
59	HH	119	SER
59	HH	120	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	HH	121	THR
59	HH	145	ARG
59	HH	148	LEU
59	HH	153	LEU
59	HH	172	THR
60	II	12	ARG
60	II	21	TYR
60	II	23	LYS
60	II	52	ASN
60	II	70	GLU
60	II	74	ARG
60	II	76	THR
60	II	82	VAL
60	II	86	SER
60	II	88	ASN
60	II	96	LEU
60	II	100	CYS
60	II	111	GLN
60	II	115	SER
60	II	123	ARG
60	II	130	THR
60	II	140	LYS
60	II	153	LYS
60	II	162	LEU
60	II	168	GLN
60	II	196	GLU
60	II	203	LYS
60	II	206	LYS
61	JJ	21	GLU
61	JJ	29	LEU
61	JJ	39	ASN
61	JJ	42	GLU
61	JJ	45	ARG
61	JJ	65	GLU
61	JJ	69	ARG
61	JJ	86	VAL
61	JJ	101	LYS
61	JJ	110	LEU
61	JJ	116	LYS
61	JJ	127	ARG
61	JJ	131	ARG
61	JJ	133	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
61	JJ	135	ILE
61	JJ	136	ARG
61	JJ	138	ARG
61	JJ	162	ARG
61	JJ	172	ARG
61	JJ	176	LYS
62	KK	1	MET
62	KK	2	LEU
62	KK	13	GLU
62	KK	16	PHE
62	KK	43	LEU
62	KK	50	GLN
62	KK	60	GLU
62	KK	65	ARG
62	KK	66	HIS
62	KK	70	TYR
62	KK	74	GLU
62	KK	80	ARG
62	KK	89	ILE
63	LL	8	ARG
63	LL	16	ILE
63	LL	18	GLN
63	LL	22	ARG
63	LL	31	GLU
63	LL	40	ILE
63	LL	56	ILE
63	LL	66	VAL
63	LL	67	SER
63	LL	69	ARG
63	LL	74	SER
63	LL	76	VAL
63	LL	78	THR
63	LL	85	THR
63	LL	90	ARG
63	LL	91	ASP
63	LL	97	ARG
63	LL	106	HIS
63	LL	109	MET
63	LL	111	VAL
63	LL	114	SER
63	LL	121	GLN
63	LL	126	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
63	LL	134	LEU
63	LL	135	SER
63	LL	147	LYS
64	MM	12	MET
64	MM	26	LEU
64	MM	27	ILE
64	MM	31	LEU
64	MM	33	ARG
64	MM	36	ARG
64	MM	45	ARG
64	MM	48	HIS
64	MM	60	MET
64	MM	73	GLN
64	MM	74	ILE
64	MM	77	ILE
64	MM	78	LYS
64	MM	83	LYS
64	MM	88	TRP
64	MM	96	ARG
64	MM	101	ARG
64	MM	114	TYR
64	MM	127	TYR
65	NN	5	HIS
65	NN	13	GLN
65	NN	25	TRP
65	NN	27	LYS
65	NN	52	VAL
65	NN	57	SER
65	NN	64	ARG
65	NN	70	LYS
65	NN	75	LEU
65	NN	76	LYS
65	NN	78	LYS
65	NN	84	LEU
65	NN	86	GLU
65	NN	94	LYS
65	NN	102	LEU
65	NN	107	LYS
65	NN	110	ASP
65	NN	114	ARG
65	NN	120	SER
65	NN	121	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
65	NN	125	LEU
65	NN	142	GLU
66	OO	34	PHE
66	OO	38	ASN
66	OO	39	ASP
66	OO	50	LYS
66	OO	51	GLU
66	OO	53	ILE
66	OO	61	LYS
66	OO	65	ASP
66	OO	69	SER
66	OO	80	ASP
66	OO	81	VAL
66	OO	85	CYS
66	OO	100	THR
66	OO	104	ARG
66	OO	106	LYS
66	OO	107	THR
66	OO	121	ARG
66	OO	128	ARG
66	OO	130	GLU
66	OO	131	ASP
66	OO	133	THR
66	OO	137	SER
66	OO	142	ARG
66	OO	146	ARG
66	OO	151	LEU
67	PP	5	GLU
67	PP	7	LYS
67	PP	10	ARG
67	PP	17	TYR
67	PP	21	ASP
67	PP	28	MET
67	PP	29	SER
67	PP	30	TYR
67	PP	37	TYR
67	PP	40	ARG
67	PP	43	ARG
67	PP	44	ARG
67	PP	52	LYS
67	PP	65	LYS
67	PP	88	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	PP	100	LYS
67	PP	107	ILE
67	PP	121	ILE
68	QQ	20	THR
68	QQ	26	LYS
68	QQ	41	MET
68	QQ	47	LEU
68	QQ	73	LYS
68	QQ	85	ARG
68	QQ	89	SER
68	QQ	90	LYS
68	QQ	97	GLN
68	QQ	119	LEU
68	QQ	126	ARG
68	QQ	131	LYS
68	QQ	140	ARG
68	QQ	145	TYR
68	QQ	146	ARG
69	RR	43	SER
69	RR	47	ARG
69	RR	58	MET
69	RR	77	GLU
69	RR	78	ARG
69	RR	79	GLU
69	RR	82	ASP
69	RR	87	GLU
69	RR	88	VAL
69	RR	99	ASP
69	RR	101	ASP
69	RR	109	LEU
69	RR	118	GLN
69	RR	121	GLN
69	RR	127	ASN
70	SS	7	GLU
70	SS	8	LYS
70	SS	10	GLN
70	SS	14	ARG
70	SS	17	ASN
70	SS	34	LYS
70	SS	52	LEU
70	SS	59	LEU
70	SS	63	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
70	SS	78	LYS
70	SS	81	ASP
70	SS	82	TRP
70	SS	86	ARG
70	SS	113	ARG
70	SS	115	LYS
70	SS	118	ARG
70	SS	131	VAL
70	SS	134	GLN
70	SS	136	THR
71	TT	4	VAL
71	TT	8	ASP
71	TT	28	LEU
71	TT	35	ASP
71	TT	37	VAL
71	TT	39	LEU
71	TT	62	ARG
71	TT	67	ARG
71	TT	74	SER
71	TT	84	ARG
71	TT	92	PHE
71	TT	93	SER
71	TT	102	ARG
71	TT	108	GLU
71	TT	121	ARG
71	TT	123	LEU
71	TT	124	THR
71	TT	128	GLN
72	UU	31	SER
72	UU	33	GLU
72	UU	36	CYS
72	UU	48	LEU
72	UU	49	LYS
72	UU	51	LYS
72	UU	55	ARG
72	UU	56	MET
72	UU	62	ARG
72	UU	68	THR
72	UU	81	GLN
72	UU	84	ILE
72	UU	93	SER
72	UU	111	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
72	UU	118	ASP
73	VV	9	VAL
73	VV	11	LEU
73	VV	31	SER
73	VV	38	GLU
73	VV	40	ASP
73	VV	74	LYS
74	WW	3	ARG
74	WW	22	LYS
74	WW	23	ARG
74	WW	25	VAL
74	WW	36	ARG
74	WW	74	VAL
74	WW	80	ASP
74	WW	83	LEU
74	WW	103	VAL
74	WW	104	LEU
74	WW	110	ILE
74	WW	111	MET
74	WW	117	ARG
75	XX	3	LYS
75	XX	4	CYS
75	XX	5	ARG
75	XX	9	THR
75	XX	12	LYS
75	XX	14	ARG
75	XX	29	LYS
75	XX	37	LYS
75	XX	61	GLN
75	XX	67	ARG
75	XX	68	LYS
75	XX	71	ARG
75	XX	98	ASP
75	XX	105	PHE
75	XX	112	VAL
75	XX	115	ILE
75	XX	123	VAL
75	XX	128	VAL
75	XX	130	LEU
76	YY	7	ILE
76	YY	10	ARG
76	YY	14	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
76	YY	16	ARG
76	YY	20	ARG
76	YY	32	LYS
76	YY	40	ILE
76	YY	44	LEU
76	YY	46	LYS
76	YY	61	ARG
76	YY	62	THR
76	YY	69	THR
76	YY	72	PHE
76	YY	74	MET
76	YY	87	PRO
76	YY	98	GLU
76	YY	99	LYS
76	YY	100	LYS
76	YY	107	ARG
76	YY	111	LYS
77	ZZ	44	LEU
77	ZZ	74	SER
77	ZZ	83	LEU
77	ZZ	89	GLN
77	ZZ	93	SER
77	ZZ	110	THR
77	ZZ	114	LYS
78	aa	19	GLN
78	aa	23	CYS
78	aa	26	CYS
78	aa	33	ASP
78	aa	41	ILE
78	aa	51	ARG
78	aa	52	ASP
78	aa	94	ASP
79	bb	3	LEU
79	bb	17	ARG
79	bb	27	SER
79	bb	36	LYS
79	bb	37	CYS
79	bb	44	THR
79	bb	51	GLN
79	bb	60	SER
79	bb	63	LEU
79	bb	72	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	bb	81	ARG
79	bb	83	GLN
79	bb	84	HIS
80	cc	31	ARG
80	cc	34	PHE
80	cc	35	MET
80	cc	58	LEU
80	cc	60	GLU
80	cc	61	SER
80	cc	62	GLU
80	cc	63	ARG
80	cc	67	ARG
80	cc	68	LEU
81	dd	5	GLN
81	dd	6	LEU
81	dd	16	GLN
81	dd	26	ASN
81	dd	27	ARG
81	dd	39	CYS
81	dd	54	LYS
82	ee	15	GLN
82	ee	18	LYS
82	ee	24	LYS
82	ee	34	ARG
82	ee	36	MET
82	ee	41	ARG
82	ee	43	VAL
82	ee	52	LYS
83	ff	81	THR
84	gg	20	GLN
84	gg	29	ASP
84	gg	36	ARG
84	gg	44	LYS
84	gg	47	ARG
84	gg	49	GLU
84	gg	63	SER
84	gg	64	HIS
84	gg	65	PHE
84	gg	93	THR
84	gg	99	ARG
84	gg	100	ARG
84	gg	107	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
84	gg	143	GLN
84	gg	156	PHE
84	gg	172	LYS
84	gg	186	THR
84	gg	234	ASP
84	gg	282	GLU
84	gg	289	LEU
84	gg	298	LEU
84	gg	306	LEU
86	ii	45	ILE
86	ii	61	ASN
86	ii	65	ARG
86	ii	67	ASN
86	ii	80	GLN
86	ii	82	LEU
86	ii	86	ASN
86	ii	103	GLU
86	ii	111	ASN
86	ii	112	ILE
86	ii	128	ASP
86	ii	136	LEU
86	ii	139	LEU
86	ii	164	ASN
86	ii	165	THR
86	ii	167	GLU
86	ii	179	LYS
86	ii	180	HIS
86	ii	182	ARG
86	ii	186	SER
86	ii	211	GLN
86	ii	212	LEU
86	ii	231	ASP
86	ii	232	PHE
86	ii	241	MET
86	ii	246	LEU
86	ii	255	ASP
86	ii	300	LYS
86	ii	333	LEU
86	ii	339	GLU
86	ii	340	GLU
86	ii	361	GLU
86	ii	368	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
86	ii	415	TYR
87	jj	52	GLU
87	jj	75	LEU
87	jj	90	ASN
87	jj	106	LEU
87	jj	131	LEU
87	jj	161	GLU
87	jj	248	ASP
87	jj	250	LYS
87	jj	289	LEU
87	jj	296	TYR
87	jj	320	GLU
87	jj	374	ILE
87	jj	399	ASP
87	jj	411	TYR
87	jj	455	ILE
87	jj	486	ASP
87	jj	494	SER
87	jj	567	ARG
87	jj	574	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	217	GLN
7	G	29	ASN
42	r	103	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	20 (27%)	1 (1%)
47	3	72/75 (96%)	36 (50%)	7 (9%)
48	5	3645/3662 (99%)	1179 (32%)	269 (7%)
49	7	119/120 (99%)	19 (15%)	1 (0%)
50	8	155/156 (99%)	52 (33%)	6 (3%)
51	9	1711/1719 (99%)	608 (35%)	129 (7%)
85	hh	11/12 (91%)	7 (63%)	0
All	All	5787/5820 (99%)	1921 (33%)	413 (7%)

