



## Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 08:24 pm BST

PDB ID : 5LZZ  
EMDB ID : EMD-4137  
Title : Structure of the mammalian rescue complex with Pelota and Hbs1l (combined)  
Authors : Shao, S.; Murray, J.; Brown, A.; Taunton, J.; Ramakrishnan, V.; Hegde, R.S.  
Deposited on : 2016-10-02  
Resolution : 3.47 Å(reported)

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

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

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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 : 1.8.4, CSD as541be (2020)  
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

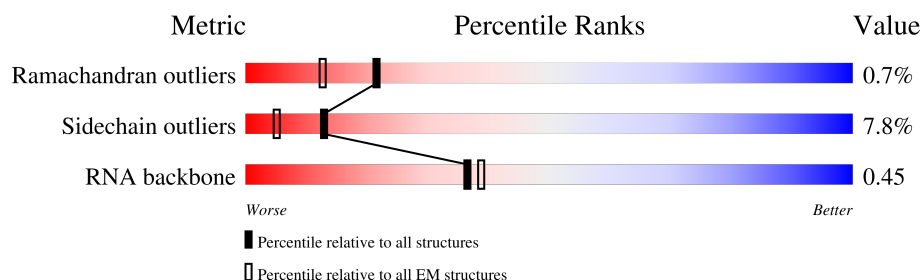
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.47 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.













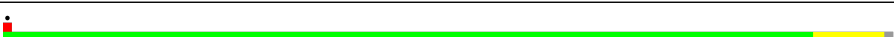


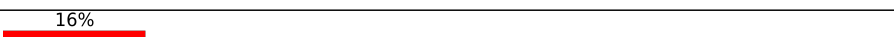
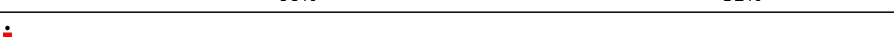
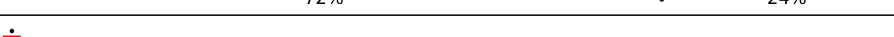

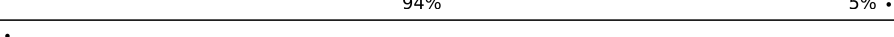
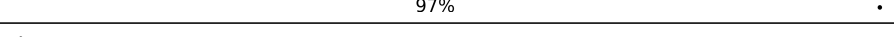
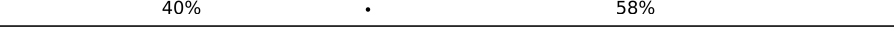





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	<div> <div>90%</div> <div>6%</div> <div>.</div> </div>
2	B	403	<div> <div>90%</div> <div>8%</div> <div>.</div> </div>
3	C	425	<div> <div>78%</div> <div>7%</div> <div>15%</div> </div>
4	D	297	<div> <div>94%</div> <div>.</div> <div>.</div> </div>
5	E	291	<div> <div>70%</div> <div>.</div> <div>26%</div> </div>
6	F	247	<div> <div>82%</div> <div>9%</div> <div>9%</div> </div>
7	G	319	<div> <div>5%</div> <div>68%</div> <div>.</div> <div>27%</div> </div>
8	H	192	<div> <div>92%</div> <div>7%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
9	I	214	
10	J	178	
11	L	211	
12	M	218	
13	N	204	
14	O	203	
15	P	184	
16	Q	188	
17	R	196	
18	S	176	
19	T	160	
20	U	128	
21	V	140	
22	W	157	
23	X	156	
24	Y	145	
25	Z	136	
26	a	148	
27	b	245	
28	c	115	
29	d	125	
30	e	135	
31	f	110	
32	g	117	
33	h	123	

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Mol	Chain	Length	Quality of chain
34	i	105	
35	j	97	
36	k	70	
37	l	51	
38	m	102	
39	n	25	
40	o	106	
41	p	92	
42	r	137	
43	s	318	
44	t	165	
45	1	7	
46	2	76	
47	3	75	
48	5	3543	
49	7	120	
50	8	156	
51	9	1869	
52	AA	295	
53	BB	264	
54	CC	293	
55	DD	243	
56	EE	263	
57	FF	204	
58	GG	249	

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Mol	Chain	Length	Quality of chain
59	HH	194	
60	II	208	
61	JJ	194	
62	KK	165	
63	LL	158	
64	MM	132	
65	NN	151	
66	OO	168	
67	PP	145	
68	QQ	146	
69	RR	135	
70	SS	152	
71	TT	145	
72	UU	119	
73	VV	83	
74	WW	130	
75	XX	143	
76	YY	130	
77	ZZ	125	
78	aa	115	
79	bb	84	
80	cc	69	
81	dd	56	
82	ee	133	
83	ff	156	

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Mol	Chain	Length	Quality of chain
84	gg	317	<div><div></div><div>5%</div><div>93%</div><div>6%</div><div></div></div>
85	hh	8	<div><div></div><div>88%</div><div>50%</div><div>50%</div><div></div></div>
86	ii	403	<div><div></div><div>12%</div><div>88%</div><div></div><div>8%</div></div>
87	jj	710	<div><div></div><div>5%</div><div>56%</div><div></div><div>40%</div></div>

## 2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 222005 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called uL2.

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

- Molecule 2 is a protein called uL3.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called uL4.

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 6 is a protein called uL30.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 7 is a protein called 60S ribosomal protein L7a,eL8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 8 is a protein called uL6.

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

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

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

- Molecule 10 is a protein called uL5.



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

- Molecule 11 is a protein called eL13.

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

- Molecule 12 is a protein called eL14.

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

- Molecule 13 is a protein called Ribosomal protein L15.

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

- Molecule 14 is a protein called uL13.

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

- Molecule 15 is a protein called uL22.

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

- Molecule 16 is a protein called eL18.

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

- Molecule 17 is a protein called eL19.

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

- Molecule 18 is a protein called eL20.

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

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called eL22.

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

- Molecule 21 is a protein called uL14.

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

- Molecule 22 is a protein called eL24.

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

- Molecule 23 is a protein called uL23.

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

- Molecule 24 is a protein called uL24.

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

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

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

- Molecule 26 is a protein called uL15.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 27 is a protein called eL29.

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

- Molecule 28 is a protein called eL30.

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

- Molecule 29 is a protein called eL31.

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

- Molecule 30 is a protein called eL32.

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

- Molecule 31 is a protein called eL33.

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

- Molecule 32 is a protein called eL34.

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

- Molecule 33 is a protein called uL29.

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

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

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

- Molecule 35 is a protein called Ribosomal protein L37.

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

- Molecule 36 is a protein called eL38.

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

- Molecule 37 is a protein called eL39.

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

- Molecule 38 is a protein called eL40.

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

- Molecule 39 is a protein called eL41.

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

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

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

- Molecule 43 is a protein called uL10.

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

- Molecule 44 is a protein called uL11.

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

- Molecule 45 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	1	7	Total	C	N	O	0	0
			49	31	8	10		

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 52 is a protein called uS2.

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

- Molecule 53 is a protein called 40S ribosomal protein S3a.

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

- Molecule 54 is a protein called uS5.

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

- Molecule 55 is a protein called uS3.

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

- Molecule 56 is a protein called eS4.

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

- Molecule 57 is a protein called uS7.

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

- Molecule 58 is a protein called 40S ribosomal protein S6.

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

- Molecule 59 is a protein called eS7.

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

- Molecule 60 is a protein called 40S ribosomal protein S8.

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 Ribosomal protein S9 (Predicted).

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

- Molecule 62 is a protein called eS10.

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

- Molecule 63 is a protein called uS17.

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

- Molecule 64 is a protein called 40S ribosomal protein S12.



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

- Molecule 65 is a protein called uS15.

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

- Molecule 66 is a protein called uS11.

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

- Molecule 67 is a protein called uS19.

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

- Molecule 68 is a protein called uS9.

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

- Molecule 69 is a protein called eS17.

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

- Molecule 70 is a protein called uS13.

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

- Molecule 71 is a protein called eS19.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 72 is a protein called uS10.

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

- Molecule 73 is a protein called eS21.

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

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called 40S ribosomal protein S24.

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

- Molecule 77 is a protein called eS25.

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

- Molecule 78 is a protein called eS26.

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

- Molecule 79 is a protein called 40S ribosomal protein S27.

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

- Molecule 80 is a protein called eS28.

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

- Molecule 81 is a protein called uS14.

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

- Molecule 82 is a protein called eS30.

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

- Molecule 83 is a protein called eS31.

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

- Molecule 84 is a protein called RACK1.

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

- Molecule 85 is a RNA chain called mRNA.

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

- Molecule 86 is a protein called Protein pelota homolog.

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

There are 19 discrepancies between the modelled and reference sequences:

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

- Molecule 87 is a protein called HBS1-like protein.

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

There are 26 discrepancies between the modelled and reference sequences:

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

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

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

*Continued on next page...*

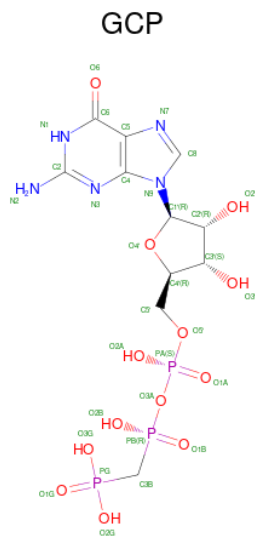
*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
88	e	1	Total 1	Mg 1	0
88	g	1	Total 1	Mg 1	0
88	j	1	Total 1	Mg 1	0
88	5	178	Total 178	Mg 178	0
88	7	5	Total 5	Mg 5	0
88	8	5	Total 5	Mg 5	0
88	9	66	Total 66	Mg 66	0
88	jj	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 PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

### 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.

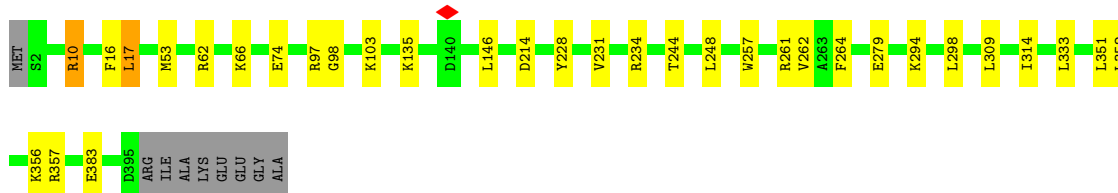
#### • Molecule 1: uL2

Chain A: 




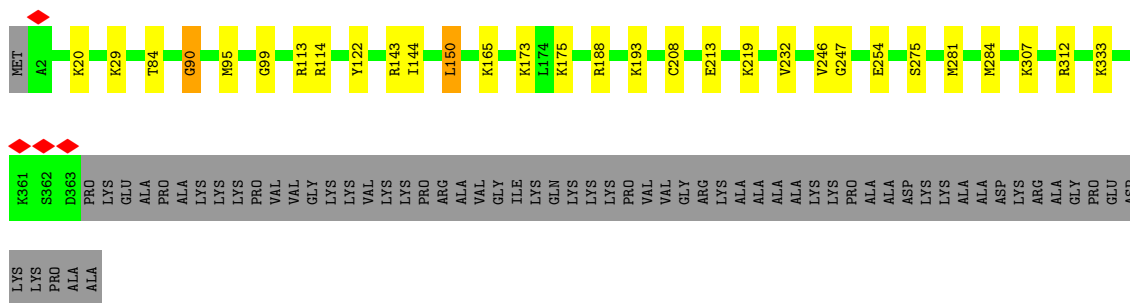
#### • Molecule 2: uL3

Chain B: 



#### • Molecule 3: uL4

Chain C: 



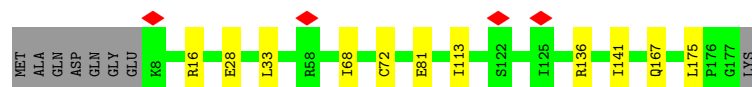
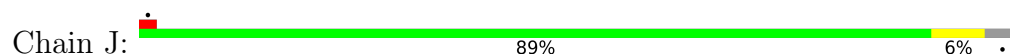
#### • Molecule 4: 60S ribosomal protein L5

Chain D: 

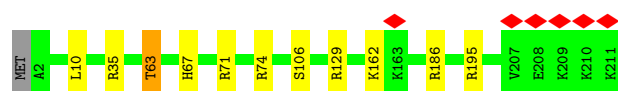




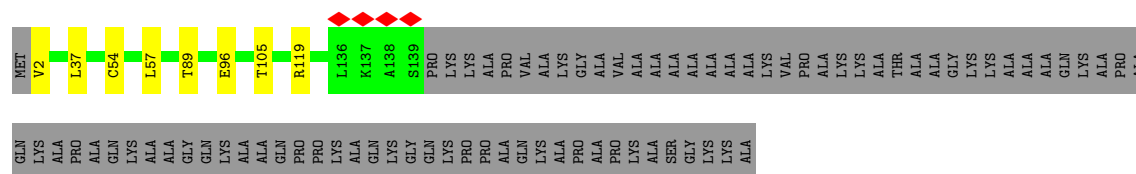
- Molecule 10: uL5



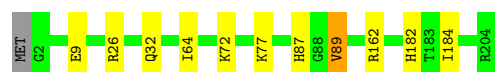
- Molecule 11: eL13



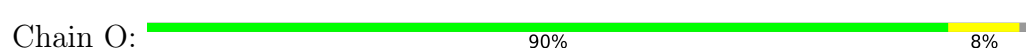
- Molecule 12: eL14



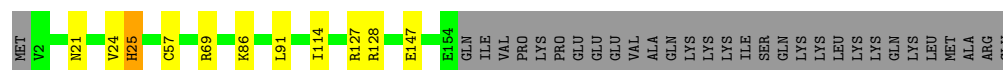
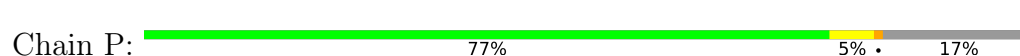
- Molecule 13: Ribosomal protein L15