All (1921) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	7	G
46	2	8	U
46	2	9	A
46	2	13	U
46	2	16	C
46	2	19	G
46	2	20(A)	U
46	2	21	A
46	2	31	C
46	2	35	A
46	2	42	A
46	2	47	U
46	2	49	C
46	2	58	A
46	2	60	A
46	2	61	C
46	2	67	G
46	2	72	C
46	2	75	C
46	2	76	A
47	3	2	C
47	3	5	G
47	3	7	A
47	3	8	U
47	3	9	A
47	3	10	G
47	3	13	C
47	3	21	A
47	3	22	G
47	3	29	A
47	3	30	G
47	3	31	A
47	3	34	U
47	3	35	U
47	3	38	A
47	3	39	U
47	3	41	U
47	3	42	G
47	3	47	U
47	3	48	C
47	3	49	C
47	3	58	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	3	60	U
47	3	61	C
47	3	63	C
47	3	65	G
47	3	67	U
47	3	68	C
47	3	69	G
47	3	70	G
47	3	71	G
47	3	72	C
47	3	73	G
47	3	74	C
47	3	75	C
47	3	76	A
48	5	2	G
48	5	8	U
48	5	9	C
48	5	10	A
48	5	12	A
48	5	13	U
48	5	21	G
48	5	25	A
48	5	30	C
48	5	39	A
48	5	42	A
48	5	43	U
48	5	44	A
48	5	48	G
48	5	49	U
48	5	56	A
48	5	58	G
48	5	59	A
48	5	64	A
48	5	65	A
48	5	69	A
48	5	71	C
48	5	72	C
48	5	73	A
48	5	74	G
48	5	91	G
48	5	93	G
48	5	94	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	95	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	121	A
48	5	126	C
48	5	128	C
48	5	129	C
48	5	134	G
48	5	135	G
48	5	136	C
48	5	143	C
48	5	144	G
48	5	146	G
48	5	157	U
48	5	159	C
48	5	160	G
48	5	161	G
48	5	164	G
48	5	166	C
48	5	167	C
48	5	170	C
48	5	171	U
48	5	172	C
48	5	173	C
48	5	174	C
48	5	175	C
48	5	177	G
48	5	183	C
48	5	184	U
48	5	185	C
48	5	186	G
48	5	187	U
48	5	188	G
48	5	189	G
48	5	197	A
48	5	200	U
48	5	201	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	203	U
48	5	205	C
48	5	209	U
48	5	210	C
48	5	216	C
48	5	217	C
48	5	218	A
48	5	219	G
48	5	220	C
48	5	221	C
48	5	224	U
48	5	226	G
48	5	227	A
48	5	233	U
48	5	234	G
48	5	246	G
48	5	253	G
48	5	255	C
48	5	257	C
48	5	265	C
48	5	266	C
48	5	267	G
48	5	272	U
48	5	276	C
48	5	277	G
48	5	278	G
48	5	280	G
48	5	286	U
48	5	296	A
48	5	297	U
48	5	300	A
48	5	306	A
48	5	309	C
48	5	315	G
48	5	316	U
48	5	319	A
48	5	321	U
48	5	322	C
48	5	326	C
48	5	328	A
48	5	334	A
48	5	337	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	340	C
48	5	347	A
48	5	349	A
48	5	350	C
48	5	353	A
48	5	357	U
48	5	361	C
48	5	362	A
48	5	363	A
48	5	385	A
48	5	386	A
48	5	387	G
48	5	399	G
48	5	405	U
48	5	406	C
48	5	407	A
48	5	409	G
48	5	410	A
48	5	412	G
48	5	413	G
48	5	424	U
48	5	429	A
48	5	431	G
48	5	432	U
48	5	434	A
48	5	446	C
48	5	448	G
48	5	449	C
48	5	451	C
48	5	452	A
48	5	453	G
48	5	454	U
48	5	455	C
48	5	458	C
48	5	465	G
48	5	467	U
48	5	468	U
48	5	469	C
48	5	470	A
48	5	473	C
48	5	485	C
48	5	486	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	487	G
48	5	498	C
48	5	499	G
48	5	500	G
48	5	501	C
48	5	502	C
48	5	503	C
48	5	504	G
48	5	506	C
48	5	509	A
48	5	510	U
48	5	513	U
48	5	514	U
48	5	515	C
48	5	519	C
48	5	649	A
48	5	654	C
48	5	655	C
48	5	663	G
48	5	664	G
48	5	665	C
48	5	666	G
48	5	667	A
48	5	668	C
48	5	682	G
48	5	684	G
48	5	685	C
48	5	686	A
48	5	690	C
48	5	694	C
48	5	695	G
48	5	696	C
48	5	697	G
48	5	701	G
48	5	703	G
48	5	707	C
48	5	718	C
48	5	721	G
48	5	722	G
48	5	724	C
48	5	728	U
48	5	729	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	730	G
48	5	737	C
48	5	742	G
48	5	745	G
48	5	746	A
48	5	747	A
48	5	748	G
48	5	749	G
48	5	756	G
48	5	911	U
48	5	914	U
48	5	915	A
48	5	917	A
48	5	918	G
48	5	919	C
48	5	920	C
48	5	925	C
48	5	927	G
48	5	928	C
48	5	929	A
48	5	930	G
48	5	931	C
48	5	932	A
48	5	933	G
48	5	934	C
48	5	935	A
48	5	936	C
48	5	937	U
48	5	938	C
48	5	939	G
48	5	940	C
48	5	942	G
48	5	943	A
48	5	944	A
48	5	945	U
48	5	946	C
48	5	947	C
48	5	957	G
48	5	958	G
48	5	960	A
48	5	961	G
48	5	962	C

Continued on next page...

Continued from previous page...