- Molecule 14: uL13



- Molecule 15: uL22




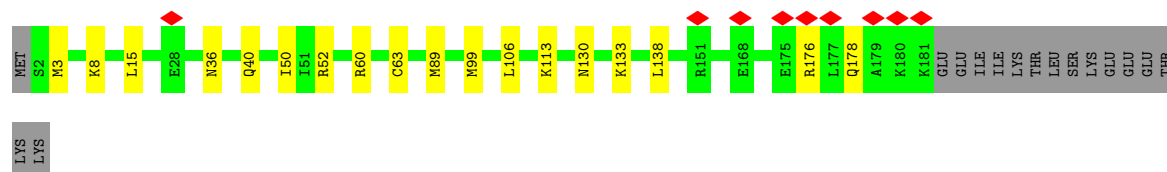
- Molecule 16: eL18

Chain Q:  91% 9%



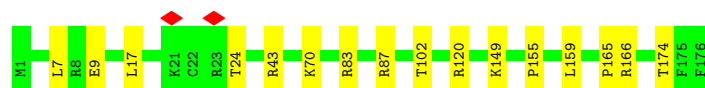
• Molecule 17: eL19

Chain R:  5% 83% 9% 8%



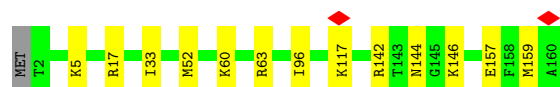
• Molecule 18: eL20

Chain S:  91% 9%




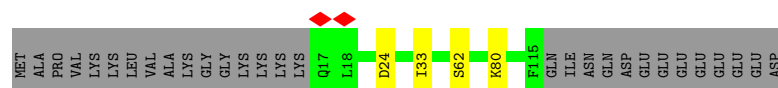
• Molecule 19: eL21

Chain T:  91% 8%




• Molecule 20: eL22

Chain U:  74% 23%



• Molecule 21: uL14

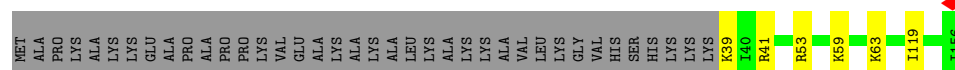
Chain V:  86% 8% 6%



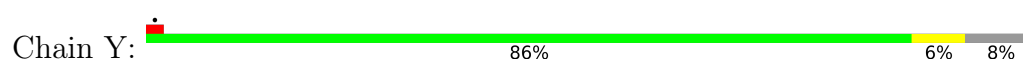
• Molecule 22: eL24

Chain W:  16% 66% 32%

- Molecule 23: uL23



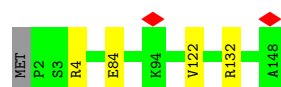
- Molecule 24: uL24



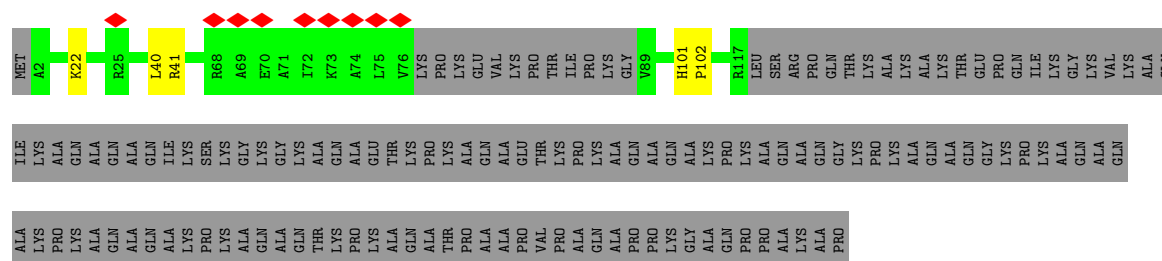
- Molecule 25: 60S ribosomal protein L27



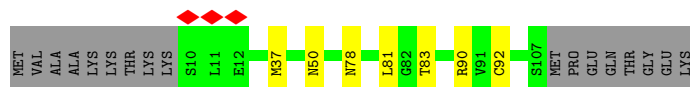
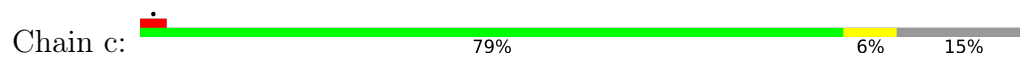
- Molecule 26: uL15



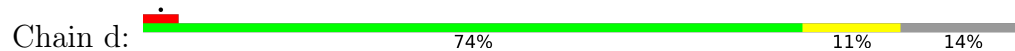
- Molecule 27: eL29



- Molecule 28: eL30



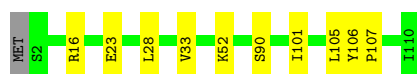
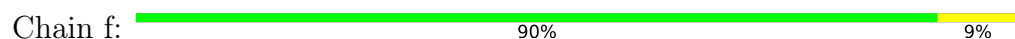
- Molecule 29: eL31



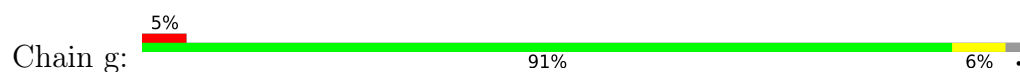
- Molecule 30: eL32



- Molecule 31: eL33



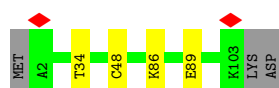
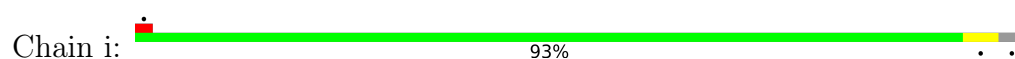
- Molecule 32: eL34




- Molecule 33: uL29

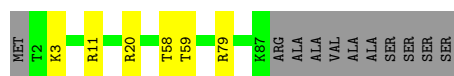


- Molecule 34: 60S ribosomal protein L36



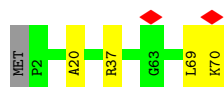
- Molecule 35: Ribosomal protein L37

Chain j:  82% 6% 11%



- Molecule 36: eL38

Chain k:  93% 6%



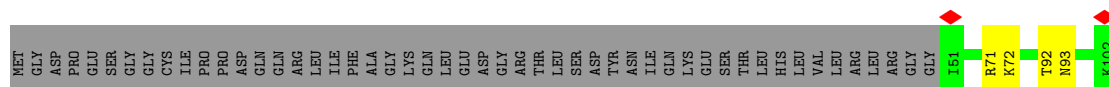
- Molecule 37: eL39

Chain l:  94%



- Molecule 38: eL40

Chain m:  47% 49%



- Molecule 39: eL41

Chain n:  8% 92% 8%




- Molecule 40: eL42

Chain o:  94%




- Molecule 41: eL43

Chain p:  92% 7%



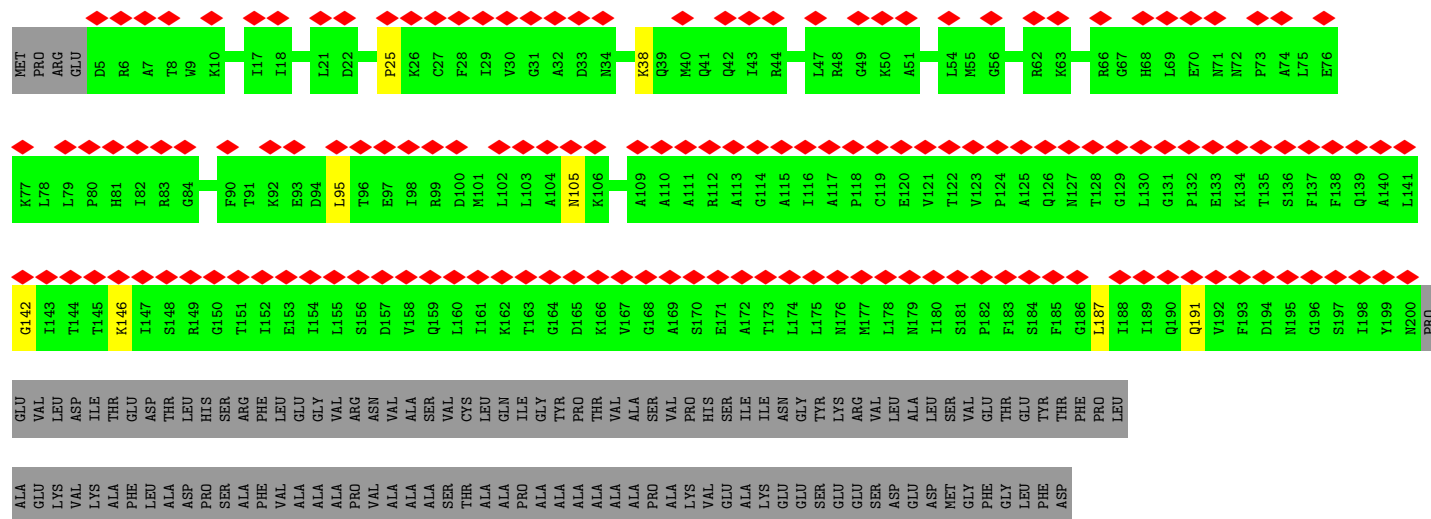
- Molecule 42: eL28

Chain r: 

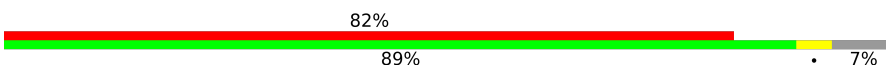


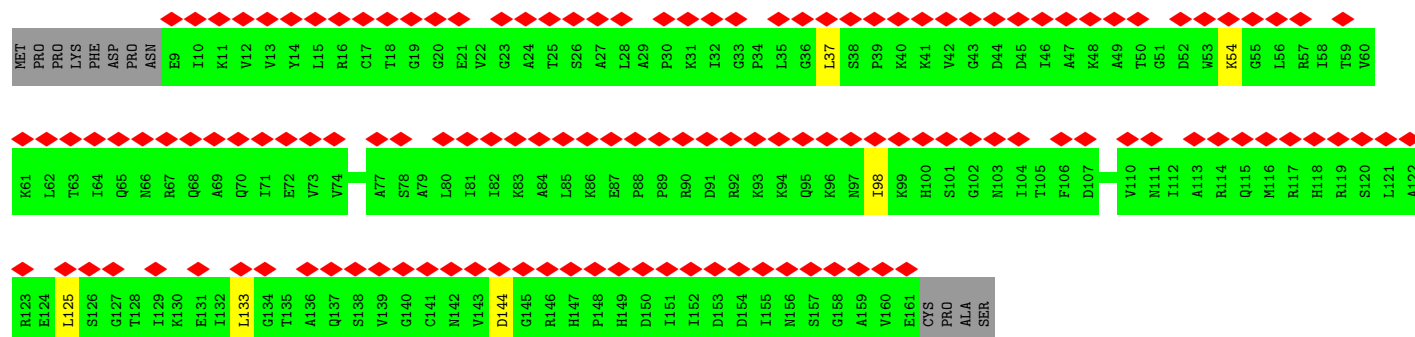
- Molecule 43: uL10

Chain s: 




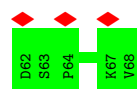
- Molecule 44: uL11

Chain t: 




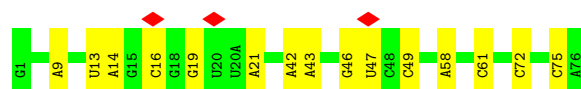
- Molecule 45: Nascent chain

Chain 1: 