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	970	G
48	5	971	U
48	5	972	C
48	5	973	G
48	5	976	G
48	5	977	C
48	5	978	G
48	5	979	C
48	5	982	U
48	5	983	C
48	5	984	C
48	5	989	U
48	5	990	C
48	5	992	C
48	5	1051	G
48	5	1070	G
48	5	1072	C
48	5	1073	G
48	5	1075	G
48	5	1076	C
48	5	1083	U
48	5	1097	C
48	5	1175	A
48	5	1176	C
48	5	1177	U
48	5	1181	C
48	5	1182	C
48	5	1183	C
48	5	1193	C
48	5	1204	C
48	5	1209	U
48	5	1211	G
48	5	1212	G
48	5	1214	C
48	5	1215	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	1219	G
48	5	1221	G
48	5	1222	A
48	5	1233	G
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	1240	G
48	5	1241	C
48	5	1242	G
48	5	1243	C
48	5	1244	G
48	5	1245	C
48	5	1255	A
48	5	1256	G
48	5	1259	G
48	5	1266	G
48	5	1267	C
48	5	1268	G
48	5	1269	G
48	5	1270	A
48	5	1272	C
48	5	1273	G
48	5	1274	A
48	5	1275	G
48	5	1279	A
48	5	1280	C
48	5	1281	G
48	5	1285	U
48	5	1286	C
48	5	1287	G
48	5	1288	G
48	5	1289	C
48	5	1293	G
48	5	1294	A
48	5	1295	C
48	5	1296	G
48	5	1297	U
48	5	1301	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	1303	A
48	5	1304	C
48	5	1313	C
48	5	1326	A
48	5	1330	A
48	5	1337	A
48	5	1344	C
48	5	1354	A
48	5	1358	G
48	5	1364	U
48	5	1365	C
48	5	1366	G
48	5	1367	C
48	5	1368	A
48	5	1369	C
48	5	1370	G
48	5	1371	A
48	5	1372	A
48	5	1376	C
48	5	1377	G
48	5	1378	C
48	5	1379	C
48	5	1380	G
48	5	1381	U
48	5	1387	A
48	5	1390	G
48	5	1394	G
48	5	1397	A
48	5	1398	A
48	5	1399	G
48	5	1407	C
48	5	1408	G
48	5	1409	C
48	5	1410	U
48	5	1411	C
48	5	1413	C
48	5	1414	C
48	5	1416	G
48	5	1418	C
48	5	1420	A
48	5	1421	G
48	5	1429	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	1432	G
48	5	1435	G
48	5	1436	C
48	5	1439	C
48	5	1440	U
48	5	1441	C
48	5	1442	C
48	5	1445	U
48	5	1446	C
48	5	1448	G
48	5	1449	C
48	5	1455	G
48	5	1456	C
48	5	1457	G
48	5	1475	G
48	5	1477	C
48	5	1478	C
48	5	1481	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	1501	C
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	1524	A
48	5	1533	A
48	5	1534	A
48	5	1547	A
48	5	1563	A
48	5	1564	A
48	5	1566	C
48	5	1568	C
48	5	1578	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	1582	U
48	5	1586	G
48	5	1591	U
48	5	1592	G
48	5	1596	U
48	5	1602	U
48	5	1612	G
48	5	1613	A
48	5	1614	C
48	5	1624	G
48	5	1625	G
48	5	1631	A
48	5	1633	G
48	5	1634	A
48	5	1636	U
48	5	1638	A
48	5	1641	G
48	5	1654	G
48	5	1655	C
48	5	1656	U
48	5	1661	C
48	5	1670	G
48	5	1676	C
48	5	1677	U
48	5	1691	G
48	5	1692	C
48	5	1696	C
48	5	1697	G
48	5	1698	C
48	5	1699	A
48	5	1719	A
48	5	1720	C
48	5	1721	G
48	5	1722	C
48	5	1724	G
48	5	1725	U
48	5	1733	G
48	5	1734	G
48	5	1735	U
48	5	1742	A
48	5	1746	A
48	5	1750	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	1753	G
48	5	1754	U
48	5	1755	C
48	5	1756	U
48	5	1757	U
48	5	1758	G
48	5	1760	G
48	5	1761	G
48	5	1764	G
48	5	1767	A
48	5	1768	C
48	5	1772	C
48	5	1776	A
48	5	1777	C
48	5	1781	U
48	5	1787	A
48	5	1799	G
48	5	1800	U
48	5	1803	G
48	5	1804	A
48	5	1805	A
48	5	1812	C
48	5	1815	G
48	5	1818	G
48	5	1819	G
48	5	1820	C
48	5	1821	G
48	5	1822	U
48	5	1828	C
48	5	1830	G
48	5	1832	C
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1836	G
48	5	1847	C
48	5	1848	C
48	5	1855	G
48	5	1867	A
48	5	1869	G
48	5	1882	U
48	5	1885	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	1886	G
48	5	1889	U
48	5	1892	A
48	5	1897	A
48	5	1899	G
48	5	1900	C
48	5	1910	G
48	5	1918	U
48	5	1919	G
48	5	1920	C
48	5	1921	C
48	5	1922	G
48	5	1923	A
48	5	1931	C
48	5	1947	U
48	5	1952	G
48	5	1955	G
48	5	1956	A
48	5	1957	U
48	5	1958	A
48	5	1959	U
48	5	1960	A
48	5	1961	G
48	5	1964	A
48	5	1968	G
48	5	1969	G
48	5	1975	G
48	5	1976	G
48	5	1977	C
48	5	1979	A
48	5	1980	U
48	5	1981	G
48	5	1983	A
48	5	1984	A
48	5	1985	G
48	5	1986	U
48	5	1987	C
48	5	1988	G
48	5	1990	A
48	5	1991	A
48	5	1992	U
48	5	1993	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	1997	U
48	5	1998	A
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	2010	A
48	5	2011	C
48	5	2019	C
48	5	2020	U
48	5	2021	G
48	5	2024	G
48	5	2025	A
48	5	2026	A
48	5	2027	U
48	5	2028	C
48	5	2044	U
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	2071	A
48	5	2079	G
48	5	2084	C
48	5	2085	G
48	5	2089	G
48	5	2090	U
48	5	2091	C
48	5	2092	G
48	5	2093	A
48	5	2094	G
48	5	2095	A
48	5	2097	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	2100	A
48	5	2101	C
48	5	2103	G
48	5	2107	C
48	5	2108	G
48	5	2109	G
48	5	2110	C
48	5	2111	G
48	5	2112	G
48	5	2113	G
48	5	2114	G
48	5	2115	G
48	5	2116	C
48	5	2117	G
48	5	2118	G
48	5	2119	C
48	5	2120	G
48	5	2122	G
48	5	2123	C
48	5	2124	G
48	5	2125	C
48	5	2126	G
48	5	2127	C
48	5	2129	C
48	5	2130	G
48	5	2131	C
48	5	2247	C
48	5	2248	C
48	5	2250	C
48	5	2251	G
48	5	2252	G
48	5	2253	A
48	5	2254	G
48	5	2255	C
48	5	2256	C
48	5	2257	C
48	5	2258	C
48	5	2259	G
48	5	2260	C
48	5	2261	G
48	5	2263	A
48	5	2264	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	2265	G
48	5	2266	C
48	5	2267	U
48	5	2268	A
48	5	2269	C
48	5	2270	G
48	5	2274	C
48	5	2275	G
48	5	2279	A
48	5	2288	G
48	5	2289	C
48	5	2299	G
48	5	2300	A
48	5	2301	G
48	5	2312	U
48	5	2313	A
48	5	2314	G
48	5	2324	C
48	5	2331	G
48	5	2332	A
48	5	2333	G
48	5	2335	C
48	5	2337	C
48	5	2348	G
48	5	2351	C
48	5	2360	A
48	5	2364	G
48	5	2370	A
48	5	2382	A
48	5	2383	C
48	5	2395	A
48	5	2396	A
48	5	2399	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	2434	G
48	5	2440	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	2441	C
48	5	2447	U
48	5	2450	G
48	5	2458	C
48	5	2469	C
48	5	2471	G
48	5	2473	A
48	5	2474	G
48	5	2475	G
48	5	2485	U
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	2499	C
48	5	2503	G
48	5	2504	C
48	5	2505	C
48	5	2506	G
48	5	2507	A
48	5	2512	A
48	5	2513	A
48	5	2514	G
48	5	2519	U
48	5	2521	G
48	5	2527	A
48	5	2530	U
48	5	2536	A
48	5	2537	A
48	5	2544	G
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	2568	C
48	5	2571	C
48	5	2575	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	2577	C
48	5	2583	C
48	5	2587	A
48	5	2588	C
48	5	2589	C
48	5	2591	A
48	5	2601	A
48	5	2602	G
48	5	2611	A
48	5	2620	G
48	5	2623	A
48	5	2627	C
48	5	2638	G
48	5	2640	G
48	5	2647	A
48	5	2653	C
48	5	2661	U
48	5	2662	G
48	5	2663	G
48	5	2669	C
48	5	2673	G
48	5	2676	A
48	5	2679	G
48	5	2681	G
48	5	2686	G
48	5	2687	U
48	5	2688	G
48	5	2695	A
48	5	2696	A
48	5	2704	C
48	5	2708	U
48	5	2710	C
48	5	2711	G
48	5	2712	G
48	5	2714	G
48	5	2716	C
48	5	2721	G
48	5	2724	G
48	5	2725	A
48	5	2726	G
48	5	2733	C
48	5	2740	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	2743	A
48	5	2754	G
48	5	2755	A
48	5	2756	G
48	5	2760	G
48	5	2761	U
48	5	2762	G
48	5	2767	U
48	5	2768	C
48	5	2769	U
48	5	2770	C
48	5	2772	C
48	5	2787	A
48	5	2788	U
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	2806	A
48	5	2807	A
48	5	2814	C
48	5	2824	C
48	5	2825	A
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	2859	G
48	5	2862	G
48	5	2869	U
48	5	2896	G
48	5	2897	G
48	5	2898	G
48	5	2904	U
48	5	2905	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	2910	G
48	5	3594	C
48	5	3595	U
48	5	3596	A
48	5	3597	G
48	5	3598	C
48	5	3605	C
48	5	3606	U
48	5	3615	G
48	5	3617	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	3668	C
48	5	3670	C
48	5	3671	G
48	5	3673	C
48	5	3674	G
48	5	3680	U
48	5	3682	A
48	5	3689	G
48	5	3692	A
48	5	3696	C
48	5	3698	G
48	5	3702	A
48	5	3709	U
48	5	3710	G
48	5	3711	A
48	5	3712	A
48	5	3717	A
48	5	3718	A
48	5	3722	G
48	5	3728	A
48	5	3729	U
48	5	3737	A
48	5	3740	G
48	5	3748	A
48	5	3750	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	3752	C
48	5	3753	G
48	5	3755	G
48	5	3756	A
48	5	3759	A
48	5	3760	A
48	5	3764	U
48	5	3773	U
48	5	3774	A
48	5	3775	A
48	5	3776	G
48	5	3777	G
48	5	3778	U
48	5	3780	G
48	5	3783	A
48	5	3784	A
48	5	3786	U
48	5	3788	C
48	5	3798	U
48	5	3799	A
48	5	3802	U
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	3836	A
48	5	3838	U
48	5	3839	G
48	5	3840	U
48	5	3859	G
48	5	3867	A
48	5	3877	A
48	5	3878	C
48	5	3879	G
48	5	3889	G
48	5	3897	G
48	5	3900	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	3901	A
48	5	3905	A
48	5	3906	A
48	5	3907	G
48	5	3912	U
48	5	3915	U
48	5	3916	G
48	5	3917	A
48	5	3924	C
48	5	3925	U
48	5	3926	C
48	5	3927	U
48	5	3938	G
48	5	3939	G
48	5	3943	A
48	5	3946	G
48	5	4069	U
48	5	4070	U
48	5	4076	G
48	5	4084	G
48	5	4085	A
48	5	4086	G
48	5	4087	G
48	5	4088	C
48	5	4091	G
48	5	4092	G
48	5	4093	G
48	5	4094	G
48	5	4097	G
48	5	4104	G
48	5	4105	A
48	5	4107	G
48	5	4112	C
48	5	4114	C
48	5	4115	G
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	4125	C
48	5	4127	A
48	5	4134	C
48	5	4143	G
48	5	4144	C
48	5	4145	C
48	5	4155	C
48	5	4161	G
48	5	4162	C
48	5	4163	U
48	5	4165	C
48	5	4166	G
48	5	4168	G
48	5	4170	A
48	5	4171	C
48	5	4182	G
48	5	4183	G
48	5	4184	G
48	5	4191	G
48	5	4203	A
48	5	4208	U
48	5	4212	A
48	5	4213	A
48	5	4216	G
48	5	4217	G
48	5	4218	U
48	5	4219	A
48	5	4225	G
48	5	4226	G
48	5	4229	U
48	5	4232	U
48	5	4233	A
48	5	4238	G
48	5	4241	C
48	5	4251	A
48	5	4254	G
48	5	4258	C
48	5	4265	U
48	5	4266	G
48	5	4267	G
48	5	4268	A
48	5	4271	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	4273	A
48	5	4282	A
48	5	4291	G
48	5	4297	G
48	5	4302	U
48	5	4303	C
48	5	4304	A
48	5	4305	G
48	5	4306	U
48	5	4307	A
48	5	4311	A
48	5	4312	U
48	5	4313	A
48	5	4314	C
48	5	4317	A
48	5	4318	C
48	5	4319	C
48	5	4329	G
48	5	4330	G
48	5	4331	G
48	5	4332	C
48	5	4335	C
48	5	4336	A
48	5	4349	C
48	5	4350	C
48	5	4354	U
48	5	4355	G
48	5	4360	U
48	5	4367	G
48	5	4368	G
48	5	4372	U
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	4394	A
48	5	4395	U
48	5	4396	A
48	5	4398	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	4405	G
48	5	4419	U
48	5	4420	U
48	5	4421	C
48	5	4422	A
48	5	4424	A
48	5	4426	C
48	5	4430	G
48	5	4433	G
48	5	4438	U
48	5	4439	U
48	5	4441	A
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	4464	A
48	5	4471	U
48	5	4472	G
48	5	4473	A
48	5	4475	G
48	5	4476	C
48	5	4481	U
48	5	4482	U
48	5	4484	A
48	5	4488	A
48	5	4491	G
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
48	5	4524	G
48	5	4527	G
48	5	4528	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	4529	G
48	5	4535	A
48	5	4548	A
48	5	4549	G
48	5	4550	G
48	5	4557	U
48	5	4567	G
48	5	4570	G
48	5	4573	G
48	5	4575	G
48	5	4577	U
48	5	4583	C
48	5	4584	A
48	5	4585	U
48	5	4586	G
48	5	4590	A
48	5	4591	U
48	5	4606	G
48	5	4618	G
48	5	4636	U
48	5	4637	G
48	5	4641	U
48	5	4647	G
48	5	4648	A
48	5	4656	A
48	5	4657	U
48	5	4661	G
48	5	4670	C
48	5	4672	A
48	5	4677	U
48	5	4687	A
48	5	4694	G
48	5	4695	C
48	5	4700	A
48	5	4701	A
48	5	4702	G
48	5	4709	U
48	5	4719	G
48	5	4720	C
48	5	4721	G
48	5	4730	C
48	5	4731	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	4732	G
48	5	4733	C
48	5	4734	A
48	5	4737	G
48	5	4741	C
48	5	4745	G
48	5	4746	C
48	5	4749	C
48	5	4750	G
48	5	4753	U
48	5	4754	G
48	5	4756	C
48	5	4758	U
48	5	4760	G
48	5	4764	A
48	5	4768	G
48	5	4770	U
48	5	4771	C
48	5	4774	C
48	5	4869	U
48	5	4871	C
48	5	4872	G
48	5	4873	G
48	5	4874	A
48	5	4875	G
48	5	4876	U
48	5	4877	G
48	5	4878	C
48	5	4883	C
48	5	4884	G
48	5	4885	U
48	5	4886	C
48	5	4889	G
48	5	4890	G
48	5	4893	A
48	5	4895	C
48	5	4896	G
48	5	4898	G
48	5	4900	C
48	5	4901	G
48	5	4904	G
48	5	4906	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	4910	G
48	5	4911	A
48	5	4912	G
48	5	4913	G
48	5	4924	C
48	5	4926	C
48	5	4927	G
48	5	4930	C
48	5	4931	G
48	5	4932	U
48	5	4934	A
48	5	4935	C
48	5	4936	G
48	5	4939	C
48	5	4942	C
48	5	4945	G
48	5	4948	C
48	5	4949	G
48	5	4950	U
48	5	4951	G
48	5	4952	G
48	5	4959	U
48	5	4964	C
48	5	4965	U
48	5	4966	A
48	5	4967	A
48	5	4975	G
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	5007	A
48	5	5013	C
48	5	5014	A
48	5	5017	G
48	5	5018	C
48	5	5022	U
48	5	5023	C
48	5	5024	C
48	5	5025	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	5026	U
48	5	5027	C
48	5	5028	G
48	5	5031	G
48	5	5033	G
48	5	5041	G
48	5	5047	C
48	5	5050	C
48	5	5052	C
48	5	5053	U
48	5	5054	C
48	5	5056	A
48	5	5058	A
48	5	5060	A
48	5	5061	A
48	5	5062	G
48	5	5066	U
49	7	7	G
49	7	11	A
49	7	21	G
49	7	25	G
49	7	33	U
49	7	40	U
49	7	51	G
49	7	53	U
49	7	54	A
49	7	64	G
49	7	74	A
49	7	76	U
49	7	97	G
49	7	99	G
49	7	100	A
49	7	106	G
49	7	110	G
49	7	111	C
49	7	120	U
50	8	2	G
50	8	3	A
50	8	34	U
50	8	35	C
50	8	38	U
50	8	39	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	8	49	G
50	8	51	U
50	8	52	A
50	8	55	U
50	8	57	C
50	8	59	A
50	8	62	A
50	8	63	U
50	8	74	U
50	8	75	G
50	8	79	G
50	8	80	A
50	8	81	C
50	8	82	A
50	8	83	C
50	8	84	A
50	8	85	U
50	8	86	U
50	8	87	G
50	8	94	G
50	8	95	A
50	8	99	U
50	8	101	C
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	113	C
50	8	114	G
50	8	115	G
50	8	117	C
50	8	121	G
50	8	122	G
50	8	123	U
50	8	124	U
50	8	125	C
50	8	126	C
50	8	127	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	8	137	A
50	8	143	G
50	8	150	C
50	8	156	U
51	9	2	A
51	9	3	C
51	9	4	C
51	9	6	G
51	9	9	U
51	9	10	G
51	9	11	A
51	9	17	C
51	9	19	A
51	9	25	A
51	9	26	U
51	9	33	G
51	9	37	C
51	9	41	G
51	9	42	A
51	9	44	U
51	9	45	A
51	9	46	A
51	9	49	C
51	9	56	G
51	9	58	C
51	9	59	U
51	9	60	A
51	9	61	A
51	9	63	U
51	9	65	C
51	9	66	G
51	9	67	C
51	9	68	A
51	9	70	G
51	9	71	G
51	9	72	C
51	9	73	C
51	9	74	G
51	9	75	G
51	9	76	U
51	9	77	A
51	9	78	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	9	79	A
51	9	80	G
51	9	93	U
51	9	95	G
51	9	99	A
51	9	100	U
51	9	103	A
51	9	109	U
51	9	110	U
51	9	111	A
51	9	113	G
51	9	114	G
51	9	115	U
51	9	116	U
51	9	119	U
51	9	124	U
51	9	126	G
51	9	140	C
51	9	141	A
51	9	142	C
51	9	147	A
51	9	150	A
51	9	155	G
51	9	158	A
51	9	161	U
51	9	162	C
51	9	163	U
51	9	164	A
51	9	165	G
51	9	167	G
51	9	168	C
51	9	173	A
51	9	180	G
51	9	183	G
51	9	184	G
51	9	185	G
51	9	188	C
51	9	189	U
51	9	190	G
51	9	191	A
51	9	192	C
51	9	202	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	9	206	G
51	9	213	G
51	9	215	G
51	9	216	C
51	9	225	G
51	9	289	G
51	9	291	G
51	9	292	A
51	9	293	C
51	9	294	U
51	9	302	A
51	9	304	C
51	9	305	U
51	9	306	C
51	9	307	G
51	9	308	G
51	9	309	G
51	9	310	C
51	9	312	G
51	9	313	A
51	9	314	U
51	9	320	G
51	9	321	C
51	9	322	C
51	9	323	C
51	9	324	C
51	9	326	C
51	9	327	G
51	9	328	U
51	9	338	G
51	9	339	A
51	9	343	A
51	9	347	G
51	9	350	C
51	9	351	G
51	9	355	G
51	9	360	A
51	9	362	C
51	9	364	A
51	9	368	U
51	9	370	G
51	9	373	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	9	385	G
51	9	386	C
51	9	400	C
51	9	407	G
51	9	408	A
51	9	409	C
51	9	416	U
51	9	417	C
51	9	418	A
51	9	428	U
51	9	432	G
51	9	435	A
51	9	438	G
51	9	441	C
51	9	447	A
51	9	448	A
51	9	449	A
51	9	450	C
51	9	457	C
51	9	459	C
51	9	460	A
51	9	464	A
51	9	465	A
51	9	466	G
51	9	467	G
51	9	469	A
51	9	472	C
51	9	473	A
51	9	474	G
51	9	482	G
51	9	483	C
51	9	487	U
51	9	488	U
51	9	489	A
51	9	492	C
51	9	493	A
51	9	503	C
51	9	508	A
51	9	511	U
51	9	512	A
51	9	523	A
51	9	525	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	9	528	A
51	9	530	U
51	9	532	C
51	9	533	A
51	9	535	G
51	9	539	C
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	552	G
51	9	554	A
51	9	556	U
51	9	557	U
51	9	559	G
51	9	560	A
51	9	562	U
51	9	563	G
51	9	568	C
51	9	576	A
51	9	577	U
51	9	579	C
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	593	C
51	9	594	A
51	9	595	U
51	9	596	U
51	9	597	G
51	9	598	G
51	9	603	C
51	9	604	A
51	9	605	A
51	9	606	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	9	607	U
51	9	608	C
51	9	609	U
51	9	613	G
51	9	614	C
51	9	620	G
51	9	621	C
51	9	623	G
51	9	627	U
51	9	628	A
51	9	629	A
51	9	631	U
51	9	632	C
51	9	643	A
51	9	644	G
51	9	654	A
51	9	658	U
51	9	659	G
51	9	660	C
51	9	663	C
51	9	664	A
51	9	668	A
51	9	669	A
51	9	671	A
51	9	672	A
51	9	673	G
51	9	684	G
51	9	688	U
51	9	689	U
51	9	698	G
51	9	731	G
51	9	735	C
51	9	737	G
51	9	738	C
51	9	747	U
51	9	748	C
51	9	749	U
51	9	752	G
51	9	753	C
51	9	788	G
51	9	791	C
51	9	794	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	9	796	G
51	9	797	C
51	9	798	G
51	9	799	U
51	9	800	U
51	9	810	A
51	9	811	A
51	9	812	A
51	9	821	G
51	9	822	U
51	9	830	A
51	9	833	C
51	9	834	C
51	9	835	C
51	9	836	G
51	9	837	A
51	9	838	G
51	9	839	C
51	9	840	C
51	9	844	U
51	9	845	G
51	9	847	A
51	9	859	G
51	9	869	A
51	9	870	A
51	9	871	U
51	9	872	A
51	9	873	G
51	9	875	A
51	9	877	C
51	9	878	G
51	9	879	C
51	9	880	G
51	9	887	U
51	9	888	U
51	9	890	U
51	9	892	U
51	9	893	U
51	9	901	G
51	9	902	G
51	9	903	A
51	9	909	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	9	910	G
51	9	912	C
51	9	913	A
51	9	914	U
51	9	917	U
51	9	919	A
51	9	920	A
51	9	921	G
51	9	922	A
51	9	930	C
51	9	933	G
51	9	934	G
51	9	938	A
51	9	943	U
51	9	956	G
51	9	958	G
51	9	971	G
51	9	978	G
51	9	985	G
51	9	990	A
51	9	992	A
51	9	996	A
51	9	999	G
51	9	1002	U
51	9	1016	U
51	9	1017	U
51	9	1023	A
51	9	1033	G
51	9	1040	G
51	9	1041	G
51	9	1044	G
51	9	1045	U
51	9	1049	A
51	9	1058	A
51	9	1060	A
51	9	1083	A
51	9	1085	C
51	9	1089	G
51	9	1096	G
51	9	1099	G
51	9	1100	A
51	9	1109	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	9	1110	G
51	9	1111	U
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	1120	U
51	9	1121	G
51	9	1126	G
51	9	1131	G
51	9	1133	A
51	9	1137	U
51	9	1138	C
51	9	1139	C
51	9	1143	A
51	9	1144	A
51	9	1146	C
51	9	1148	A
51	9	1149	A
51	9	1150	A
51	9	1153	C
51	9	1154	U
51	9	1161	U
51	9	1165	G
51	9	1166	G
51	9	1170	A
51	9	1181	A
51	9	1195	A
51	9	1207	G
51	9	1208	A
51	9	1209	A
51	9	1211	G
51	9	1212	G
51	9	1213	C
51	9	1215	C
51	9	1221	G
51	9	1224	G
51	9	1227	G
51	9	1240	A
51	9	1242	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	9	1243	U
51	9	1244	U
51	9	1247	C
51	9	1248	U
51	9	1250	A
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	1267	C
51	9	1268	C
51	9	1270	G
51	9	1271	C
51	9	1274	G
51	9	1275	G
51	9	1276	A
51	9	1280	G
51	9	1283	C
51	9	1284	A
51	9	1285	G
51	9	1286	G
51	9	1288	U
51	9	1289	U
51	9	1291	A
51	9	1292	C
51	9	1293	A
51	9	1294	G
51	9	1295	A
51	9	1299	A
51	9	1301	A
51	9	1302	G
51	9	1303	C
51	9	1308	U
51	9	1309	C
51	9	1310	U
51	9	1312	G
51	9	1314	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	9	1315	U
51	9	1316	C
51	9	1322	G
51	9	1330	G
51	9	1331	C
51	9	1342	U
51	9	1343	U
51	9	1345	G
51	9	1347	U
51	9	1348	G
51	9	1364	U
51	9	1371	U
51	9	1372	U
51	9	1378	A
51	9	1386	A
51	9	1394	G
51	9	1395	C
51	9	1396	A
51	9	1397	U
51	9	1398	G
51	9	1401	A
51	9	1402	A
51	9	1403	C
51	9	1404	U
51	9	1405	A
51	9	1407	U
51	9	1408	U
51	9	1410	C
51	9	1412	C
51	9	1413	G
51	9	1414	A
51	9	1417	C
51	9	1418	C
51	9	1419	C
51	9	1420	G
51	9	1422	G
51	9	1424	G
51	9	1426	U
51	9	1427	C
51	9	1432	U
51	9	1433	C
51	9	1434	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	9	1437	C
51	9	1438	A
51	9	1439	A
51	9	1440	C
51	9	1442	U
51	9	1447	G
51	9	1448	A
51	9	1449	G
51	9	1450	G
51	9	1452	A
51	9	1454	A
51	9	1455	A
51	9	1456	G
51	9	1459	G
51	9	1462	U
51	9	1463	U
51	9	1464	C
51	9	1466	G
51	9	1473	G
51	9	1474	A
51	9	1475	G
51	9	1476	A
51	9	1477	U
51	9	1478	U
51	9	1489	A
51	9	1490	G
51	9	1494	U
51	9	1495	G
51	9	1496	U
51	9	1498	A
51	9	1499	U
51	9	1500	G
51	9	1507	G
51	9	1510	G
51	9	1521	C
51	9	1522	A
51	9	1523	C
51	9	1525	C
51	9	1531	A
51	9	1533	A
51	9	1535	U
51	9	1536	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	9	1544	C
51	9	1545	A
51	9	1548	G
51	9	1552	G
51	9	1553	C
51	9	1554	C
51	9	1555	U
51	9	1556	A
51	9	1558	C
51	9	1560	U
51	9	1563	G
51	9	1564	C
51	9	1565	C
51	9	1567	G
51	9	1570	G
51	9	1574	C
51	9	1575	G
51	9	1580	A
51	9	1581	C
51	9	1582	C
51	9	1585	U
51	9	1586	U
51	9	1587	G
51	9	1588	A
51	9	1589	A
51	9	1594	A
51	9	1595	U
51	9	1596	U
51	9	1599	U
51	9	1600	G
51	9	1601	A
51	9	1603	G
51	9	1604	G
51	9	1606	G
51	9	1618	C
51	9	1621	U
51	9	1622	U
51	9	1623	A
51	9	1624	U
51	9	1625	U
51	9	1630	A
51	9	1632	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	9	1633	A
51	9	1637	A
51	9	1638	G
51	9	1639	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	1672	U
51	9	1680	G
51	9	1681	U
51	9	1682	C
51	9	1683	C
51	9	1686	G
51	9	1688	C
51	9	1689	C
51	9	1695	A
51	9	1698	C
51	9	1699	A
51	9	1706	G
51	9	1715	A
51	9	1721	U
51	9	1722	G
51	9	1725	U
51	9	1728	U
51	9	1729	U
51	9	1739	C
51	9	1742	C
51	9	1745	A
51	9	1746	U
51	9	1750	C
51	9	1753	C
51	9	1756	C
51	9	1757	G
51	9	1758	G
51	9	1783	C
51	9	1786	U
51	9	1789	G
51	9	1800	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	9	1802	C
51	9	1809	A
51	9	1812	U
51	9	1813	A
51	9	1823	A
51	9	1824	A
51	9	1825	A
51	9	1826	G
51	9	1827	U
51	9	1829	G
51	9	1831	A
51	9	1835	A
51	9	1836	G
51	9	1837	G
51	9	1838	U
51	9	1839	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	1867	U
85	hh	42	C
85	hh	43	A
85	hh	45	A
85	hh	46	G
85	hh	49	U
85	hh	50	A
85	hh	52	G

All (413) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
46	2	34	A
47	3	7	A
47	3	9	A
47	3	29	A
47	3	30	G
47	3	60	U
47	3	69	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	3	74	C
48	5	1	C
48	5	12	A
48	5	20	U
48	5	39	A
48	5	42	A
48	5	47	A
48	5	48	G
48	5	58	G
48	5	64	A
48	5	72	C
48	5	90	G
48	5	93	G
48	5	119	G
48	5	120	A
48	5	125	C
48	5	126	C
48	5	134	G
48	5	143	C
48	5	157	U
48	5	159	C
48	5	170	C
48	5	187	U
48	5	215	C
48	5	216	C
48	5	218	A
48	5	219	G
48	5	224	U
48	5	226	G
48	5	245	C
48	5	253	G
48	5	265	C
48	5	266	C
48	5	275	C
48	5	286	U
48	5	296	A
48	5	361	C
48	5	385	A
48	5	387	G
48	5	406	C
48	5	451	C
48	5	454	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	486	C
48	5	497	G
48	5	505	G
48	5	509	A
48	5	664	G
48	5	684	G
48	5	693	C
48	5	727	C
48	5	728	U
48	5	733	A
48	5	746	A
48	5	747	A
48	5	917	A
48	5	930	G
48	5	931	C
48	5	932	A
48	5	935	A
48	5	943	A
48	5	956	A
48	5	957	G
48	5	965	G
48	5	977	C
48	5	978	G
48	5	989	U
48	5	1071	C
48	5	1176	C
48	5	1211	G
48	5	1214	C
48	5	1232	G
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1239	C
48	5	1241	C
48	5	1266	G
48	5	1268	G
48	5	1272	C
48	5	1279	A
48	5	1280	C
48	5	1292	C
48	5	1296	G
48	5	1329	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	1354	A
48	5	1357	C
48	5	1365	C
48	5	1370	G
48	5	1371	A
48	5	1376	C
48	5	1379	C
48	5	1380	G
48	5	1390	G
48	5	1398	A
48	5	1407	C
48	5	1410	U
48	5	1419	G
48	5	1420	A
48	5	1435	G
48	5	1440	U
48	5	1445	U
48	5	1455	G
48	5	1474	C
48	5	1477	C
48	5	1481	C
48	5	1485	C
48	5	1500	A
48	5	1523	A
48	5	1533	A
48	5	1563	A
48	5	1625	G
48	5	1633	G
48	5	1654	G
48	5	1678	C
48	5	1696	C
48	5	1697	G
48	5	1724	G
48	5	1733	G
48	5	1741	G
48	5	1755	C
48	5	1756	U
48	5	1804	A
48	5	1818	G
48	5	1819	G
48	5	1835	G
48	5	1839	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	1891	A
48	5	1892	A
48	5	1921	C
48	5	1935	C
48	5	1956	A
48	5	1957	U
48	5	1958	A
48	5	1959	U
48	5	1960	A
48	5	1961	G
48	5	1968	G
48	5	1969	G
48	5	1974	U
48	5	1975	G
48	5	1986	U
48	5	2009	A
48	5	2019	C
48	5	2046	G
48	5	2068	C
48	5	2083	C
48	5	2084	C
48	5	2088	A
48	5	2089	G
48	5	2093	A
48	5	2107	C
48	5	2110	C
48	5	2116	C
48	5	2119	C
48	5	2122	G
48	5	2123	C
48	5	2125	C
48	5	2246	C
48	5	2251	G
48	5	2253	A
48	5	2256	C
48	5	2257	C
48	5	2260	C
48	5	2262	G
48	5	2265	G
48	5	2266	C
48	5	2269	C
48	5	2278	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	2313	A
48	5	2333	G
48	5	2370	A
48	5	2396	A
48	5	2398	U
48	5	2467	U
48	5	2468	U
48	5	2473	A
48	5	2474	G
48	5	2490	U
48	5	2502	G
48	5	2505	C
48	5	2506	G
48	5	2513	A
48	5	2546	G
48	5	2553	A
48	5	2554	U
48	5	2587	A
48	5	2588	C
48	5	2623	A
48	5	2661	U
48	5	2687	U
48	5	2695	A
48	5	2724	G
48	5	2739	C
48	5	2754	G
48	5	2769	U
48	5	2782	U
48	5	2794	C
48	5	2806	A
48	5	2827	G
48	5	2858	A
48	5	3593	C
48	5	3625	G
48	5	3670	C
48	5	3673	C
48	5	3697	U
48	5	3702	A
48	5	3709	U
48	5	3710	G
48	5	3713	U
48	5	3715	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	3717	A
48	5	3752	C
48	5	3784	A
48	5	3876	A
48	5	3878	C
48	5	3888	G
48	5	3904	G
48	5	4069	U
48	5	4075	U
48	5	4084	G
48	5	4086	G
48	5	4115	G
48	5	4119	C
48	5	4121	G
48	5	4124	G
48	5	4144	C
48	5	4170	A
48	5	4232	U
48	5	4254	G
48	5	4331	G
48	5	4349	C
48	5	4378	A
48	5	4395	U
48	5	4404	U
48	5	4448	G
48	5	4449	A
48	5	4463	U
48	5	4475	G
48	5	4510	A
48	5	4512	U
48	5	4527	G
48	5	4528	G
48	5	4548	A
48	5	4583	C
48	5	4656	A
48	5	4694	G
48	5	4699	U
48	5	4718	G
48	5	4719	G
48	5	4730	C
48	5	4872	G
48	5	4885	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	5	4888	U
48	5	4889	G
48	5	4895	C
48	5	4900	C
48	5	4926	C
48	5	4935	C
48	5	4948	C
48	5	4951	G
48	5	4965	U
48	5	4975	G
48	5	4990	C
48	5	5022	U
48	5	5026	U
48	5	5027	C
48	5	5047	C
48	5	5059	C
48	5	5060	A
48	5	5061	A
49	7	109	U
50	8	2	G
50	8	51	U
50	8	94	G
50	8	110	U
50	8	111	U
50	8	124	U
51	9	1	U
51	9	2	A
51	9	3	C
51	9	43	U
51	9	44	U
51	9	58	C
51	9	62	G
51	9	72	C
51	9	92	A
51	9	102	A
51	9	110	U
51	9	113	G
51	9	139	C
51	9	140	C
51	9	143	U
51	9	146	G
51	9	160	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	9	164	A
51	9	180	G
51	9	183	G
51	9	191	A
51	9	215	G
51	9	291	G
51	9	292	A
51	9	304	C
51	9	305	U
51	9	312	G
51	9	321	C
51	9	322	C
51	9	327	G
51	9	369	C
51	9	400	C
51	9	407	G
51	9	434	G
51	9	447	A
51	9	448	A
51	9	464	A
51	9	465	A
51	9	473	A
51	9	488	U
51	9	500	A
51	9	532	C
51	9	550	C
51	9	559	G
51	9	589	G
51	9	594	A
51	9	606	G
51	9	620	G
51	9	627	U
51	9	642	U
51	9	656	G
51	9	670	A
51	9	688	U
51	9	746	C
51	9	747	U
51	9	752	G
51	9	797	C
51	9	798	G
51	9	833	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	9	844	U
51	9	869	A
51	9	870	A
51	9	887	U
51	9	912	C
51	9	913	A
51	9	970	G
51	9	1016	U
51	9	1087	A
51	9	1109	C
51	9	1113	A
51	9	1115	U
51	9	1137	U
51	9	1138	C
51	9	1165	G
51	9	1212	G
51	9	1234	C
51	9	1247	C
51	9	1253	A
51	9	1265	A
51	9	1275	G
51	9	1283	C
51	9	1294	G
51	9	1298	G
51	9	1302	G
51	9	1308	U
51	9	1309	C
51	9	1312	G
51	9	1313	A
51	9	1330	G
51	9	1342	U
51	9	1394	G
51	9	1395	C
51	9	1396	A
51	9	1407	U
51	9	1418	C
51	9	1419	C
51	9	1432	U
51	9	1438	A
51	9	1448	A
51	9	1454	A
51	9	1455	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	9	1475	G
51	9	1477	U
51	9	1489	A
51	9	1508	A
51	9	1534	C
51	9	1555	U
51	9	1580	A
51	9	1601	A
51	9	1621	U
51	9	1623	A
51	9	1632	G
51	9	1636	G
51	9	1637	A
51	9	1638	G
51	9	1646	C
51	9	1647	A
51	9	1664	A
51	9	1665	G
51	9	1679	A
51	9	1680	G
51	9	1721	U
51	9	1724	A
51	9	1728	U
51	9	1824	A
51	9	1826	G
51	9	1830	U
51	9	1835	A
51	9	1837	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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 207 ligands modelled in this entry, 203 are monoatomic - leaving 4 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	SF4	jj	600	87	0,12,12	-	-	-		
91	ADP	jj	602	-	24,29,29	1.04	3 (12%)	29,45,45	1.29	2 (6%)
90	SF4	jj	601	87	0,12,12	-	-	-		
91	ADP	jj	603	-	24,29,29	1.03	3 (12%)	29,45,45	1.29	2 (6%)