- Molecule 46: P-site tRNA

Chain 2:  80% 20%



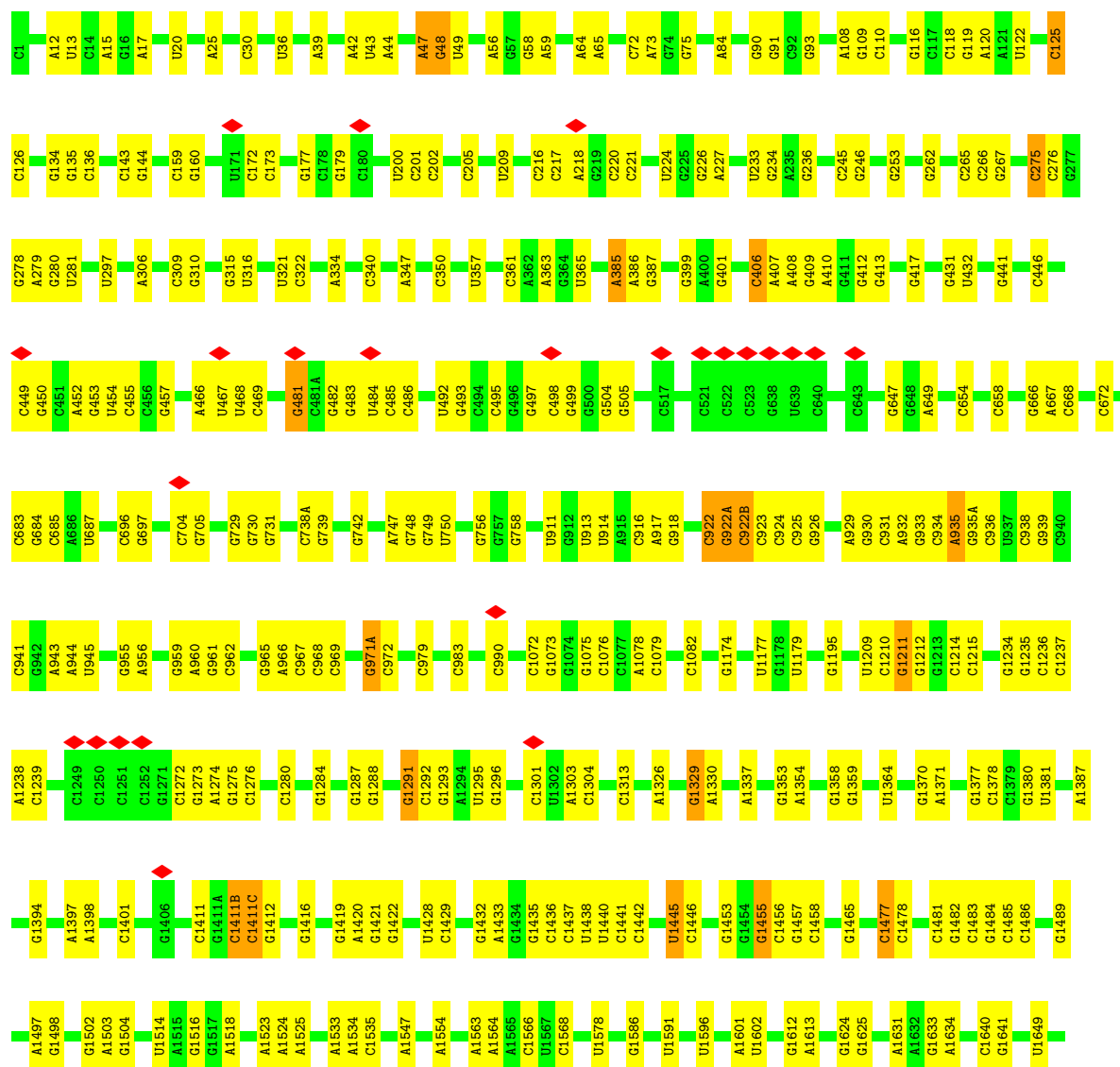
• Molecule 47: E-site tRNA

Chain 3:  23% 71% 29%



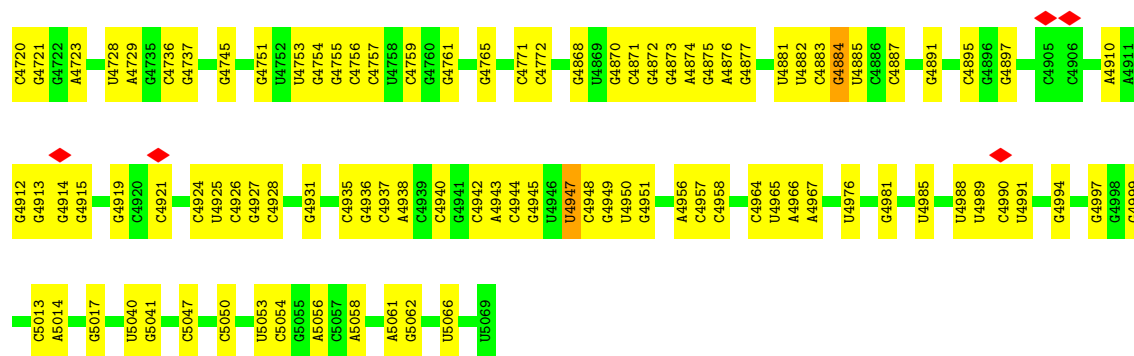
• Molecule 48: 28S ribosomal RNA

Chain 5:  73% 26%

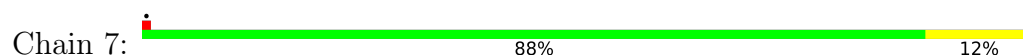




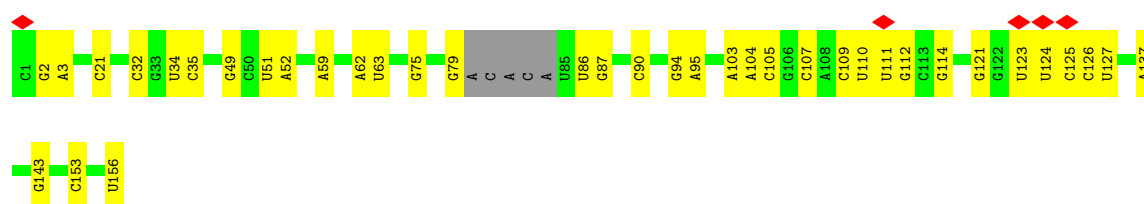
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A4548	G4391	C4237	G4084	U3831	A3692	A2807	A2676	A2502	G2348	G2085	G1976	A1804	A1653
A4549	G4392	A4251	A4085	U3832	C3696	C2814	G2681	C2502	C2351	A2088	C1978	A1805	G1654
A4394	A4393	G4251	G4086	U3833	U3697	C3839	G2686	C2504	G2351	G2089	G1979	G1818	U1656
A4395	U4395	G4254	C4088	U3840	G3698	U2826	U2687	C2505	A2360	U2090	U1980	G1819	C1661
A4396	A4397	A4255	G4092	C3843	G3710	G2827	A2695	A2511	G2364	G2092	G1981	U1821	C1676
A4398	C4398	A4257	A4098	A3859	A3711	U2828	A2696	A2512	G2365	G2093	G1982	U1677	C1678
A4567	G4401	C4258	A4099	G3859	A3712	U2829	A2696	A2513	A2366	C2094	A1983	U1822	G1678
A4570	U4401	U4265	A4098	A3867	G3722	A2835	C2704	A2514	A2395	A2095	A1984	C1828	A1679
A4571	U4404	G4266	C4100	A3867	G3722	A2836	C2704	G2521	A2396	A2097	G1985	G1833	G1691
A4572	U4404	A4267	C4101	G3874	U3729	U2837	U2707	G2521	G2397	U2098	U1986	U1834	U1834
A4573	A4415	A4268	G4107	G3875	G3740	U2838	G2708	A2529	G2397	C2099	C1987	G1835	C1694
A4575	U4419	A4271	A4108	A3876	G3740	U2839	G2709	U2530	G2399	G2100	G1988	G1836	G1694
A4584	U4420	G4272	C4116	A3877	A3748	G2842	G2710	A2537	G2402	A2101	G1989	A1837	G1724
U4585	A4421	A4273	U4117	G3878	A3749	U2843	G2711	G2537	G2402	G2102	A1990	G1842	A1729
U4586	A4422	A4281	U4118	G3879	G3750	A2844	G2712	U2545	G2416	A2103	A1991	G1855	G1733
A4590	G4440	A4281	U4119	G3888	G3751	A2845	G2713	G2546	G2417	A2105	U1992	G1855	G1733
A4599	C4444	G4291	U4120	G3889	G3753	G2855	G2715	G2547	G2421	G2106	C1993	G1869	G1734
A4606	U4448	G4297	G4121	U3892	A3759	U2874	G2716	G2549	G2422	G2108	C1994	U1882	C1740
A4618	A4449	A4304	C4122	G3897	A3760	G2884	G2719	A2553	G2424	A2109	U1997	G1890	G1741
U4619	U4450	G4305	C4125	G3898	C3761	G2884	G2720	U2554	U2425	G2260	G2001	A1891	G1750
U4620	C4453	U4306	C4126	A3901	G3765	G2896	G2721	U2555	A2428	G2261	G2002	A1892	G1750
C4621	C4314	C4314	C4138	G3904	A3766	G2897	G2726	G2563	G2433	G2262	U2004	A1897	G1753
A4622	A4317	A4317	C4162	A3905	U3773	C3598	G2735	G2564	C2441	G2265	G2008	G1910	U1754
U4636	C4318	C4318	U4163	A3906	A3775	G3603	G2735	A2566	G2441	G2266	U2008	G1910	C1755
C4637	C4319	C4319	U4164	G3907	G3776	A3604	G2739	A2566	U2447	U2267	C2011	U1918	U1756
U4652	A4472	G4329	C4165	U3915	G3777	C3605	G2740	U2575	G2450	C2268	G2015	G1919	U1757
C4653	A4474	G4330	G4166	G3916	U3778	U3606	G2743	C2583	G2467	C2269	U2016	C1920	G1762
A4656	C4476	C4331	A4170	A3917	A3779	G3615	A2744	C2583	U2468	G2270	C2017	C1921	G1763
C4661	A4488	C4332	C4171	U3927	G3780	G3618	G2754	A2587	C2469	C2274	A2017	C1922	G1764
C4670	G4496	C4335	G4183	A3938	A3784	G3625	G2760	A2601	G2470	G2275	G2024	C1931	A1765
A4672	U4500	A4336	G4184	G3939	A3785	G3626	U2761	A2611	G2471	A2025	A2026	C1935	A1766
A4510	A4510	C4349	G4191	U3940	U3798	A3630	G2762	G2620	G2475	C2289	U2044	C1938	A1767
A4511	U4512	C4350	G4201	A3942	A3799	A3635	U2763	G2627	G2479	G2045	G2046	G1769	G1768
A4513	A4513	A4355	U4202	A3943	A3799	A3635	U2764	C2627	G2479	G2047	U2048	A1770	U1771
G4514	G4514	G4368	A4203	C3948	G3809	U3644	A2769	G2638	G2483	G2300	G2052	G1951	U1772
G4515	U4067	U4068	A4212	U4067	C3810	A3653	A2787	A2647	G2487	G2301	G2052	G1952	U1773
C4519	U4069	U4069	U4218	U4069	C3811	A3662	U2788	G2647	G2488	A2313	G2055	G1961	A1776
G4520	U4070	U4070	U4218	U4070	C3812	A3667	A2789	A2660	C2489	G2314	G2056	C1962	U1781
A4524	U4071	U4071	C4221	G3817	G3813	C3672	U2794	U2661	U2490	C2325	G2062	C1966	C1785
G4527	A4072	A4072	C4222	G3671	C3819	G3672	A2795	G2662	C2491	C2325	G2063	C1966	A1786
U4709	A4073	A4073	A4379	G3672	U3822	C3673	G2796	G2663	G2493	A2332	G2064	C1967	A1787
C4719	C4074	U4075	U4229	C3673	U3822	C3673	G2797	C2669	U2494	C2068	A2069	G1799	
	U4075		U4232		A2798		A2798	C2670			C2072		



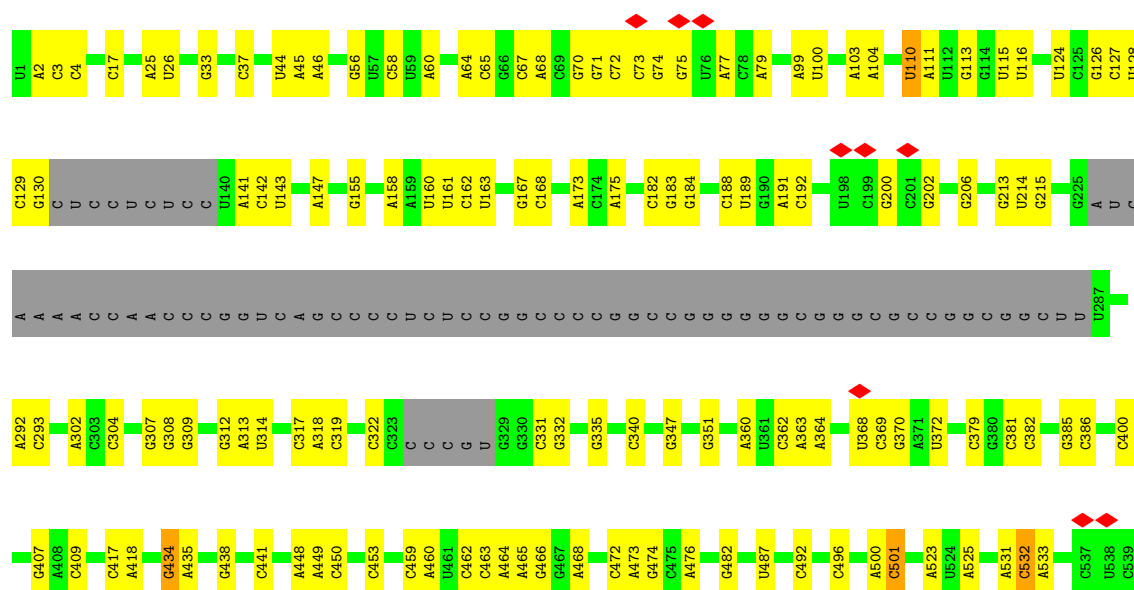
• Molecule 49: 5S ribosomal RNA

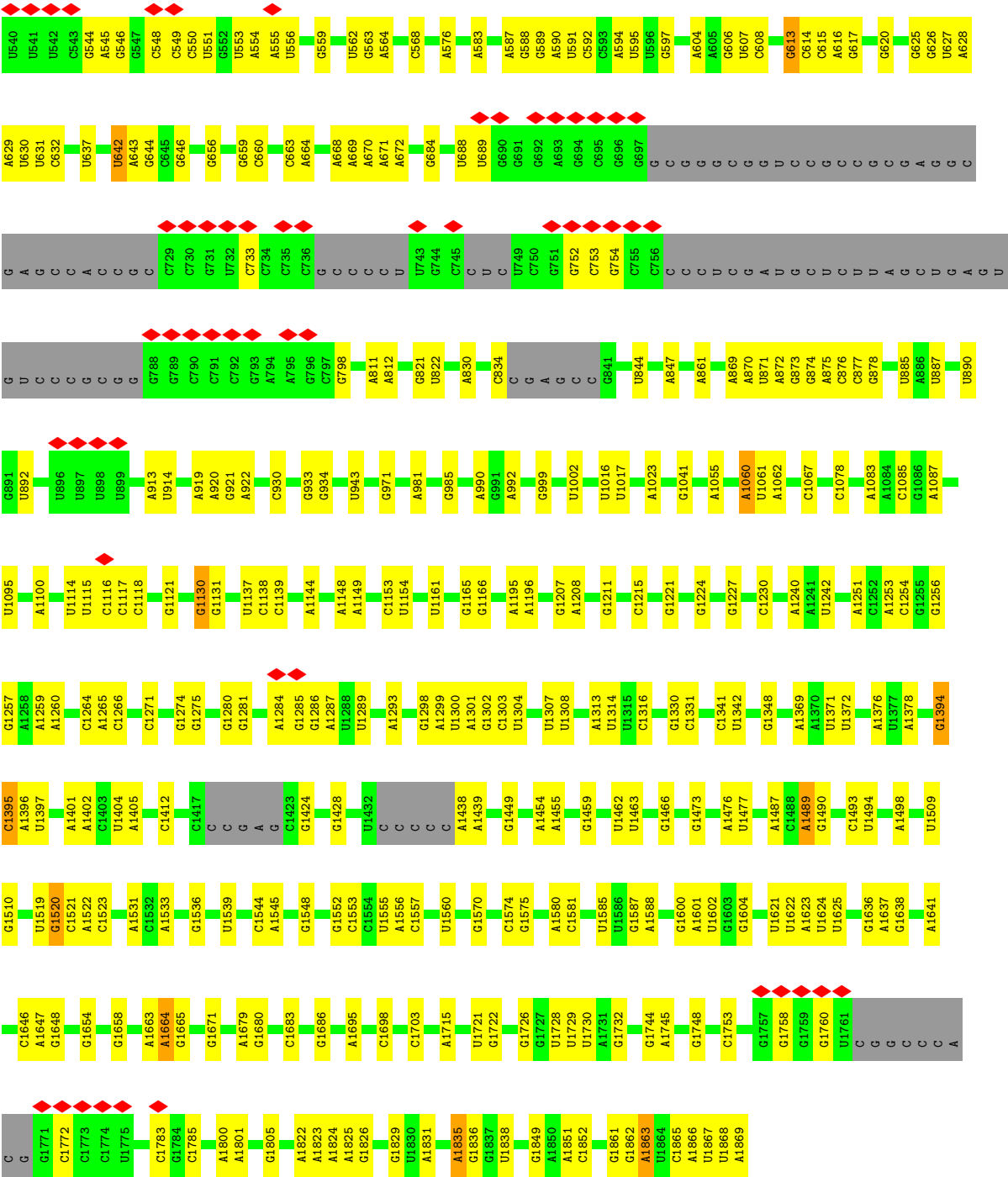


• Molecule 50: 5.8S ribosomal RNA

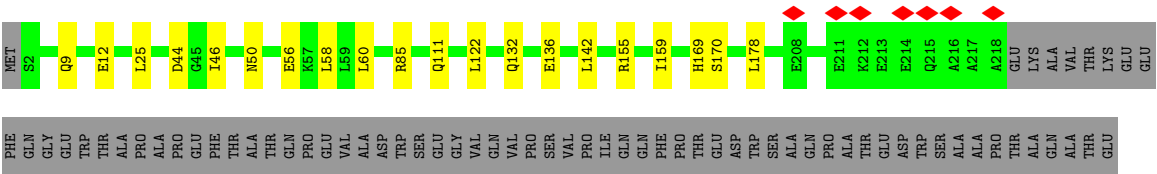


• Molecule 51: 18S ribosomal RNA

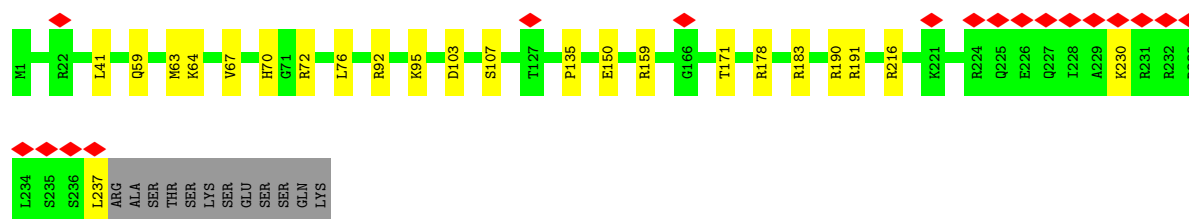




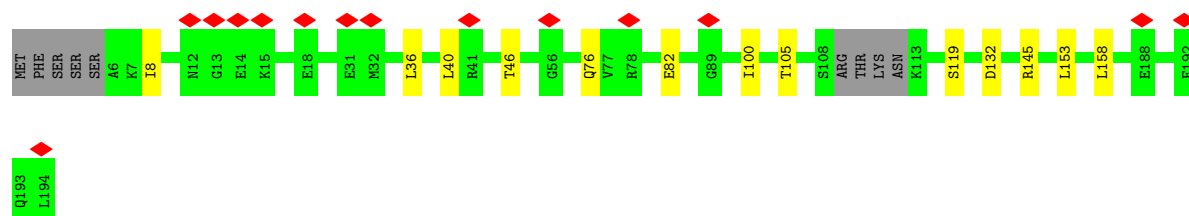
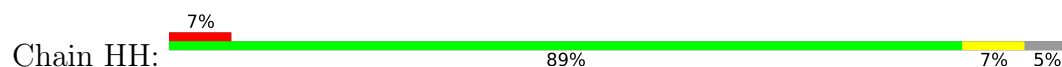
• Molecule 52: uS2