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	SF4	jj	600	87	-	-	0/6/5/5
91	ADP	jj	602	-	-	1/12/32/32	0/3/3/3
90	SF4	jj	601	87	-	-	0/6/5/5
91	ADP	jj	603	-	-	1/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	jj	603	ADP	C2-N3	2.39	1.35	1.32
91	jj	602	ADP	C2-N3	2.29	1.35	1.32
91	jj	602	ADP	PA-O3A	2.27	1.61	1.59
91	jj	602	ADP	O4'-C1'	2.14	1.43	1.40
91	jj	603	ADP	PA-O3A	2.13	1.61	1.59
91	jj	603	ADP	O4'-C1'	2.08	1.43	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	jj	602	ADP	N3-C2-N1	-4.33	122.80	128.67
91	jj	603	ADP	N3-C2-N1	-4.32	122.81	128.67
91	jj	603	ADP	C4-C5-N7	-2.74	106.45	109.34
91	jj	602	ADP	C4-C5-N7	-2.74	106.45	109.34

There are no chirality outliers.

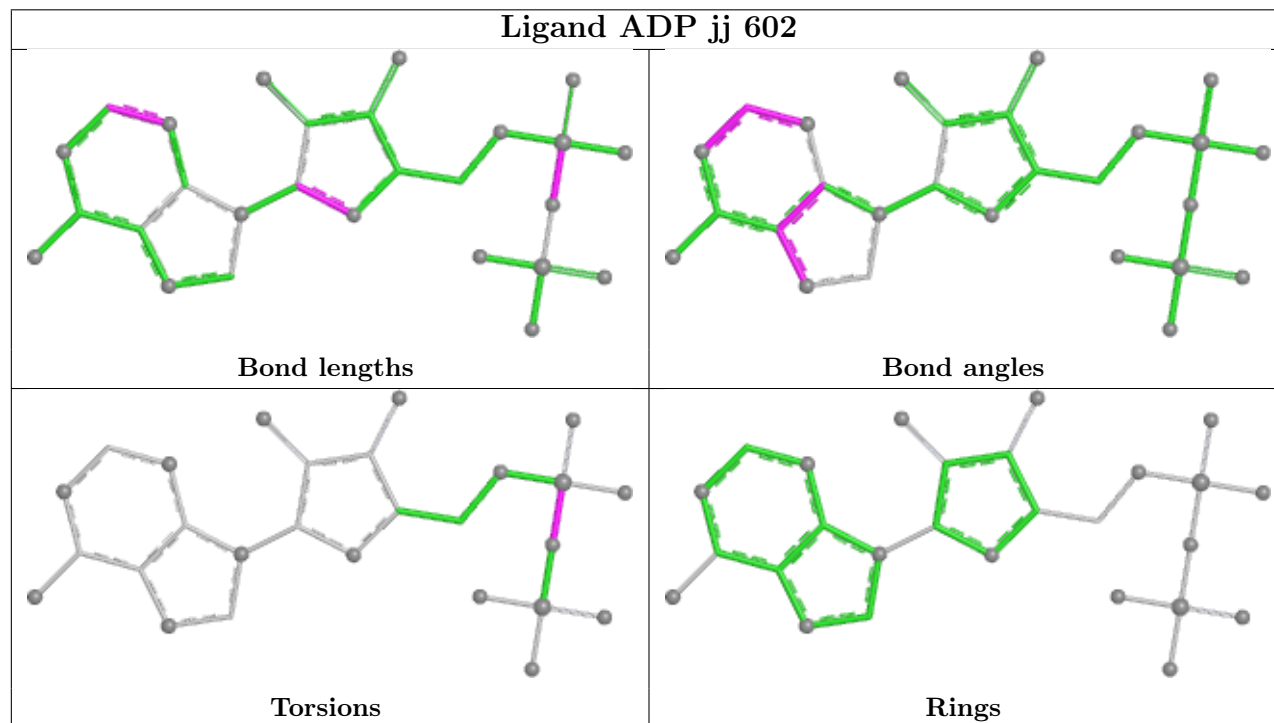
All (2) torsion outliers are listed below:

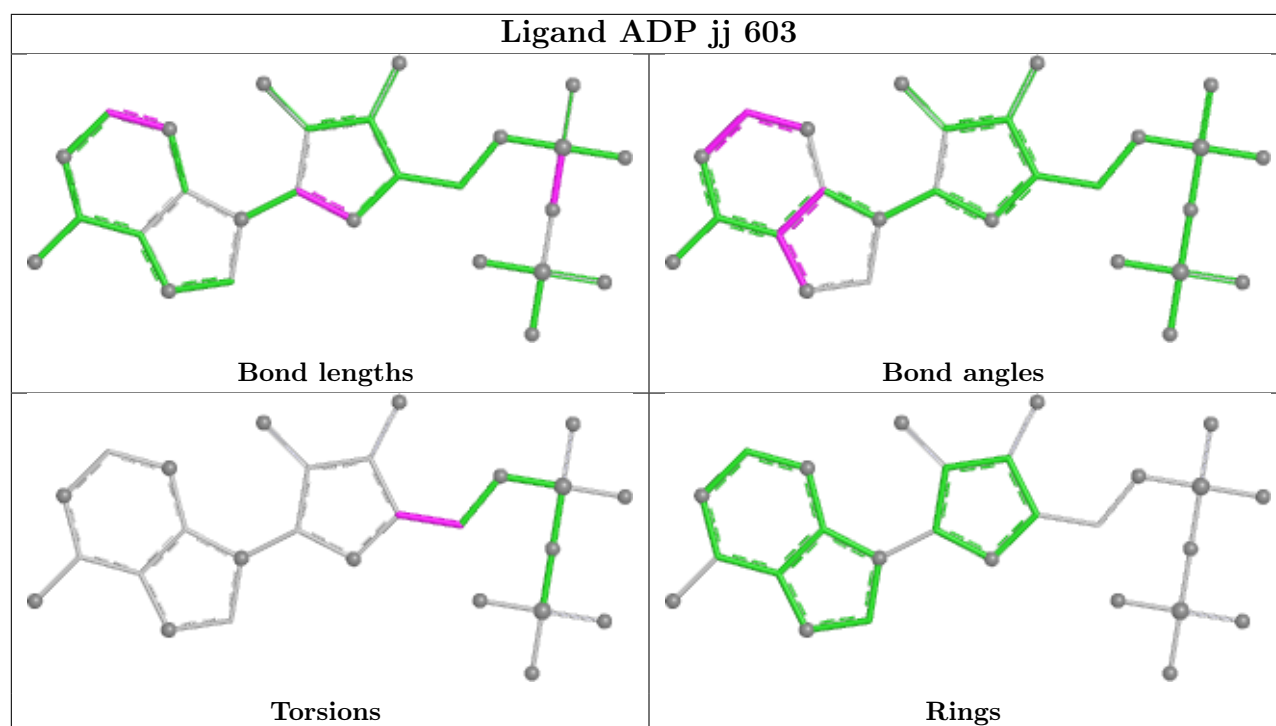
Mol	Chain	Res	Type	Atoms
91	jj	603	ADP	O4'-C4'-C5'-O5'
91	jj	602	ADP	PB-O3A-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [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	17
51	9	8
47	3	2
46	2	1
87	jj	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	9	753:C	O3'	785:C	P	23.16
1	9	126:G	O3'	139:C	P	22.33
1	9	698:G	O3'	730:C	P	19.62
1	5	4776:G	O3'	4859:C	P	17.95
1	9	1761:U	O3'	1771:G	P	17.55
1	5	757:G	O3'	906:C	P	17.49

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	519:C	O3'	642:G	P	16.73
1	5	2910:G	O3'	3583:U	P	16.46
1	5	2131:C	O3'	2243:C	P	14.50
1	5	3950:U	O3'	4065:G	P	14.39
1	5	997:C	O3'	1047:C	P	13.95
1	5	1051:G	O3'	1064:G	P	8.98
1	9	225:G	O3'	287:U	P	7.38
1	9	739:C	O3'	744:G	P	6.44
1	3	19:G	O3'	20:U	P	6.06
1	5	1222:A	O3'	1232:G	P	5.15
1	5	2016:C	O3'	2017:A	P	4.53
1	5	1100:U	O3'	1167:C	P	4.42
1	3	16:C	O3'	18:U	P	4.26
1	5	1699:A	O3'	1718:C	P	4.00
1	2	16:C	O3'	18:G	P	3.75
1	jj	416:ILE	C	417:SER	N	3.69
1	9	873:G	O3'	874:G	P	3.24
1	9	340:C	O3'	342:C	P	3.08
1	5	1840:G	O3'	1842:G	P	2.91
1	5	4939:C	O3'	4941:G	P	2.80
1	5	4942:C	O3'	4944:C	P	2.73
1	5	1823:G	O3'	1825:A	P	2.56
1	5	1965:G	O3'	1966:C	P	1.33

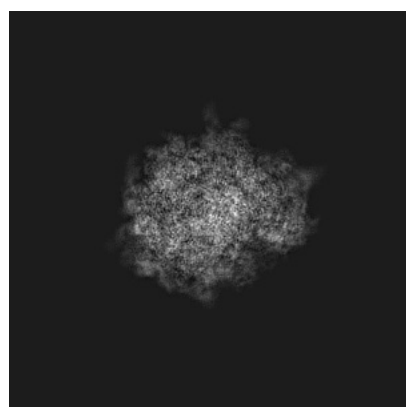
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3039. These allow visual inspection of the internal detail of the map and identification of artifacts.

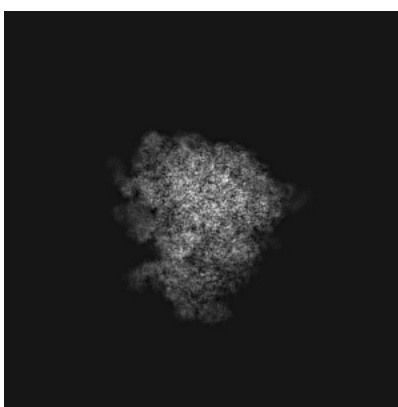
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

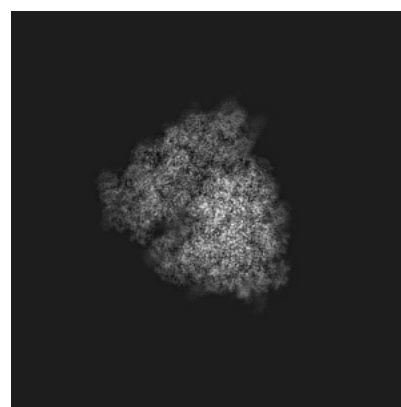
6.1.1 Primary map



X



Y

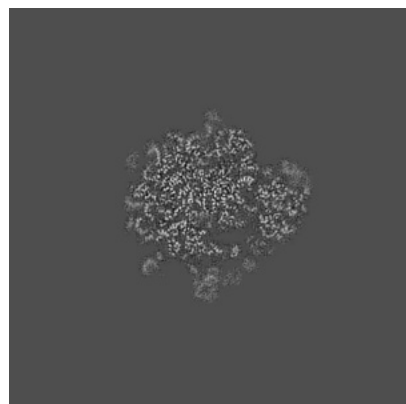


Z

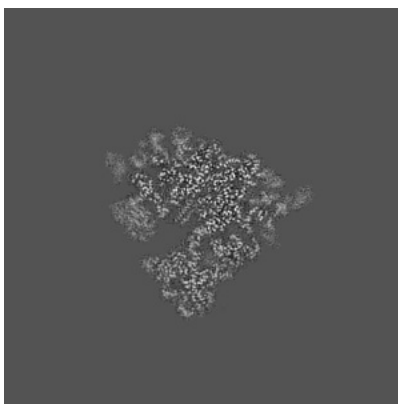
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

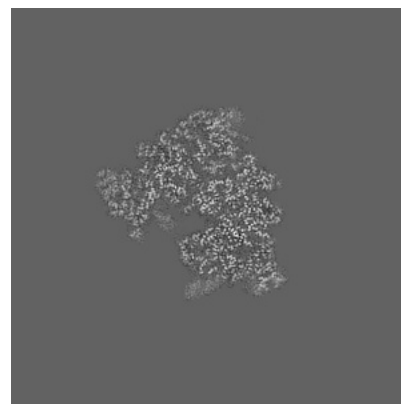
6.2.1 Primary map



X Index: 210



Y Index: 210

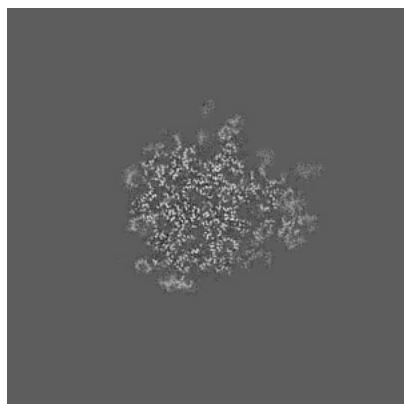


Z Index: 210

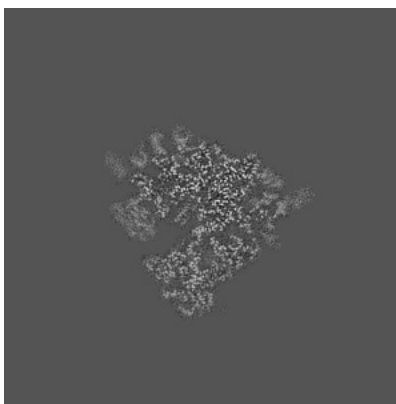
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

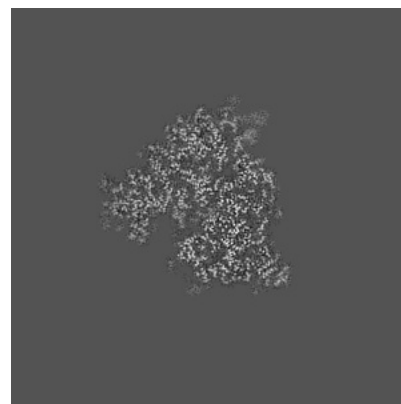
6.3.1 Primary map



X Index: 228



Y Index: 211

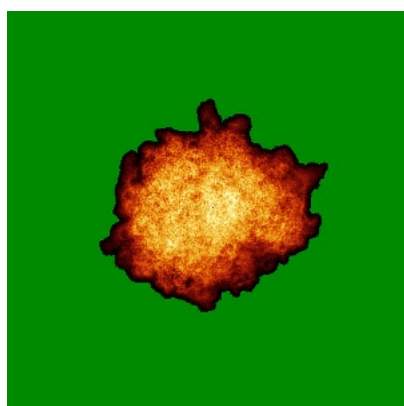


Z Index: 203

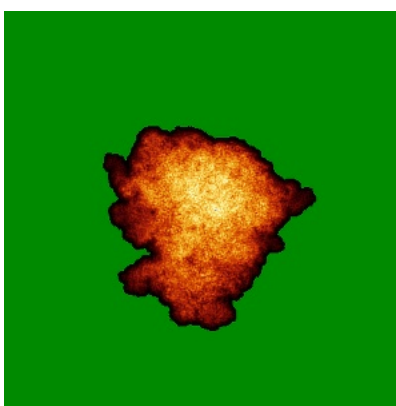
The images above show the largest variance slices of the map in three orthogonal directions.

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

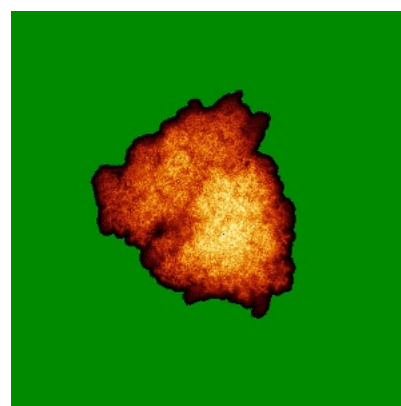
6.4.1 Primary map



X



Y



Z

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 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

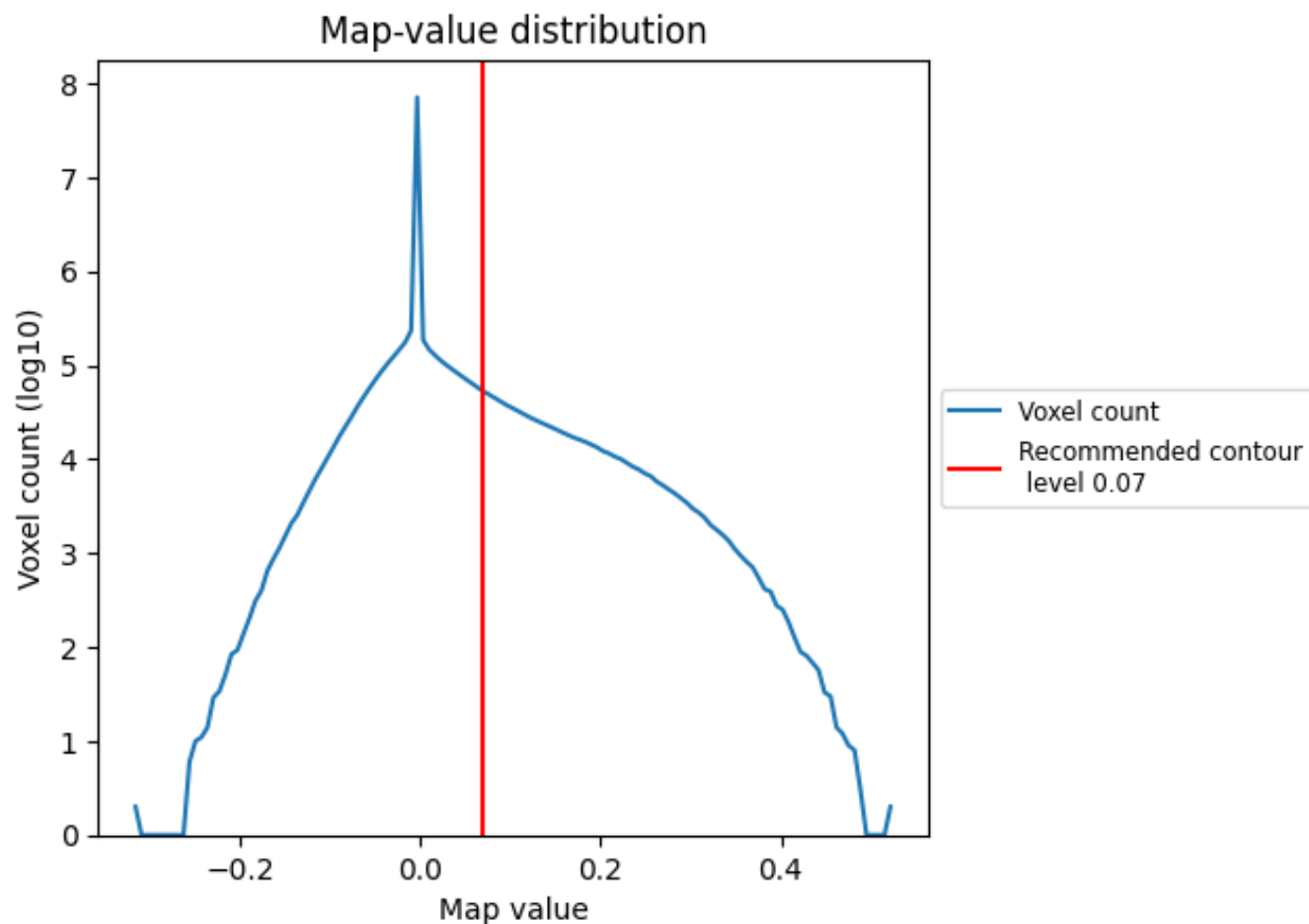
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