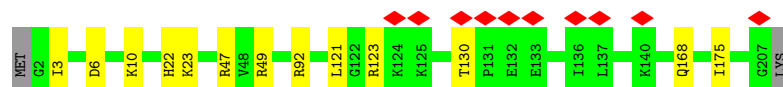




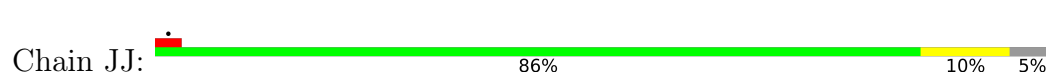
- Molecule 59: eS7



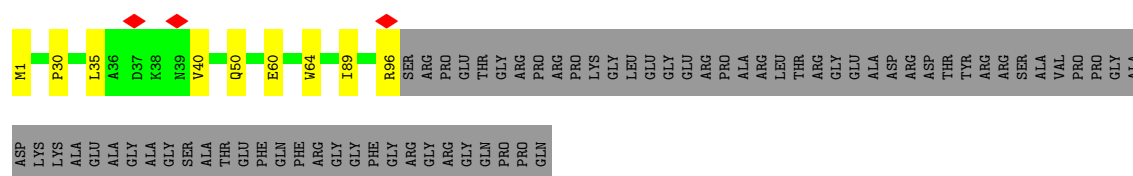
- Molecule 60: 40S ribosomal protein S8



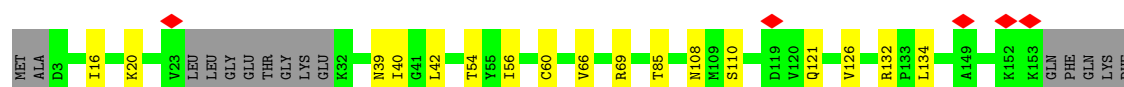
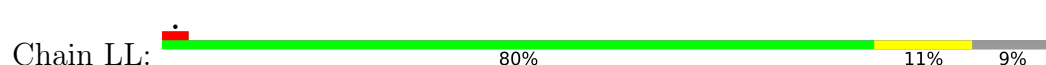
- Molecule 61: Ribosomal protein S9 (Predicted)



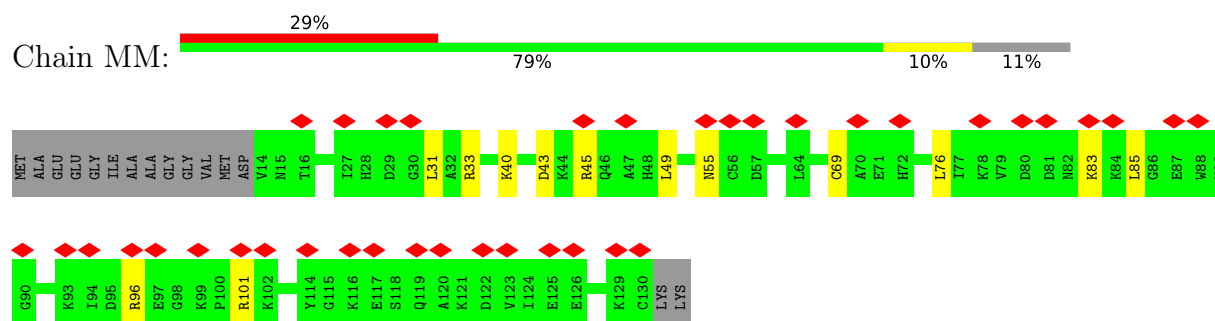
- Molecule 62: eS10



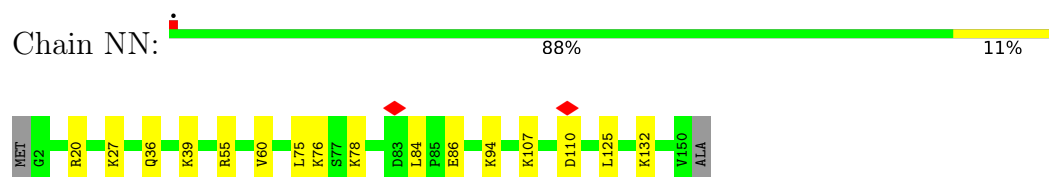
- Molecule 63: uS17



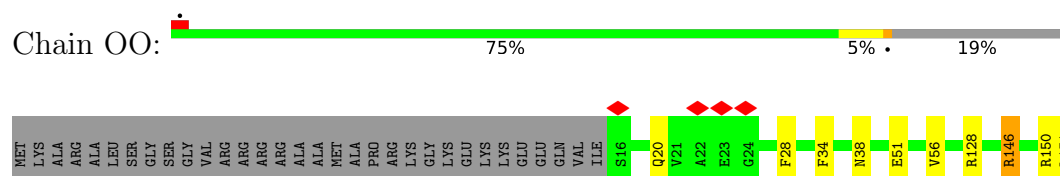
- Molecule 64: 40S ribosomal protein S12



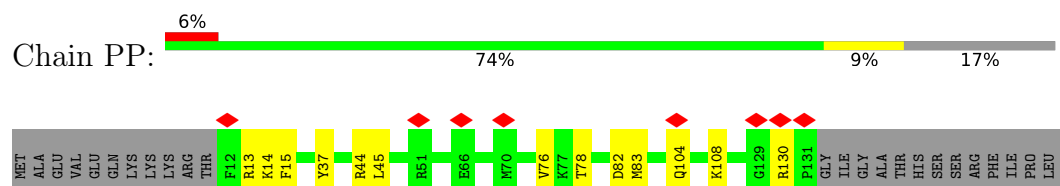
- Molecule 65: uS15



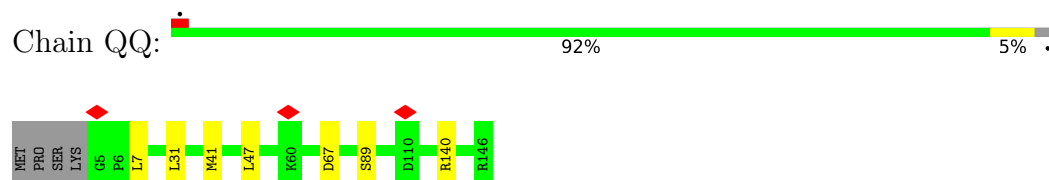
- Molecule 66: uS11



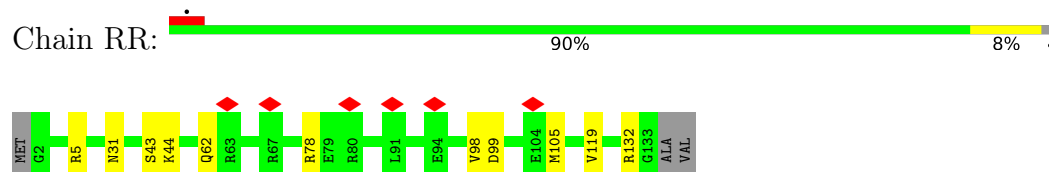
- Molecule 67: uS19



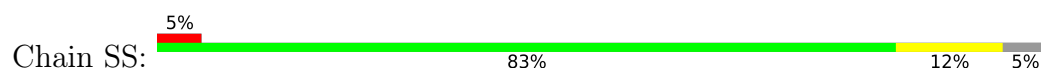
- Molecule 68: uS9



- Molecule 69: eS17



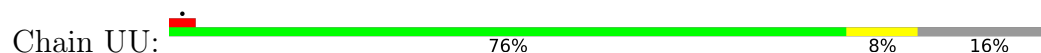
- Molecule 70: uS13



- Molecule 71: eS19



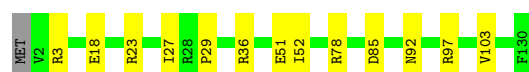
- Molecule 72: uS10



- Molecule 73: eS21



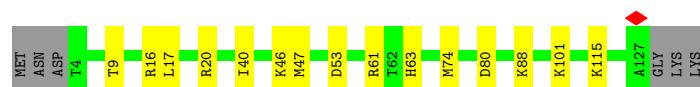
- Molecule 74: uS8



- Molecule 75: uS12

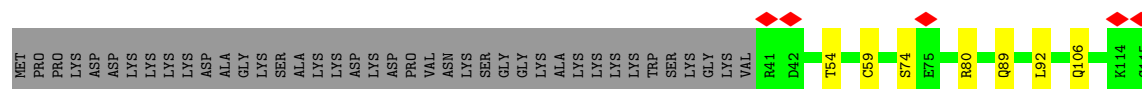


- Molecule 76: 40S ribosomal protein S24




- Molecule 77: eS25

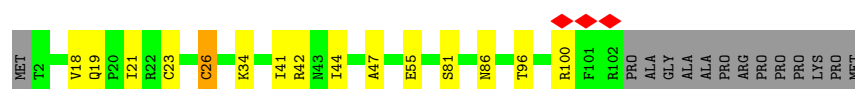
Chain ZZ: 




GLY  
ASP  
ALA  
PRO  
ALA  
ALA  
GLY  
GLU  
ASP  
ALA

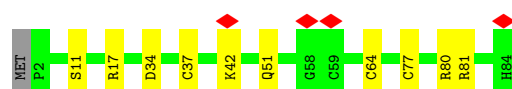
• Molecule 78: eS26

Chain aa: 




• Molecule 79: 40S ribosomal protein S27

Chain bb: 



• Molecule 80: eS28

Chain cc: 




• Molecule 81: uS14

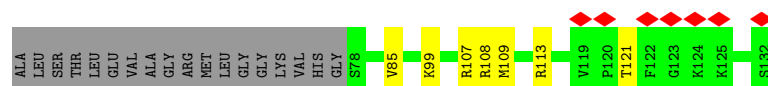
Chain dd: 



• Molecule 82: eS30

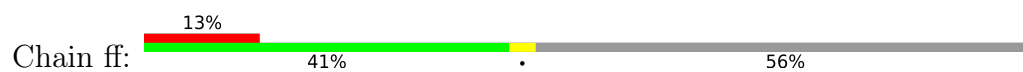
Chain ee: 

MET, GLN, LEU, PHE, VAL, ARG, ALA, GLN, GLU, LEU, HIS, THR, LEU, GLU, VAL, THR, GLY, ARG, GLU, THR, VAL, VAL, ALA, GLN, ILE, LYS, ALA, HIS, VAL, ALA, SER, LEU, GLU, GLY, ILE, ALA, PRO, GLU, ASP, GLN, VAL, VAL, LEU, LEU, ALA, GLY, THR, PRO, LEU, GLU, ASP, GLU, ALA, THR, LEU, LEU, GLN, CYS, GLY, VAL, GLU

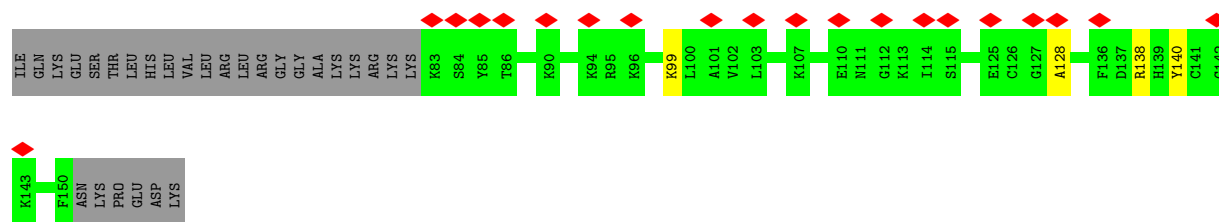


• Molecule 83: eS31

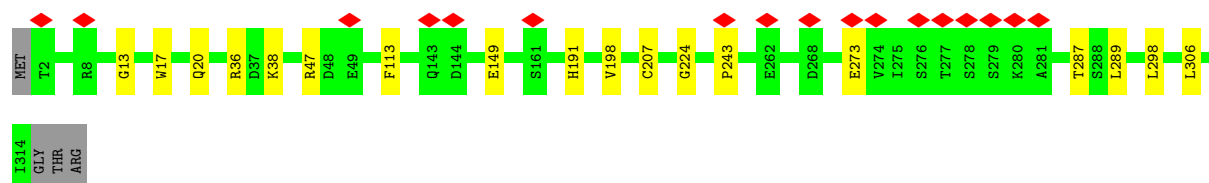
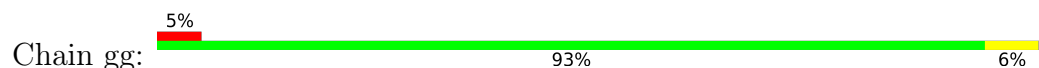




MET GLN ILE PHE VAL SER THR LEU THR GLY LYS THR ILE THR GLY VAL GLU VAL PRO SER ASP THR ILE GLU ASN VAL LYS ALA ILE ILE GLN ASP LYS GLU ILE PRO PRO ASP GLN GLN ARG LEU ILE PHE ALA GLY LYS GLN LEU GLU ASP GLY ARG THR LEU SER ASP TYR ASN



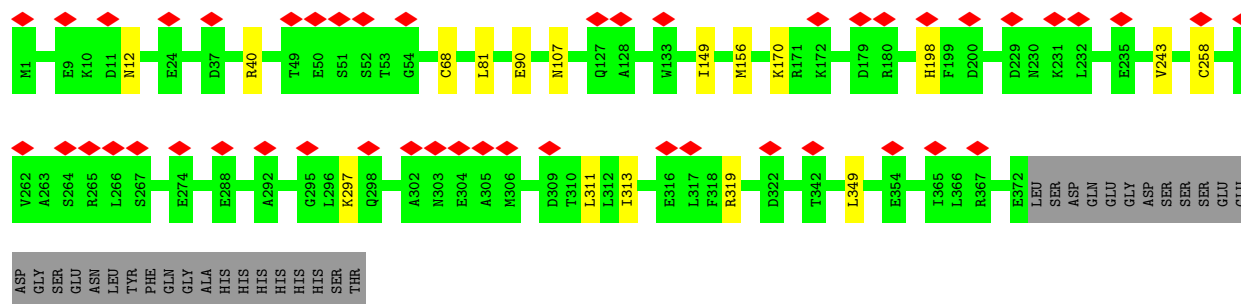
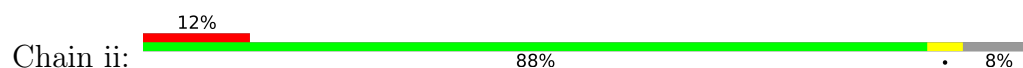
• Molecule 84: RACK1



• Molecule 85: mRNA



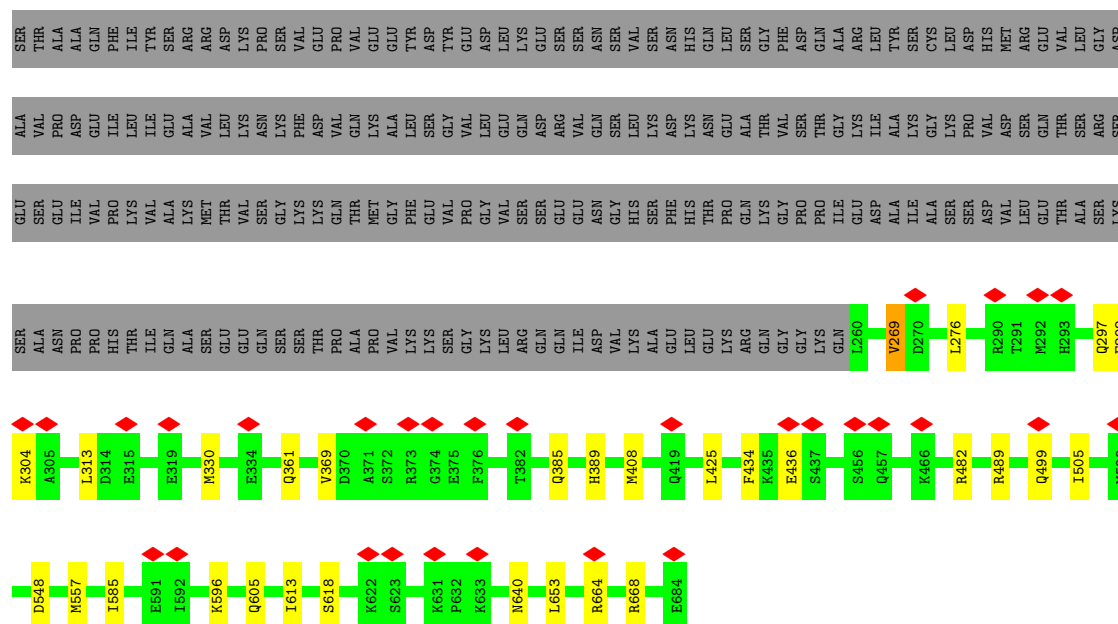
• Molecule 86: Protein pelota homolog



• Molecule 87: HBS1-like protein



MET ASP TYR LYS ASP HIS ASP GLY TYR LYS ASP HIS ASP ILE ASP TYR LYS ASP ASP MET ARG HIS ARG ASN VAL ARG TYR ASN TYR ASP PHE ASP ASP ASP LEU TYR GLY GLN SER VAL ASP ASP ASP CYS ILE SER PRO



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58773	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.747	Depositor
Minimum map value	-0.536	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	562.8, 562.8, 562.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3399999, 1.3399999, 1.3399999	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GCP, 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	0.44	0/1936	0.79	0/2596
2	B	0.48	0/3240	0.75	1/4339 (0.0%)
3	C	0.46	0/2937	0.77	2/3946 (0.1%)
4	D	0.39	0/2437	0.69	2/3264 (0.1%)
5	E	0.38	0/1762	0.69	0/2362
6	F	0.54	0/1911	0.79	0/2549
7	G	0.40	0/1910	0.68	0/2569
8	H	0.42	0/1535	0.69	0/2063
9	I	0.43	0/1702	0.69	0/2272
10	J	0.40	0/1385	0.70	0/1852
11	L	0.41	0/1733	0.74	0/2316
12	M	0.44	0/1158	0.72	0/1547
13	N	0.43	0/1746	0.78	0/2338
14	O	0.44	0/1662	0.73	0/2222
15	P	0.49	0/1268	0.73	0/1700
16	Q	0.44	0/1539	0.82	0/2054
17	R	0.41	0/1524	0.74	1/2013 (0.0%)
18	S	0.54	0/1501	0.79	1/2012 (0.0%)
19	T	0.42	0/1326	0.70	0/1770
20	U	0.39	0/823	0.64	0/1104
21	V	0.45	0/993	0.72	0/1332
22	W	0.45	0/873	0.62	0/1158
23	X	0.37	0/984	0.66	0/1323
24	Y	0.42	0/1132	0.72	0/1504
25	Z	0.44	0/1130	0.70	0/1507
26	a	0.44	0/1191	0.72	0/1590
27	b	0.37	0/861	0.63	0/1138
28	c	0.40	0/771	0.60	0/1034
29	d	0.44	0/903	0.75	0/1216
30	e	0.45	0/1071	0.74	0/1429
31	f	0.48	0/895	0.78	0/1198
32	g	0.42	0/916	0.74	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	h	0.36	0/1021	0.66	0/1348
34	i	0.43	0/841	0.69	0/1112
35	j	0.45	0/720	0.77	0/952
36	k	0.35	0/575	0.60	0/761
37	l	0.43	0/459	0.70	0/608
38	m	0.47	0/435	0.72	0/575
39	n	0.39	0/240	0.77	0/305
40	o	0.44	0/864	0.70	0/1140
41	p	0.47	0/718	0.70	0/953
42	r	0.47	0/1010	0.76	0/1354
43	s	0.37	0/1530	0.49	0/2064
44	t	0.36	0/1174	0.52	0/1582
45	1	0.48	0/49	0.59	0/65
46	2	0.26	0/1805	0.66	0/2809
47	3	0.23	0/1777	0.66	0/2763
48	5	0.41	15/84961 (0.0%)	0.78	53/132460 (0.0%)
49	7	0.37	0/2858	0.67	0/4455
50	8	0.38	0/3581	0.70	0/5577
51	9	0.37	3/40523 (0.0%)	0.73	14/63130 (0.0%)
52	AA	0.40	0/1747	0.67	0/2374
53	BB	0.38	0/1756	0.64	0/2350
54	CC	0.40	0/1753	0.70	0/2369
55	DD	0.37	0/1796	0.65	0/2417
56	EE	0.37	0/2118	0.69	0/2849
57	FF	0.35	0/1492	0.66	0/2005
58	GG	0.37	0/1946	0.69	0/2590
59	HH	0.36	0/1510	0.61	0/2022
60	II	0.40	0/1715	0.72	0/2287
61	JJ	0.40	0/1550	0.76	0/2069
62	KK	0.39	0/834	0.61	0/1125
63	LL	0.41	0/1195	0.73	0/1597
64	MM	0.37	0/918	0.62	0/1233
65	NN	0.40	0/1226	0.74	0/1649
66	OO	0.42	0/1029	0.83	1/1380 (0.1%)
67	PP	0.40	0/1017	0.71	0/1358
68	QQ	0.36	0/1146	0.66	0/1534
69	RR	0.37	0/1082	0.65	0/1452
70	SS	0.37	0/1208	0.70	0/1618
71	TT	0.37	0/1115	0.66	0/1493
72	UU	0.37	0/805	0.68	0/1081
73	VV	0.41	0/643	0.73	0/860
74	WW	0.45	0/1051	0.79	2/1406 (0.1%)
75	XX	0.43	0/1116	0.75	1/1490 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	YY	0.37	0/1028	0.67	0/1366
77	ZZ	0.36	0/604	0.66	0/810
78	aa	0.42	0/828	0.80	0/1109
79	bb	0.37	0/665	0.65	0/891
80	cc	0.37	0/490	0.73	0/656
81	dd	0.43	0/470	0.72	0/623
82	ee	0.38	0/447	0.70	0/587
83	ff	0.37	0/567	0.53	0/753
84	gg	0.34	0/2493	0.59	0/3394
85	hh	0.28	0/188	0.79	0/290
86	ii	0.34	0/2996	0.58	0/4050
87	jj	0.34	0/3352	0.57	0/4523
All	All	0.40	18/237792 (0.0%)	0.73	78/348210 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
3	C	0	1
11	L	0	1
13	N	0	1
31	f	0	1
48	5	0	2
56	EE	0	1
74	WW	0	1
75	XX	0	1
78	aa	0	1
80	cc	0	1
All	All	0	13

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	935	A	C5-C6	-15.99	1.26	1.41
48	5	935	A	C6-N1	-12.18	1.27	1.35
48	5	935	A	C2-N3	10.23	1.42	1.33
48	5	481	G	N1-C2	-9.91	1.29	1.37
48	5	922(A)	G	O3'-P	9.08	1.72	1.61
48	5	481	G	C5-C6	8.94	1.51	1.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	481	G	C2-N2	-8.56	1.25	1.34
48	5	935	A	N3-C4	7.10	1.39	1.34
48	5	1411(B)	C	O3'-P	7.03	1.69	1.61
48	5	481	G	C2-N3	-6.41	1.27	1.32
48	5	935	A	C6-N6	-6.09	1.29	1.33
48	5	922	C	O3'-P	5.78	1.68	1.61
51	9	613	G	O3'-P	-5.73	1.54	1.61
48	5	441	G	O3'-P	-5.60	1.54	1.61
48	5	4622	A	O3'-P	-5.42	1.54	1.61
51	9	1658	G	O3'-P	-5.20	1.54	1.61
48	5	2836	A	O3'-P	-5.12	1.55	1.61
51	9	1095	U	O3'-P	-5.09	1.55	1.61