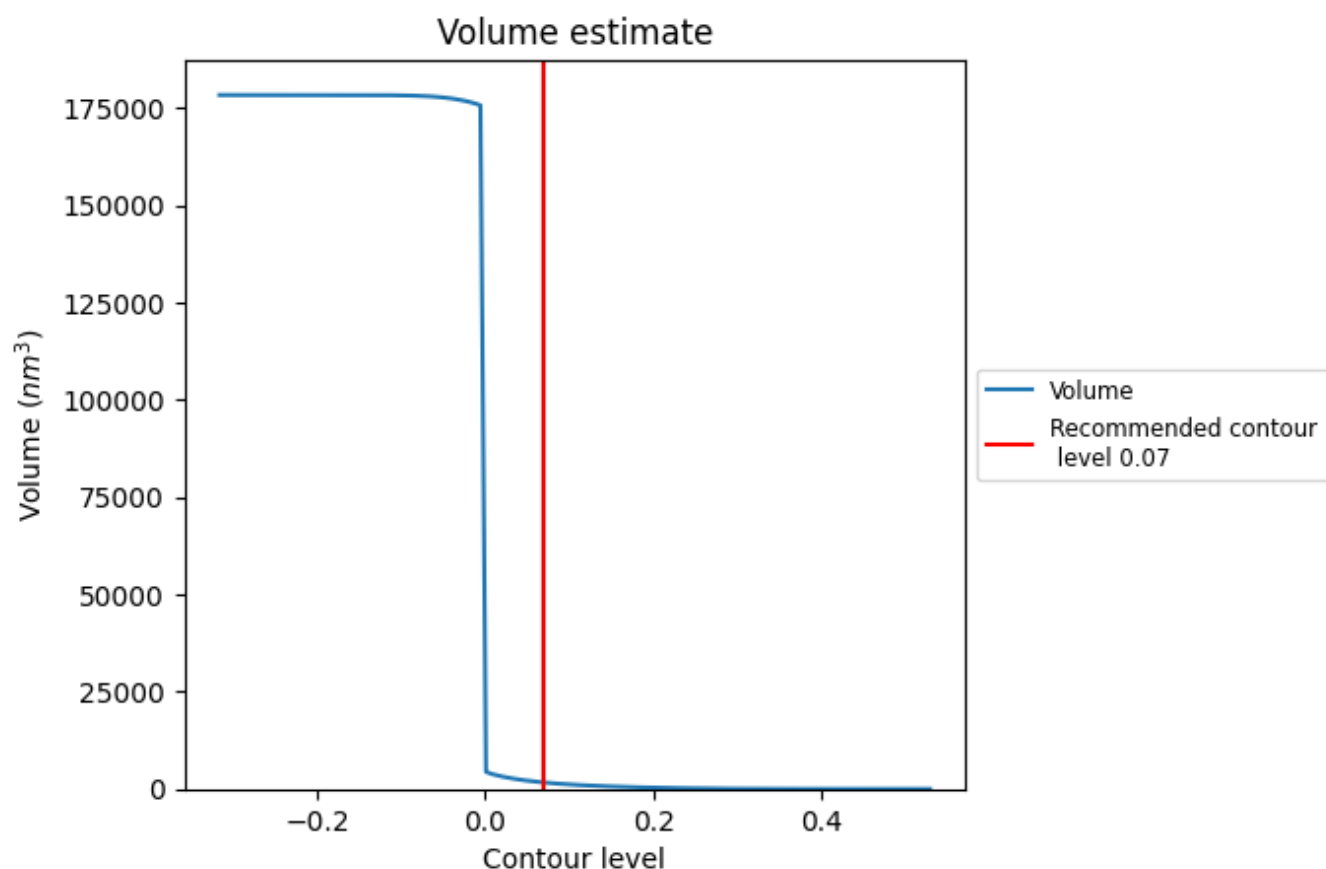
This section contains the results of statistical analysis of the map.

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.

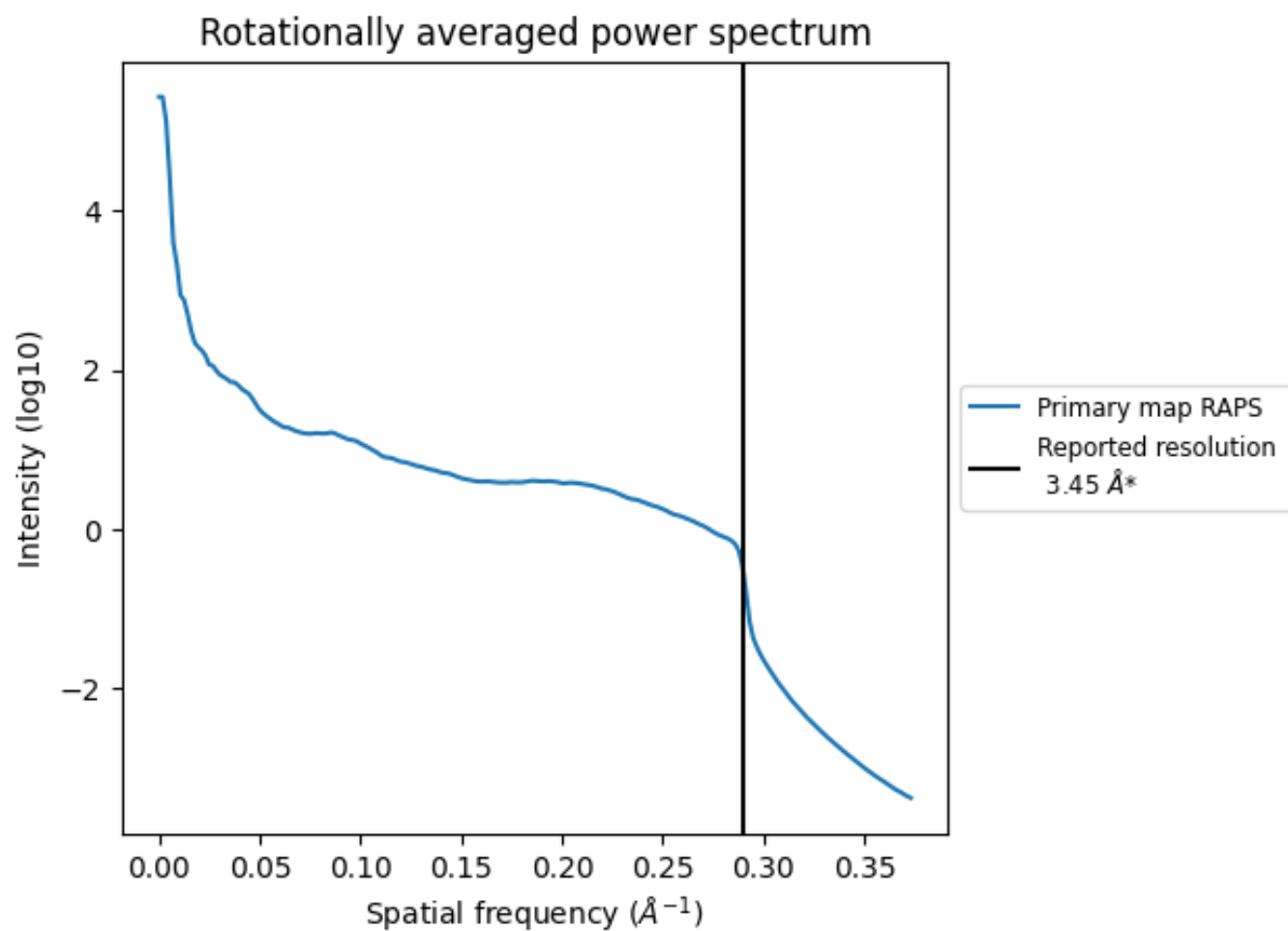
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1656 nm³; this corresponds to an approximate mass of 1496 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 ⓘ