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	481	G	N1-C2-N2	-52.63	68.83	116.20
48	5	935	A	C5-C6-N6	-48.73	84.72	123.70
48	5	935	A	N1-C6-N6	-35.80	97.12	118.60
48	5	935	A	C6-N1-C2	-31.95	99.43	118.60
48	5	481	G	N3-C2-N2	-29.88	98.98	119.90
48	5	935	A	C4-C5-C6	-26.98	103.51	117.00
48	5	481	G	C6-N1-C2	-21.12	112.42	125.10
48	5	481	G	C2-N3-C4	-17.67	103.06	111.90
48	5	922	C	C2'-C3'-O3'	12.68	137.40	109.50
48	5	935	A	N3-C4-C5	-11.67	118.63	126.80
48	5	935	A	N1-C2-N3	-10.89	123.86	129.30
51	9	1835	A	C2'-C3'-O3'	9.70	130.85	109.50
4	D	22	ARG	NE-CZ-NH1	8.98	124.79	120.30
48	5	922	C	N1-C1'-C2'	-8.89	102.22	112.00
48	5	922	C	O4'-C4'-C3'	-8.40	95.60	104.00
48	5	3697	U	C2'-C3'-O3'	8.21	127.57	109.50
51	9	1394	G	C2'-C3'-O3'	8.13	127.38	109.50
48	5	1455	G	C2'-C3'-O3'	8.08	127.27	109.50
48	5	3888	G	C2'-C3'-O3'	7.92	126.94	109.50
48	5	2046	G	C2'-C3'-O3'	7.86	126.80	109.50
48	5	1211	G	C2'-C3'-O3'	7.44	125.86	109.50
51	9	434	G	C2'-C3'-O3'	7.40	125.78	109.50
48	5	922	C	C4'-C3'-C2'	-7.20	95.41	102.60
48	5	1834	U	C2'-C3'-O3'	7.16	125.24	109.50
48	5	406	C	C2'-C3'-O3'	7.14	125.21	109.50
48	5	481	G	N3-C4-C5	-7.10	125.05	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	1477	C	C2'-C3'-O3'	7.10	125.11	109.50
48	5	1411	C	C2'-C3'-O3'	-7.04	94.00	109.50
51	9	110	U	C2'-C3'-O3'	6.99	124.88	113.70
48	5	1411	C	C4'-C3'-O3'	6.92	126.84	113.00
48	5	922	C	C5'-C4'-O4'	6.77	117.23	109.10
48	5	125	C	C2'-C3'-O3'	6.64	124.32	113.70
48	5	1428	U	C2'-C3'-O3'	6.62	124.29	113.70
48	5	4947	U	C2'-C3'-O3'	6.61	124.28	113.70
4	D	22	ARG	NE-CZ-NH2	-6.41	117.09	120.30
51	9	1520	G	C4'-C3'-O3'	6.24	125.48	113.00
48	5	922(A)	G	N9-C1'-C2'	6.15	122.00	114.00
2	B	10	ARG	NE-CZ-NH2	6.05	123.32	120.30
48	5	1329	G	C2'-C3'-O3'	6.04	123.37	113.70
48	5	4884	G	C2'-C3'-O3'	6.00	123.30	113.70
48	5	4723	A	N9-C1'-C2'	5.92	121.70	114.00
51	9	1130	G	C4'-C3'-O3'	5.92	124.83	113.00
48	5	1291	G	C2'-C3'-O3'	5.88	123.10	113.70
48	5	2474	G	C2'-C3'-O3'	5.81	123.00	113.70
48	5	481	G	C5-C6-N1	-5.80	108.60	111.50
48	5	47	A	C4'-C3'-O3'	5.76	124.52	113.00
48	5	90	G	C2'-C3'-O3'	5.74	122.88	113.70
48	5	2695	A	C2'-C3'-O3'	5.73	122.87	113.70
51	9	1489	A	C4'-C3'-O3'	5.70	124.39	113.00
48	5	275	C	C2'-C3'-O3'	5.69	122.80	113.70
48	5	385	A	C4'-C3'-O3'	5.62	124.23	113.00
51	9	642	U	C2'-C3'-O3'	5.60	122.65	113.70
51	9	1060	A	N9-C1'-C2'	5.58	121.26	114.00
48	5	922	C	O4'-C1'-N1	5.53	112.62	108.20
48	5	1411(C)	C	C5'-C4'-O4'	5.52	115.72	109.10
48	5	1445	U	C2'-C3'-O3'	5.49	122.49	113.70
17	R	60	ARG	NE-CZ-NH1	5.49	123.05	120.30
48	5	4448	G	C4'-C3'-O3'	5.48	123.95	113.00
51	9	1863	A	O4'-C1'-C2'	-5.42	100.38	105.80
51	9	1664	A	C4'-C3'-O3'	5.41	123.83	113.00
48	5	922(A)	G	P-O3'-C3'	5.39	126.17	119.70
48	5	1818	G	C2'-C3'-O3'	5.37	122.29	113.70
48	5	971(A)	G	C4'-C3'-O3'	5.29	123.58	113.00
48	5	922(B)	C	C5'-C4'-O4'	5.28	115.44	109.10
48	5	3625	G	C2'-C3'-O3'	5.27	122.13	113.70
48	5	48	G	C2'-C3'-O3'	5.20	122.02	113.70
48	5	4653	C	O5'-P-OP2	-5.17	101.05	105.70
74	WW	3	ARG	NE-CZ-NH1	5.17	122.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	150	LEU	CB-CG-CD2	5.16	119.77	111.00
51	9	532	C	C2'-C3'-O3'	5.14	121.93	113.70
51	9	1395	C	C4'-C3'-O3'	5.14	123.28	113.00
51	9	501	C	N1-C1'-C2'	5.12	120.65	114.00
66	OO	146	ARG	NE-CZ-NH1	5.11	122.86	120.30
75	XX	14	ARG	NE-CZ-NH1	5.10	122.85	120.30
48	5	1411	C	O4'-C4'-C3'	-5.07	98.93	104.00
18	S	87	ARG	NE-CZ-NH1	5.01	122.80	120.30
3	C	114	ARG	NE-CZ-NH1	5.01	122.80	120.30
74	WW	3	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	5	481	G	Sidechain
48	5	935	A	Sidechain
2	B	16	PHE	Peptide
2	B	257	TRP	Peptide
3	C	90	GLY	Peptide
56	EE	155	LYS	Peptide
11	L	71	ARG	Peptide
13	N	184	ILE	Peptide
74	WW	27	ILE	Peptide
75	XX	61	GLN	Peptide
78	aa	26	CYS	Peptide
80	cc	20	ARG	Sidechain
31	f	105	LEU	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	246/257 (96%)	220 (89%)	24 (10%)	2 (1%)	16	51
2	B	392/403 (97%)	355 (91%)	35 (9%)	2 (0%)	25	59
3	C	360/425 (85%)	332 (92%)	23 (6%)	5 (1%)	9	40
4	D	291/297 (98%)	278 (96%)	10 (3%)	3 (1%)	13	46
5	E	208/291 (72%)	189 (91%)	19 (9%)	0	100	100
6	F	223/247 (90%)	204 (92%)	16 (7%)	3 (1%)	10	41
7	G	229/319 (72%)	216 (94%)	11 (5%)	2 (1%)	14	48
8	H	188/192 (98%)	172 (92%)	16 (8%)	0	100	100
9	I	201/214 (94%)	177 (88%)	23 (11%)	1 (0%)	25	59
10	J	168/178 (94%)	157 (94%)	9 (5%)	2 (1%)	11	43
11	L	208/211 (99%)	193 (93%)	14 (7%)	1 (0%)	25	59
12	M	136/218 (62%)	125 (92%)	11 (8%)	0	100	100
13	N	201/204 (98%)	181 (90%)	19 (10%)	1 (0%)	25	59
14	O	197/203 (97%)	183 (93%)	13 (7%)	1 (0%)	25	59
15	P	151/184 (82%)	140 (93%)	9 (6%)	2 (1%)	10	41
16	Q	185/188 (98%)	168 (91%)	16 (9%)	1 (0%)	25	59
17	R	178/196 (91%)	171 (96%)	6 (3%)	1 (1%)	22	55
18	S	174/176 (99%)	159 (91%)	12 (7%)	3 (2%)	7	36
19	T	157/160 (98%)	142 (90%)	15 (10%)	0	100	100
20	U	97/128 (76%)	86 (89%)	9 (9%)	2 (2%)	5	32
21	V	129/140 (92%)	113 (88%)	16 (12%)	0	100	100
22	W	102/157 (65%)	93 (91%)	8 (8%)	1 (1%)	13	46
23	X	116/156 (74%)	109 (94%)	6 (5%)	1 (1%)	14	48
24	Y	132/145 (91%)	126 (96%)	5 (4%)	1 (1%)	16	51
25	Z	133/136 (98%)	123 (92%)	8 (6%)	2 (2%)	8	38
26	a	145/148 (98%)	135 (93%)	10 (7%)	0	100	100
27	b	100/245 (41%)	93 (93%)	6 (6%)	1 (1%)	13	46
28	c	96/115 (84%)	89 (93%)	7 (7%)	0	100	100
29	d	105/125 (84%)	94 (90%)	10 (10%)	1 (1%)	13	46
30	e	126/135 (93%)	121 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	f	107/110 (97%)	97 (91%)	8 (8%)	2 (2%)	6	34
32	g	112/117 (96%)	103 (92%)	8 (7%)	1 (1%)	14	48
33	h	120/123 (98%)	116 (97%)	3 (2%)	1 (1%)	16	51
34	i	100/105 (95%)	92 (92%)	8 (8%)	0	100	100
35	j	84/97 (87%)	74 (88%)	9 (11%)	1 (1%)	11	43
36	k	67/70 (96%)	63 (94%)	3 (4%)	1 (2%)	8	38
37	l	48/51 (94%)	41 (85%)	7 (15%)	0	100	100
38	m	50/102 (49%)	46 (92%)	4 (8%)	0	100	100
39	n	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
40	o	102/106 (96%)	92 (90%)	9 (9%)	1 (1%)	13	46
41	p	89/92 (97%)	81 (91%)	7 (8%)	1 (1%)	12	44
42	r	122/137 (89%)	104 (85%)	14 (12%)	4 (3%)	3	24
43	s	194/318 (61%)	174 (90%)	18 (9%)	2 (1%)	13	46
44	t	151/165 (92%)	134 (89%)	15 (10%)	2 (1%)	10	41
45	1	5/7 (71%)	2 (40%)	3 (60%)	0	100	100
52	AA	215/295 (73%)	195 (91%)	19 (9%)	1 (0%)	25	59
53	BB	211/264 (80%)	199 (94%)	12 (6%)	0	100	100
54	CC	219/293 (75%)	202 (92%)	16 (7%)	1 (0%)	25	59
55	DD	226/243 (93%)	206 (91%)	18 (8%)	2 (1%)	14	48
56	EE	260/263 (99%)	242 (93%)	18 (7%)	0	100	100
57	FF	181/204 (89%)	168 (93%)	10 (6%)	3 (2%)	7	36
58	GG	235/249 (94%)	217 (92%)	17 (7%)	1 (0%)	30	64
59	HH	181/194 (93%)	168 (93%)	13 (7%)	0	100	100
60	II	204/208 (98%)	191 (94%)	11 (5%)	2 (1%)	13	46
61	JJ	183/194 (94%)	175 (96%)	8 (4%)	0	100	100
62	KK	94/165 (57%)	85 (90%)	6 (6%)	3 (3%)	3	25
63	LL	139/158 (88%)	124 (89%)	14 (10%)	1 (1%)	19	53
64	MM	115/132 (87%)	99 (86%)	16 (14%)	0	100	100
65	NN	147/151 (97%)	134 (91%)	13 (9%)	0	100	100
66	OO	134/168 (80%)	120 (90%)	13 (10%)	1 (1%)	19	53
67	PP	118/145 (81%)	103 (87%)	14 (12%)	1 (1%)	16	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	QQ	140/146 (96%)	132 (94%)	8 (6%)	0	100	100
69	RR	130/135 (96%)	115 (88%)	14 (11%)	1 (1%)	16	51
70	SS	142/152 (93%)	134 (94%)	8 (6%)	0	100	100
71	TT	139/145 (96%)	131 (94%)	7 (5%)	1 (1%)	19	53
72	UU	98/119 (82%)	92 (94%)	6 (6%)	0	100	100
73	VV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
74	WW	127/130 (98%)	116 (91%)	9 (7%)	2 (2%)	8	37
75	XX	139/143 (97%)	124 (89%)	12 (9%)	3 (2%)	5	31
76	YY	122/130 (94%)	116 (95%)	6 (5%)	0	100	100
77	ZZ	73/125 (58%)	71 (97%)	2 (3%)	0	100	100
78	aa	99/115 (86%)	88 (89%)	9 (9%)	2 (2%)	6	33
79	bb	81/84 (96%)	73 (90%)	7 (9%)	1 (1%)	11	43
80	cc	60/69 (87%)	55 (92%)	3 (5%)	2 (3%)	3	24
81	dd	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
82	ee	53/133 (40%)	50 (94%)	3 (6%)	0	100	100
83	ff	66/156 (42%)	60 (91%)	5 (8%)	1 (2%)	8	38
84	gg	311/317 (98%)	284 (91%)	24 (8%)	3 (1%)	13	46
86	ii	370/403 (92%)	343 (93%)	26 (7%)	1 (0%)	37	69
87	jj	423/710 (60%)	381 (90%)	38 (9%)	4 (1%)	14	48
All	All	12317/14495 (85%)	11302 (92%)	923 (8%)	92 (1%)	21	53

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	236	GLU
18	S	155	PRO
31	f	107	PRO
75	XX	62	PRO
87	jj	605	GLN
1	A	217	GLN
11	L	63	THR
13	N	89	VAL
14	O	200	GLY
20	U	24	ASP
20	U	62	SER

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Mol	Chain	Res	Type
22	W	27	LYS
29	d	58	GLY
33	h	89	ARG
42	r	11	ARG
42	r	68	SER
43	s	142	GLY
44	t	125	LEU
66	OO	20	GLN
75	XX	61	GLN
75	XX	86	PRO
84	gg	224	GLY
87	jj	269	VAL
1	A	14	SER
3	C	275	SER
6	F	99	GLY
7	G	105	THR
10	J	141	ILE
15	P	25	HIS
18	S	166	ARG
31	f	106	TYR
35	j	59	THR
42	r	33	LYS
52	AA	159	ILE
78	aa	47	ALA
80	cc	22	GLY
87	jj	596	LYS
2	B	17	LEU
4	D	44	TYR
16	Q	14	ARG
17	R	3	MET
25	Z	90	PRO
25	Z	91	LEU
55	DD	93	THR
57	FF	21	GLY
57	FF	63	LYS
60	II	123	ARG
62	KK	64	TRP
67	PP	82	ASP
74	WW	78	ARG
78	aa	26	CYS
86	ii	12	ASN
3	C	254	GLU

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Mol	Chain	Res	Type
4	D	119	TYR
6	F	125	ASN
24	Y	78	TYR
36	k	20	ALA
40	o	96	ASP
43	s	25	PRO
44	t	54	LYS
57	FF	43	GLU
62	KK	30	PRO
63	LL	66	VAL
71	TT	109	GLY
80	cc	18	LEU
83	ff	128	ALA
7	G	216	PRO
18	S	165	PRO
27	b	102	PRO
41	p	51	ALA
69	RR	119	VAL
74	WW	29	PRO
79	bb	51	GLN
87	jj	618	SER
10	J	68	ILE
58	GG	135	PRO
3	C	90	GLY
3	C	99	GLY
4	D	125	VAL
15	P	114	ILE
23	X	119	ILE
32	g	48	VAL
55	DD	48	ILE
62	KK	40	VAL
2	B	98	GLY
3	C	247	GLY
9	I	135	ILE
54	CC	171	GLY
84	gg	13	GLY
42	r	29	PRO
60	II	3	ILE
84	gg	243	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/199 (96%)	176 (93%)	14 (7%)	11	36
2	B	342/348 (98%)	312 (91%)	30 (9%)	8	31
3	C	302/347 (87%)	278 (92%)	24 (8%)	10	34
4	D	247/250 (99%)	236 (96%)	11 (4%)	23	53
5	E	190/251 (76%)	179 (94%)	11 (6%)	17	44
6	F	196/215 (91%)	177 (90%)	19 (10%)	6	27
7	G	200/272 (74%)	186 (93%)	14 (7%)	12	39
8	H	169/171 (99%)	155 (92%)	14 (8%)	9	32
9	I	175/181 (97%)	161 (92%)	14 (8%)	10	34
10	J	143/149 (96%)	134 (94%)	9 (6%)	15	43
11	L	175/176 (99%)	165 (94%)	10 (6%)	17	45
12	M	117/161 (73%)	109 (93%)	8 (7%)	13	40
13	N	171/172 (99%)	161 (94%)	10 (6%)	17	44
14	O	171/173 (99%)	156 (91%)	15 (9%)	8	31
15	P	134/163 (82%)	124 (92%)	10 (8%)	11	36
16	Q	164/165 (99%)	149 (91%)	15 (9%)	7	30
17	R	159/175 (91%)	143 (90%)	16 (10%)	6	26
18	S	157/157 (100%)	145 (92%)	12 (8%)	11	35
19	T	139/140 (99%)	126 (91%)	13 (9%)	7	29
20	U	89/114 (78%)	87 (98%)	2 (2%)	47	70
21	V	101/107 (94%)	90 (89%)	11 (11%)	5	24
22	W	86/126 (68%)	85 (99%)	1 (1%)	67	81
23	X	106/134 (79%)	101 (95%)	5 (5%)	22	52
24	Y	124/135 (92%)	116 (94%)	8 (6%)	14	41
25	Z	117/118 (99%)	112 (96%)	5 (4%)	25	54
26	a	119/120 (99%)	115 (97%)	4 (3%)	32	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	b	84/184 (46%)	80 (95%)	4 (5%)	21	51
28	c	84/98 (86%)	77 (92%)	7 (8%)	9	32
29	d	98/110 (89%)	85 (87%)	13 (13%)	3	18
30	e	114/121 (94%)	106 (93%)	8 (7%)	12	39
31	f	88/89 (99%)	81 (92%)	7 (8%)	10	34
32	g	98/100 (98%)	92 (94%)	6 (6%)	15	43
33	h	109/110 (99%)	104 (95%)	5 (5%)	23	52
34	i	86/89 (97%)	82 (95%)	4 (5%)	22	52
35	j	73/80 (91%)	68 (93%)	5 (7%)	13	40
36	k	64/65 (98%)	61 (95%)	3 (5%)	22	52
37	l	47/48 (98%)	45 (96%)	2 (4%)	25	54
38	m	48/90 (53%)	44 (92%)	4 (8%)	9	32
39	n	24/24 (100%)	22 (92%)	2 (8%)	9	32
40	o	92/94 (98%)	89 (97%)	3 (3%)	33	61
41	p	74/75 (99%)	69 (93%)	5 (7%)	13	40
42	r	108/121 (89%)	97 (90%)	11 (10%)	6	26
43	s	164/258 (64%)	158 (96%)	6 (4%)	29	58
44	t	126/137 (92%)	122 (97%)	4 (3%)	34	62
45	1	6/6 (100%)	6 (100%)	0	100	100
52	AA	180/245 (74%)	161 (89%)	19 (11%)	5	24
53	BB	194/231 (84%)	176 (91%)	18 (9%)	7	29
54	CC	187/225 (83%)	170 (91%)	17 (9%)	7	30
55	DD	190/202 (94%)	173 (91%)	17 (9%)	8	31
56	EE	224/225 (100%)	204 (91%)	20 (9%)	8	31
57	FF	158/170 (93%)	147 (93%)	11 (7%)	12	39
58	GG	207/218 (95%)	185 (89%)	22 (11%)	5	24
59	HH	165/174 (95%)	152 (92%)	13 (8%)	10	34
60	II	178/180 (99%)	167 (94%)	11 (6%)	15	43
61	JJ	161/168 (96%)	142 (88%)	19 (12%)	4	21
62	KK	87/136 (64%)	81 (93%)	6 (7%)	13	39
63	LL	130/142 (92%)	114 (88%)	16 (12%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	MM	99/108 (92%)	86 (87%)	13 (13%)	3	18
65	NN	130/131 (99%)	114 (88%)	16 (12%)	4	20
66	OO	106/130 (82%)	97 (92%)	9 (8%)	8	32
67	PP	109/130 (84%)	97 (89%)	12 (11%)	5	24
68	QQ	117/121 (97%)	110 (94%)	7 (6%)	16	43
69	RR	119/121 (98%)	109 (92%)	10 (8%)	9	32
70	SS	125/132 (95%)	107 (86%)	18 (14%)	2	16
71	TT	111/115 (96%)	102 (92%)	9 (8%)	9	34
72	UU	92/107 (86%)	83 (90%)	9 (10%)	6	27
73	VV	67/67 (100%)	63 (94%)	4 (6%)	16	43
74	WW	112/113 (99%)	103 (92%)	9 (8%)	10	34
75	XX	113/115 (98%)	105 (93%)	8 (7%)	12	38
76	YY	107/112 (96%)	92 (86%)	15 (14%)	3	16
77	ZZ	66/103 (64%)	59 (89%)	7 (11%)	5	24
78	aa	88/98 (90%)	75 (85%)	13 (15%)	2	15
79	bb	75/76 (99%)	66 (88%)	9 (12%)	4	20
80	cc	55/62 (89%)	47 (86%)	8 (14%)	2	15
81	dd	48/49 (98%)	44 (92%)	4 (8%)	9	32
82	ee	46/106 (43%)	39 (85%)	7 (15%)	2	14
83	ff	61/140 (44%)	58 (95%)	3 (5%)	21	50
84	gg	272/275 (99%)	257 (94%)	15 (6%)	18	46
86	ii	326/353 (92%)	310 (95%)	16 (5%)	21	50
87	jj	358/608 (59%)	331 (92%)	27 (8%)	11	36
All	All	10733/12306 (87%)	9892 (92%)	841 (8%)	13	34

All (841) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	64	ARG
1	A	102	LEU
1	A	125	LYS
1	A	128	ARG
1	A	163	ARG

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Mol	Chain	Res	Type
1	A	165	VAL
1	A	175	ILE
1	A	200	ARG
1	A	209	HIS
1	A	221	LYS
1	A	227	ARG
1	A	233	ARG
1	A	242	ARG
2	B	10	ARG
2	B	17	LEU
2	B	53	MET
2	B	62	ARG
2	B	66	LYS
2	B	74	GLU
2	B	97	ARG
2	B	103	LYS
2	B	135	LYS
2	B	146	LEU
2	B	214	ASP
2	B	228	TYR
2	B	231	VAL
2	B	234	ARG
2	B	244	THR
2	B	248	LEU
2	B	261	ARG
2	B	262	VAL
2	B	264	PHE
2	B	279	GLU
2	B	294	LYS
2	B	298	LEU
2	B	309	LEU
2	B	314	ILE
2	B	333	LEU
2	B	351	LEU
2	B	352	LEU
2	B	356	LYS
2	B	357	ARG
2	B	383	GLU
3	C	20	LYS
3	C	29	LYS
3	C	84	THR
3	C	95	MET

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Mol	Chain	Res	Type
3	C	113	ARG
3	C	122	TYR
3	C	143	ARG
3	C	144	ILE
3	C	150	LEU
3	C	165	LYS
3	C	173	LYS
3	C	175	LYS
3	C	188	ARG
3	C	193	LYS
3	C	208	CYS
3	C	213	GLU
3	C	219	LYS
3	C	232	VAL
3	C	246	VAL
3	C	281	MET
3	C	284	MET
3	C	307	LYS
3	C	312	ARG
3	C	333	LYS
4	D	22	ARG
4	D	33	ARG
4	D	37	VAL
4	D	50	ARG
4	D	56	THR
4	D	89	LYS
4	D	104	LEU
4	D	124	GLU
4	D	208	MET
4	D	264	LYS
4	D	268	ARG
5	E	52	LEU
5	E	58	ARG
5	E	112	LEU
5	E	141	ARG
5	E	143	LEU
5	E	144	ARG
5	E	169	LYS
5	E	178	VAL
5	E	213	LYS
5	E	289	LEU
5	E	291	PHE

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Mol	Chain	Res	Type
6	F	30	LYS
6	F	46	ARG
6	F	65	ARG
6	F	73	MET
6	F	88	LEU
6	F	95	ARG
6	F	100	VAL
6	F	115	GLN
6	F	120	THR
6	F	123	LYS
6	F	128	SER
6	F	134	ILE
6	F	151	GLU
6	F	186	MET
6	F	187	GLU
6	F	198	LYS
6	F	211	LYS
6	F	231	ASP
6	F	245	ARG
7	G	105	THR
7	G	126	ARG
7	G	154	LYS
7	G	163	LYS
7	G	184	LYS
7	G	203	LYS
7	G	204	LYS
7	G	207	LEU
7	G	220	VAL
7	G	223	LEU
7	G	226	LEU
7	G	230	MET
7	G	242	ARG
7	G	293	ASN
8	H	1	MET
8	H	23	ARG
8	H	52	LYS
8	H	54	ARG
8	H	57	VAL
8	H	59	LYS
8	H	66	GLU
8	H	74	CYS
8	H	105	ILE

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Mol	Chain	Res	Type
8	H	108	ASN
8	H	128	MET
8	H	149	ASN
8	H	173	ARG
8	H	177	ASP
9	I	36	LEU
9	I	39	LYS
9	I	76	MET
9	I	116	ARG
9	I	123	GLN
9	I	142	LEU
9	I	153	ARG
9	I	163	GLN
9	I	164	LYS
9	I	168	SER
9	I	195	CYS
9	I	200	ILE
9	I	207	ASP
9	I	208	LYS
10	J	16	ARG
10	J	28	GLU
10	J	33	LEU
10	J	72	CYS
10	J	81	GLU
10	J	113	ILE
10	J	136	ARG
10	J	167	GLN
10	J	175	LEU
11	L	10	LEU
11	L	35	ARG
11	L	63	THR
11	L	67	HIS
11	L	74	ARG
11	L	106	SER
11	L	129	ARG
11	L	162	LYS
11	L	186	ARG
11	L	195	ARG
12	M	2	VAL
12	M	37	LEU
12	M	54	CYS
12	M	57	LEU

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Mol	Chain	Res	Type
12	M	89	THR
12	M	96	GLU
12	M	105	THR
12	M	119	ARG
13	N	9	GLU
13	N	26	ARG
13	N	32	GLN
13	N	64	ILE
13	N	72	LYS
13	N	77	LYS
13	N	87	HIS
13	N	89	VAL
13	N	162	ARG
13	N	182	HIS
14	O	18	ARG
14	O	37	ARG
14	O	49	ARG
14	O	61	ARG
14	O	67	SER
14	O	74	ARG
14	O	82	ARG
14	O	128	ARG
14	O	130	LYS
14	O	140	ARG
14	O	145	VAL
14	O	175	MET
14	O	179	LYS
14	O	188	LYS
14	O	202	LEU
15	P	21	ASN
15	P	24	VAL
15	P	25	HIS
15	P	57	CYS
15	P	69	ARG
15	P	86	LYS
15	P	91	LEU
15	P	127	ARG
15	P	128	ARG
15	P	147	GLU
16	Q	3	VAL
16	Q	5	ILE
16	Q	13	VAL

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Mol	Chain	Res	Type
16	Q	31	LEU
16	Q	61	LEU
16	Q	63	LEU
16	Q	75	ARG
16	Q	91	ARG
16	Q	95	VAL
16	Q	97	LYS
16	Q	101	CYS
16	Q	115	LYS
16	Q	138	LEU
16	Q	143	ARG
16	Q	168	ARG
17	R	8	LYS
17	R	15	LEU
17	R	36	ASN
17	R	40	GLN
17	R	50	ILE
17	R	52	ARG
17	R	63	CYS
17	R	89	MET
17	R	99	MET
17	R	106	LEU
17	R	113	LYS
17	R	130	ASN
17	R	133	LYS
17	R	138	LEU
17	R	176	ARG
17	R	178	GLN
18	S	7	LEU
18	S	9	GLU
18	S	17	LEU
18	S	24	THR
18	S	43	ARG
18	S	70	LYS
18	S	83	ARG
18	S	102	THR
18	S	120	ARG
18	S	149	LYS
18	S	159	LEU
18	S	174	THR
19	T	5	LYS
19	T	17	ARG

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Mol	Chain	Res	Type
19	T	33	ILE
19	T	52	MET
19	T	60	LYS
19	T	63	ARG
19	T	96	ILE
19	T	117	LYS
19	T	142	ARG
19	T	144	ASN
19	T	146	LYS
19	T	157	GLU
19	T	159	MET
20	U	33	ILE
20	U	80	LYS
21	V	15	ARG
21	V	18	LEU
21	V	35	LYS
21	V	45	ILE
21	V	59	ASP
21	V	60	MET
21	V	71	GLU
21	V	82	ILE
21	V	91	LYS
21	V	109	LYS
21	V	123	LYS
22	W	91	MET
23	X	39	LYS
23	X	41	ARG
23	X	53	ARG
23	X	59	LYS
23	X	63	LYS
24	Y	2	LYS
24	Y	8	THR
24	Y	28	LYS
24	Y	50	ARG
24	Y	72	GLN
24	Y	74	TYR
24	Y	104	VAL
24	Y	112	ASP
25	Z	5	MET
25	Z	65	ARG
25	Z	83	THR
25	Z	84	ARG

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Mol	Chain	Res	Type
25	Z	112	ARG
26	a	4	ARG
26	a	84	GLU
26	a	122	VAL
26	a	132	ARG
27	b	22	LYS
27	b	40	LEU
27	b	41	ARG
27	b	101	HIS
28	c	37	MET
28	c	50	ASN
28	c	78	ASN
28	c	81	LEU
28	c	83	THR
28	c	90	ARG
28	c	92	CYS
29	d	23	ARG
29	d	26	THR
29	d	31	LYS
29	d	44	ARG
29	d	48	GLU
29	d	56	GLU
29	d	78	ARG
29	d	79	ASN
29	d	83	ARG
29	d	85	ARG
29	d	90	ARG
29	d	98	SER
29	d	117	LEU
30	e	21	ILE
30	e	22	ARG
30	e	48	ARG
30	e	64	LYS
30	e	78	LEU
30	e	86	GLU
30	e	106	LYS
30	e	128	ARG
31	f	16	ARG
31	f	23	GLU
31	f	28	LEU
31	f	33	VAL
31	f	52	LYS

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Mol	Chain	Res	Type
31	f	90	SER
31	f	101	ILE
32	g	22	LEU
32	g	54	ARG
32	g	60	ARG
32	g	66	ARG
32	g	90	ARG
32	g	114	GLN
33	h	16	GLU
33	h	28	LEU
33	h	67	GLU
33	h	77	LYS
33	h	89	ARG
34	i	34	THR
34	i	48	CYS
34	i	86	LYS
34	i	89	GLU
35	j	3	LYS
35	j	11	ARG
35	j	20	ARG
35	j	58	THR
35	j	79	ARG
36	k	37	ARG
36	k	69	LEU
36	k	70	LYS
37	l	33	ASN
37	l	49	LEU
38	m	71	ARG
38	m	72	LYS
38	m	92	THR
38	m	93	ASN
39	n	1	MET
39	n	13	LEU
40	o	17	LYS
40	o	61	LYS
40	o	82	MET
41	p	8	VAL
41	p	30	GLU
41	p	47	MET
41	p	62	LYS
41	p	70	THR
42	r	8	MET

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Mol	Chain	Res	Type
42	r	14	SER
42	r	18	ILE
42	r	20	ARG
42	r	26	SER
42	r	32	LEU
42	r	35	ARG
42	r	39	ARG
42	r	67	ARG
42	r	80	THR
42	r	103	HIS
43	s	38	LYS
43	s	95	LEU
43	s	105	ASN
43	s	146	LYS
43	s	187	LEU
43	s	191	GLN
44	t	37	LEU
44	t	98	ILE
44	t	133	LEU
44	t	144	ASP
52	AA	9	GLN
52	AA	12	GLU
52	AA	25	LEU
52	AA	44	ASP
52	AA	46	ILE
52	AA	50	ASN
52	AA	56	GLU
52	AA	58	LEU
52	AA	60	LEU
52	AA	85	ARG
52	AA	111	GLN
52	AA	122	LEU
52	AA	132	GLN
52	AA	136	GLU
52	AA	142	LEU
52	AA	155	ARG
52	AA	169	HIS
52	AA	170	SER
52	AA	178	LEU
53	BB	29	ASP
53	BB	38	MET
53	BB	50	THR

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Mol	Chain	Res	Type
53	BB	71	LEU
53	BB	82	ARG
53	BB	96	CYS
53	BB	105	LEU
53	BB	125	VAL
53	BB	126	ASP
53	BB	139	CYS
53	BB	157	GLN
53	BB	175	GLU
53	BB	180	ASP
53	BB	181	LEU
53	BB	207	LEU
53	BB	209	ASP
53	BB	213	ARG
53	BB	225	LEU
54	CC	78	LEU
54	CC	114	LYS
54	CC	115	GLN
54	CC	117	ARG
54	CC	120	GLN
54	CC	121	ARG
54	CC	137	VAL
54	CC	167	ARG
54	CC	188	CYS
54	CC	192	LEU
54	CC	227	ARG
54	CC	235	ASN
54	CC	236	PHE
54	CC	244	ILE
54	CC	251	LEU
54	CC	255	LEU
54	CC	271	ASP
55	DD	28	GLU
55	DD	31	GLU
55	DD	45	ARG
55	DD	64	ARG
55	DD	65	ARG
55	DD	76	ARG
55	DD	127	MET
55	DD	134	CYS
55	DD	142	LEU
55	DD	146	ARG

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Mol	Chain	Res	Type
55	DD	160	SER
55	DD	168	VAL
55	DD	190	LEU
55	DD	206	ASP
55	DD	215	ASP
55	DD	218	LEU
55	DD	227	LYS
56	EE	17	HIS
56	EE	30	ARG
56	EE	41	CYS
56	EE	42	LEU
56	EE	51	ARG
56	EE	59	ASP
56	EE	66	MET
56	EE	77	ARG
56	EE	108	ARG
56	EE	115	THR
56	EE	145	ARG
56	EE	165	GLU
56	EE	171	ASP
56	EE	181	CYS
56	EE	205	PHE
56	EE	222	LEU
56	EE	232	ASN
56	EE	245	ARG
56	EE	246	LEU
56	EE	247	THR
57	FF	20	PHE
57	FF	36	GLN
57	FF	63	LYS
57	FF	71	ARG
57	FF	88	MET
57	FF	89	THR
57	FF	95	HIS
57	FF	122	ARG
57	FF	125	SER
57	FF	146	ARG
57	FF	204	ARG
58	GG	41	LEU
58	GG	59	GLN
58	GG	63	MET
58	GG	64	LYS