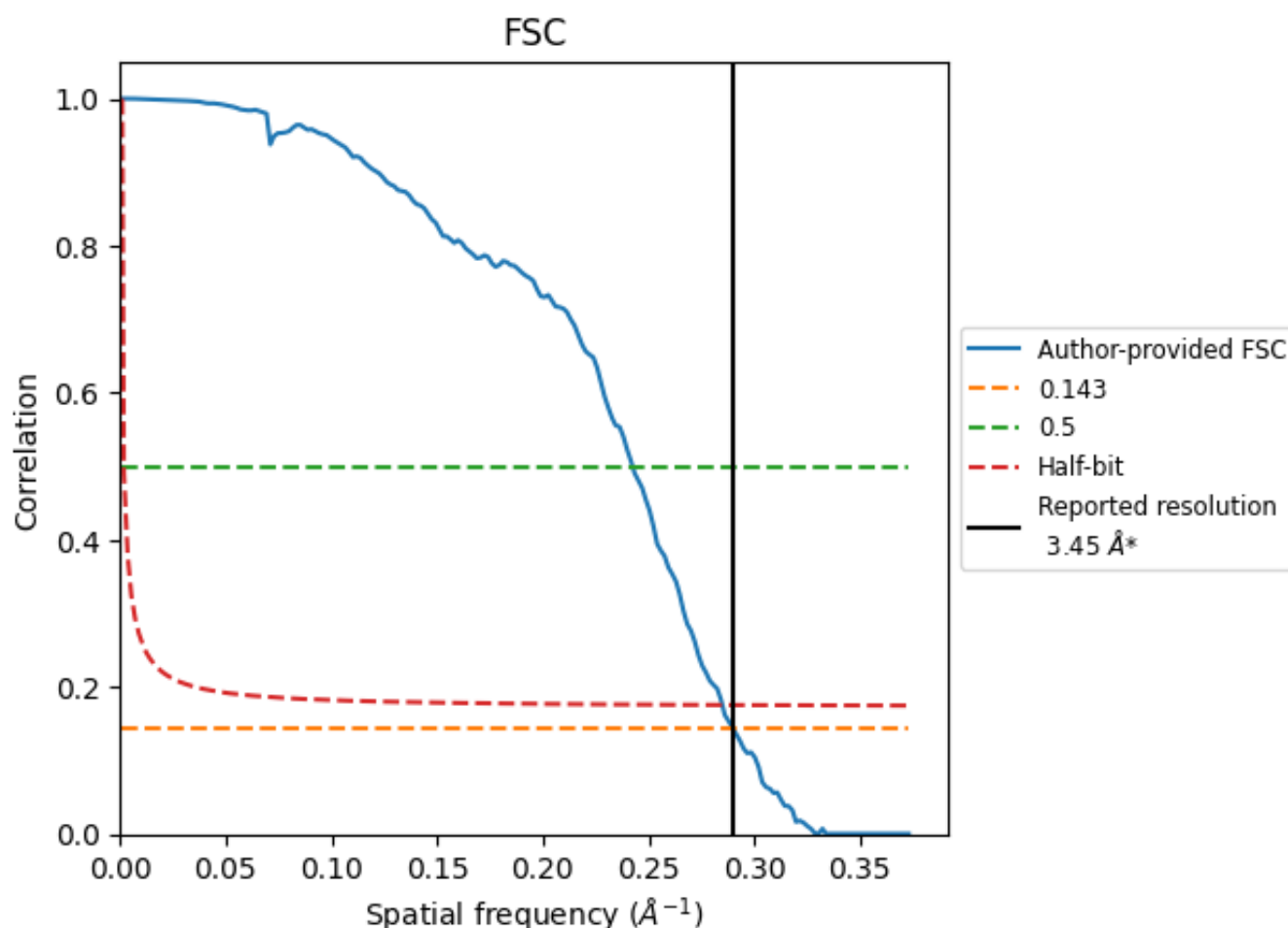


*Reported resolution corresponds to spatial frequency of 0.290 Å⁻¹

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 0.290 Å⁻¹

8.2 Resolution estimates [i](#)

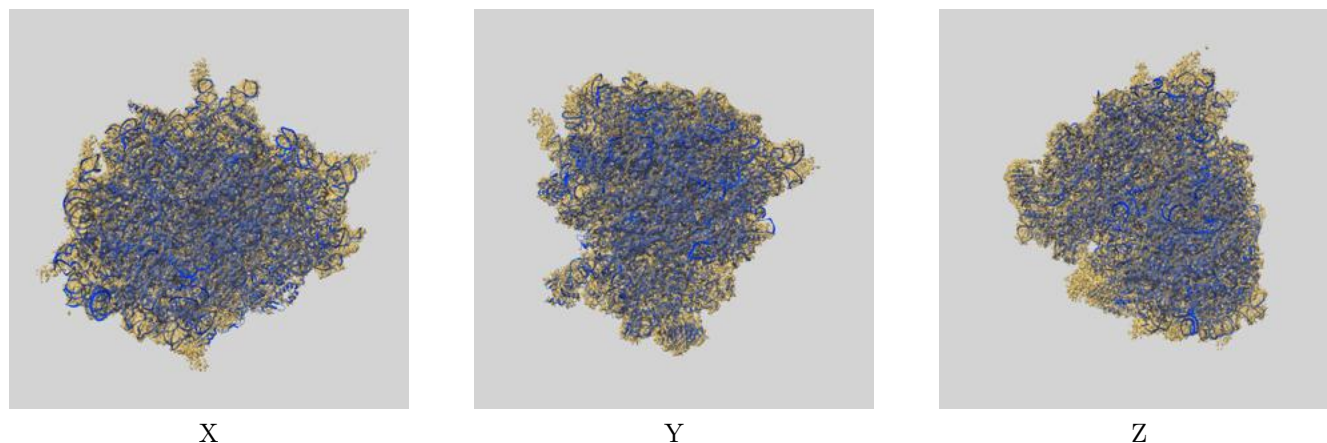
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	3.45	4.12	3.51
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

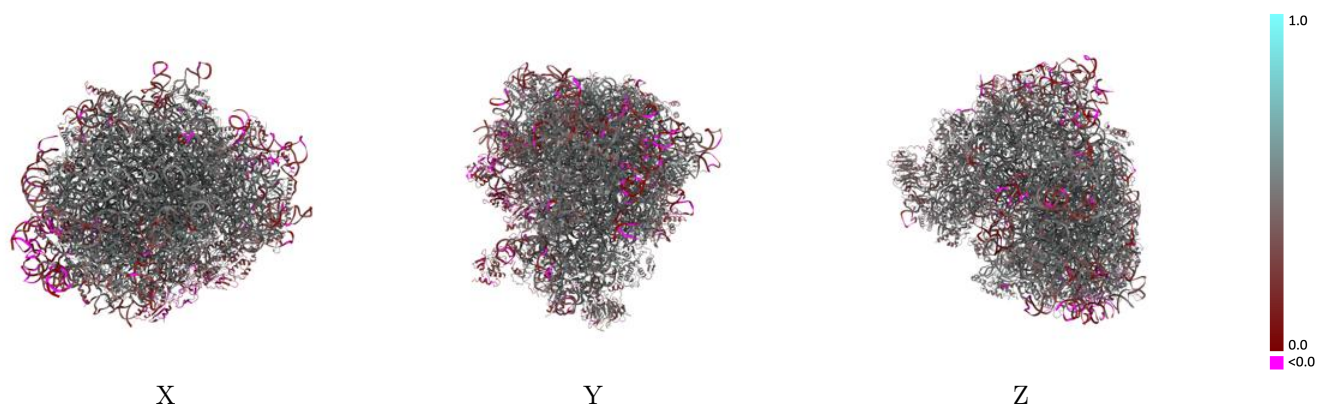
This section contains information regarding the fit between EMDB map EMD-3039 and PDB model 3JAH. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



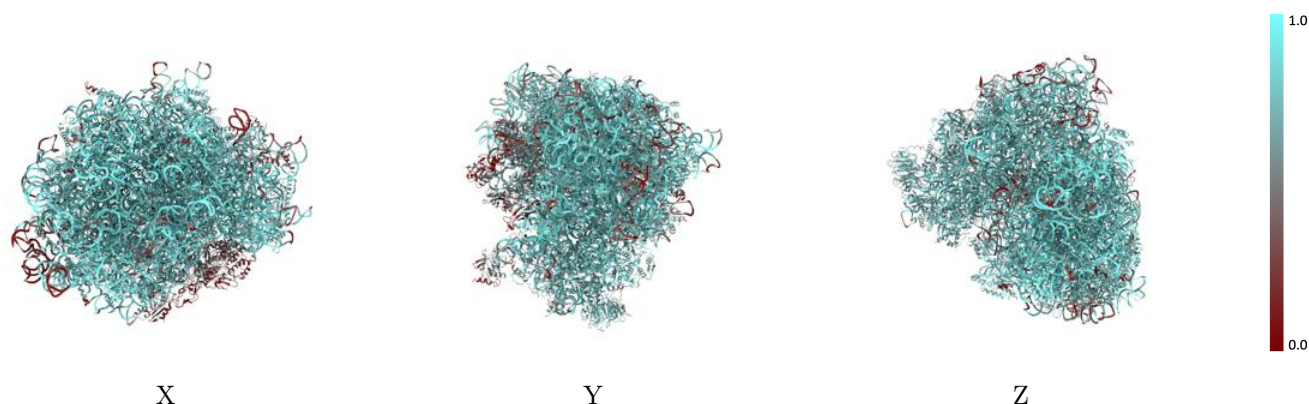
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



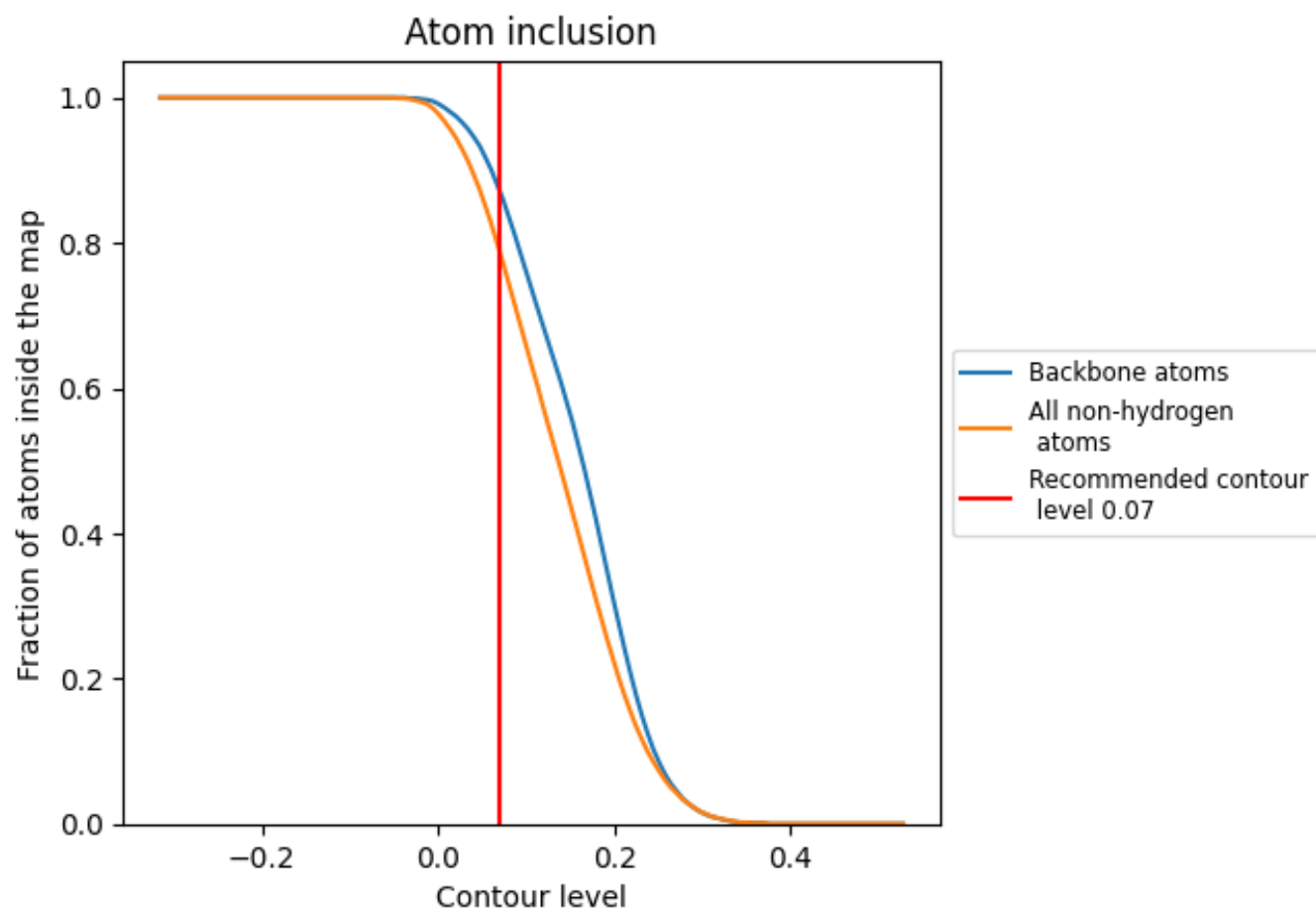
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 79% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7880	 0.4220
1	 0.5790	 0.4150
2	 0.8210	 0.3920
3	 0.5400	 0.2310
5	 0.8440	 0.4100
7	 0.9450	 0.4810
8	 0.8850	 0.4360
9	 0.8580	 0.4170
A	 0.8160	 0.5110
AA	 0.7530	 0.4540
B	 0.8160	 0.4980
BB	 0.7450	 0.4630
C	 0.8040	 0.4910
CC	 0.7680	 0.4710
D	 0.7990	 0.4550
DD	 0.6680	 0.4010
E	 0.7210	 0.4160
EE	 0.7630	 0.4700
F	 0.8050	 0.4870
FF	 0.6990	 0.4280
G	 0.6970	 0.4080
GG	 0.6780	 0.3660
H	 0.7670	 0.4690
HH	 0.6430	 0.3800
I	 0.7880	 0.4810
II	 0.7330	 0.4270
J	 0.7620	 0.4350
JJ	 0.7600	 0.4550
KK	 0.6450	 0.3440
L	 0.7780	 0.4530
LL	 0.7180	 0.4460
M	 0.8000	 0.4560
MM	 0.3720	 0.1710
N	 0.8380	 0.5080
NN	 0.7830	 0.4750

























Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
O	 0.8120	 0.4870
OO	 0.7710	 0.4790
P	 0.8190	 0.5040
PP	 0.6510	 0.3750
Q	 0.7960	 0.5000
QQ	 0.7350	 0.4470
R	 0.7630	 0.4520
RR	 0.6690	 0.3950
S	 0.8120	 0.4910
SS	 0.7430	 0.4190
T	 0.7930	 0.4790
TT	 0.7360	 0.4240
U	 0.7490	 0.4220
UU	 0.6610	 0.4020
V	 0.7630	 0.4940
VV	 0.7350	 0.4630
W	 0.8050	 0.4840
WW	 0.7900	 0.4880
X	 0.7780	 0.4670
XX	 0.7700	 0.4960
Y	 0.7910	 0.4670
YY	 0.7370	 0.4160
Z	 0.8100	 0.4740
ZZ	 0.6930	 0.3830
a	 0.8430	 0.5100
aa	 0.7910	 0.4860
b	 0.6880	 0.4000
bb	 0.7140	 0.4450
c	 0.8040	 0.4690
cc	 0.6750	 0.4260
d	 0.7950	 0.4660
dd	 0.7780	 0.4520
e	 0.8040	 0.5000
ee	 0.6540	 0.4090
f	 0.8280	 0.5090
ff	 0.4820	 0.2530
g	 0.7780	 0.4700
gg	 0.6610	 0.3850
h	 0.7890	 0.4630
hh	 0.8100	 0.4440
i	 0.7760	 0.4520
ii	 0.4330	 0.3710

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
j	 0.8440	 0.5000
jj	 0.3780	 0.3410
k	 0.7240	 0.4200
l	 0.8180	 0.4960
m	 0.7840	 0.4770
n	 0.7960	 0.4730
o	 0.7680	 0.4860
p	 0.7920	 0.4850
r	 0.8220	 0.4860
s	 0.2520	 0.1220
t	 0.2800	 0.1180