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Mol	Chain	Res	Type
58	GG	67	VAL
58	GG	70	HIS
58	GG	72	ARG
58	GG	76	LEU
58	GG	92	ARG
58	GG	95	LYS
58	GG	103	ASP
58	GG	107	SER
58	GG	150	GLU
58	GG	159	ARG
58	GG	171	THR
58	GG	178	ARG
58	GG	183	ARG
58	GG	190	ARG
58	GG	191	ARG
58	GG	216	ARG
58	GG	230	LYS
58	GG	237	LEU
59	HH	8	ILE
59	HH	36	LEU
59	HH	40	LEU
59	HH	46	THR
59	HH	76	GLN
59	HH	82	GLU
59	HH	100	ILE
59	HH	105	THR
59	HH	119	SER
59	HH	132	ASP
59	HH	145	ARG
59	HH	153	LEU
59	HH	158	LEU
60	II	6	ASP
60	II	10	LYS
60	II	22	HIS
60	II	23	LYS
60	II	47	ARG
60	II	49	ARG
60	II	92	ARG
60	II	121	LEU
60	II	130	THR
60	II	168	GLN
60	II	175	ILE

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Mol	Chain	Res	Type
61	JJ	29	LEU
61	JJ	38	ARG
61	JJ	45	ARG
61	JJ	50	LEU
61	JJ	61	LEU
61	JJ	69	ARG
61	JJ	70	ARG
61	JJ	79	ARG
61	JJ	80	ARG
61	JJ	86	VAL
61	JJ	89	GLU
61	JJ	95	ASP
61	JJ	103	GLU
61	JJ	109	ARG
61	JJ	110	LEU
61	JJ	116	LYS
61	JJ	128	VAL
61	JJ	131	ARG
61	JJ	133	ARG
62	KK	1	MET
62	KK	35	LEU
62	KK	50	GLN
62	KK	60	GLU
62	KK	89	ILE
62	KK	96	ARG
63	LL	16	ILE
63	LL	20	LYS
63	LL	39	ASN
63	LL	40	ILE
63	LL	42	LEU
63	LL	54	THR
63	LL	56	ILE
63	LL	60	CYS
63	LL	69	ARG
63	LL	85	THR
63	LL	108	ASN
63	LL	110	SER
63	LL	121	GLN
63	LL	126	VAL
63	LL	132	ARG
63	LL	134	LEU
64	MM	31	LEU

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Mol	Chain	Res	Type
64	MM	33	ARG
64	MM	40	LYS
64	MM	43	ASP
64	MM	45	ARG
64	MM	49	LEU
64	MM	55	ASN
64	MM	69	CYS
64	MM	76	LEU
64	MM	83	LYS
64	MM	85	LEU
64	MM	96	ARG
64	MM	101	ARG
65	NN	20	ARG
65	NN	27	LYS
65	NN	36	GLN
65	NN	39	LYS
65	NN	55	ARG
65	NN	60	VAL
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	107	LYS
65	NN	110	ASP
65	NN	125	LEU
65	NN	132	LYS
66	OO	28	PHE
66	OO	34	PHE
66	OO	38	ASN
66	OO	51	GLU
66	OO	56	VAL
66	OO	128	ARG
66	OO	146	ARG
66	OO	150	ARG
66	OO	151	LEU
67	PP	13	ARG
67	PP	14	LYS
67	PP	15	PHE
67	PP	37	TYR
67	PP	44	ARG

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Mol	Chain	Res	Type
67	PP	45	LEU
67	PP	76	VAL
67	PP	78	THR
67	PP	83	MET
67	PP	104	GLN
67	PP	108	LYS
67	PP	130	ARG
68	QQ	7	LEU
68	QQ	31	LEU
68	QQ	41	MET
68	QQ	47	LEU
68	QQ	67	ASP
68	QQ	89	SER
68	QQ	140	ARG
69	RR	5	ARG
69	RR	31	ASN
69	RR	43	SER
69	RR	44	LYS
69	RR	62	GLN
69	RR	78	ARG
69	RR	98	VAL
69	RR	99	ASP
69	RR	105	MET
69	RR	132	ARG
70	SS	7	GLU
70	SS	8	LYS
70	SS	13	LEU
70	SS	14	ARG
70	SS	21	ASP
70	SS	23	ARG
70	SS	46	ARG
70	SS	49	ASP
70	SS	52	LEU
70	SS	59	LEU
70	SS	60	THR
70	SS	63	GLU
70	SS	75	ARG
70	SS	81	ASP
70	SS	83	PHE
70	SS	86	ARG
70	SS	115	LYS
70	SS	132	ARG

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Mol	Chain	Res	Type
71	TT	37	VAL
71	TT	55	THR
71	TT	62	ARG
71	TT	90	SER
71	TT	102	ARG
71	TT	110	LEU
71	TT	121	ARG
71	TT	124	THR
71	TT	142	LYS
72	UU	18	HIS
72	UU	25	THR
72	UU	33	GLU
72	UU	56	MET
72	UU	68	THR
72	UU	79	ARG
72	UU	90	ASP
72	UU	106	ILE
72	UU	111	GLU
73	VV	1	MET
73	VV	10	ASP
73	VV	12	TYR
73	VV	68	SER
74	WW	18	GLU
74	WW	23	ARG
74	WW	36	ARG
74	WW	51	GLU
74	WW	52	ILE
74	WW	85	ASP
74	WW	92	ASN
74	WW	97	ARG
74	WW	103	VAL
75	XX	15	SER
75	XX	18	ARG
75	XX	48	LYS
75	XX	61	GLN
75	XX	67	ARG
75	XX	105	PHE
75	XX	115	ILE
75	XX	127	ASN
76	YY	9	THR
76	YY	16	ARG
76	YY	17	LEU

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Mol	Chain	Res	Type
76	YY	20	ARG
76	YY	40	ILE
76	YY	46	LYS
76	YY	47	MET
76	YY	53	ASP
76	YY	61	ARG
76	YY	63	HIS
76	YY	74	MET
76	YY	80	ASP
76	YY	88	LYS
76	YY	101	LYS
76	YY	115	LYS
77	ZZ	54	THR
77	ZZ	59	CYS
77	ZZ	74	SER
77	ZZ	80	ARG
77	ZZ	89	GLN
77	ZZ	92	LEU
77	ZZ	106	GLN
78	aa	18	VAL
78	aa	19	GLN
78	aa	21	ILE
78	aa	23	CYS
78	aa	34	LYS
78	aa	41	ILE
78	aa	42	ARG
78	aa	44	ILE
78	aa	55	GLU
78	aa	81	SER
78	aa	86	ASN
78	aa	96	THR
78	aa	100	ARG
79	bb	11	SER
79	bb	17	ARG
79	bb	34	ASP
79	bb	37	CYS
79	bb	42	LYS
79	bb	64	CYS
79	bb	77	CYS
79	bb	80	ARG
79	bb	81	ARG
80	cc	18	LEU

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Mol	Chain	Res	Type
80	cc	20	ARG
80	cc	31	ARG
80	cc	36	ASP
80	cc	40	ARG
80	cc	44	ARG
80	cc	51	ARG
80	cc	68	LEU
81	dd	9	SER
81	dd	11	PRO
81	dd	27	ARG
81	dd	49	ASP
82	ee	85	VAL
82	ee	99	LYS
82	ee	107	ARG
82	ee	108	ARG
82	ee	109	MET
82	ee	113	ARG
82	ee	121	THR
83	ff	99	LYS
83	ff	138	ARG
83	ff	140	TYR
84	gg	17	TRP
84	gg	20	GLN
84	gg	36	ARG
84	gg	38	LYS
84	gg	47	ARG
84	gg	113	PHE
84	gg	149	GLU
84	gg	191	HIS
84	gg	198	VAL
84	gg	207	CYS
84	gg	273	GLU
84	gg	287	THR
84	gg	289	LEU
84	gg	298	LEU
84	gg	306	LEU
86	ii	40	ARG
86	ii	68	CYS
86	ii	81	LEU
86	ii	90	GLU
86	ii	107	ASN
86	ii	149	ILE

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Mol	Chain	Res	Type
86	ii	156	MET
86	ii	170	LYS
86	ii	198	HIS
86	ii	243	VAL
86	ii	258	CYS
86	ii	297	LYS
86	ii	311	LEU
86	ii	313	ILE
86	ii	319	ARG
86	ii	349	LEU
87	jj	269	VAL
87	jj	276	LEU
87	jj	297	GLN
87	jj	298	GLU
87	jj	304	LYS
87	jj	313	LEU
87	jj	330	MET
87	jj	361	GLN
87	jj	369	VAL
87	jj	385	GLN
87	jj	389	HIS
87	jj	408	MET
87	jj	425	LEU
87	jj	434	PHE
87	jj	436	GLU
87	jj	482	ARG
87	jj	489	ARG
87	jj	499	GLN
87	jj	505	ILE
87	jj	548	ASP
87	jj	557	MET
87	jj	585	ILE
87	jj	613	ILE
87	jj	640	ASN
87	jj	653	LEU
87	jj	664	ARG
87	jj	668	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN

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Mol	Chain	Res	Type
2	B	167	GLN
2	B	204	GLN
5	E	45	HIS
5	E	194	GLN
6	F	57	HIS
6	F	79	ASN
6	F	247	ASN
7	G	134	ASN
7	G	138	GLN
8	H	15	ASN
9	I	144	ASN
9	I	147	HIS
10	J	112	HIS
14	O	65	ASN
15	P	56	GLN
17	R	130	ASN
18	S	163	HIS
19	T	131	GLN
22	W	48	GLN
23	X	93	ASN
29	d	30	HIS
32	g	14	ASN
34	i	20	ASN
38	m	91	HIS
42	r	70	GLN
42	r	103	HIS
43	s	34	ASN
52	AA	29	ASN
54	CC	115	GLN
54	CC	235	ASN
55	DD	145	GLN
56	EE	67	GLN
56	EE	98	ASN
56	EE	260	GLN
57	FF	118	ASN
58	GG	13	GLN
58	GG	186	GLN
59	HH	114	GLN
60	II	88	ASN
61	JJ	154	GLN
63	LL	39	ASN
66	OO	79	GLN

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Mol	Chain	Res	Type
68	QQ	35	ASN
68	QQ	142	GLN
69	RR	31	ASN
70	SS	10	GLN
70	SS	125	HIS
74	WW	92	ASN
75	XX	77	ASN
79	bb	26	GLN
79	bb	49	HIS
81	dd	3	HIS
81	dd	10	HIS
83	ff	93	HIS
86	ii	109	GLN
86	ii	216	GLN
87	jj	385	GLN
87	jj	389	HIS
87	jj	605	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	15 (20%)	0
47	3	72/75 (96%)	21 (29%)	1 (1%)
48	5	3506/3543 (98%)	881 (25%)	182 (5%)
49	7	119/120 (99%)	13 (10%)	1 (0%)
50	8	149/156 (95%)	38 (25%)	6 (4%)
51	9	1680/1869 (89%)	435 (25%)	85 (5%)
85	hh	7/8 (87%)	4 (57%)	0
All	All	5607/5847 (95%)	1407 (25%)	275 (4%)

All (1407) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	9	A
46	2	13	U
46	2	14	A
46	2	16	C
46	2	19	G
46	2	21	A
46	2	42	A
46	2	43	A

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Mol	Chain	Res	Type
46	2	46	G
46	2	47	U
46	2	49	C
46	2	58	A
46	2	61	C
46	2	72	C
46	2	75	C
47	3	7	A
47	3	13	C
47	3	14	A
47	3	16	C
47	3	21	A
47	3	25	C
47	3	28	C
47	3	29	A
47	3	34	U
47	3	35	U
47	3	36	U
47	3	40	C
47	3	42	G
47	3	47	U
47	3	49	C
47	3	58	A
47	3	60	U
47	3	61	C
47	3	63	C
47	3	72	C
47	3	76	A
48	5	12	A
48	5	13	U
48	5	15	A
48	5	17	A
48	5	25	A
48	5	30	C
48	5	36	U
48	5	39	A
48	5	42	A
48	5	43	U
48	5	44	A
48	5	48	G
48	5	49	U
48	5	56	A

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Mol	Chain	Res	Type
48	5	58	G
48	5	59	A
48	5	64	A
48	5	65	A
48	5	72	C
48	5	73	A
48	5	75	G
48	5	84	A
48	5	91	G
48	5	93	G
48	5	108	A
48	5	109	G
48	5	110	C
48	5	116	G
48	5	118	C
48	5	119	G
48	5	120	A
48	5	122	U
48	5	126	C
48	5	134	G
48	5	135	G
48	5	136	C
48	5	143	C
48	5	144	G
48	5	159	C
48	5	160	G
48	5	172	C
48	5	173	C
48	5	177	G
48	5	179	G
48	5	200	U
48	5	201	C
48	5	202	C
48	5	205	C
48	5	209	U
48	5	216	C
48	5	217	C
48	5	218	A
48	5	220	C
48	5	221	C
48	5	224	U
48	5	226	G

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Mol	Chain	Res	Type
48	5	227	A
48	5	233	U
48	5	234	G
48	5	236	G
48	5	245	C
48	5	246	G
48	5	253	G
48	5	262	G
48	5	265	C
48	5	266	C
48	5	267	G
48	5	276	C
48	5	279	A
48	5	280	G
48	5	281	U
48	5	297	U
48	5	306	A
48	5	309	C
48	5	310	G
48	5	315	G
48	5	316	U
48	5	321	U
48	5	322	C
48	5	334	A
48	5	340	C
48	5	347	A
48	5	350	C
48	5	357	U
48	5	361	C
48	5	363	A
48	5	365	U
48	5	386	A
48	5	387	G
48	5	399	G
48	5	401	G
48	5	407	A
48	5	409	G
48	5	410	A
48	5	412	G
48	5	413	G
48	5	431	G
48	5	432	U

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Mol	Chain	Res	Type
48	5	446	C
48	5	449	C
48	5	450	G
48	5	452	A
48	5	453	G
48	5	454	U
48	5	455	C
48	5	457	G
48	5	466	A
48	5	467	U
48	5	468	U
48	5	469	C
48	5	482	G
48	5	483	G
48	5	484	U
48	5	485	C
48	5	486	C
48	5	492	U
48	5	493	G
48	5	495	C
48	5	497	G
48	5	498	C
48	5	499	G
48	5	505	G
48	5	647	G
48	5	649	A
48	5	654	C
48	5	658	C
48	5	666	G
48	5	667	A
48	5	668	C
48	5	672	C
48	5	683	C
48	5	684	G
48	5	685	C
48	5	687	U
48	5	696	C
48	5	697	G
48	5	704	C
48	5	705	G
48	5	729	G
48	5	730	G

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Mol	Chain	Res	Type
48	5	731	G
48	5	739	G
48	5	742	G
48	5	747	A
48	5	748	G
48	5	749	G
48	5	750	U
48	5	756	G
48	5	758	G
48	5	911	U
48	5	913	U
48	5	914	U
48	5	917	A
48	5	918	G
48	5	922(A)	G
48	5	922(B)	C
48	5	923	C
48	5	924	C
48	5	925	C
48	5	926	G
48	5	929	A
48	5	931	C
48	5	932	A
48	5	933	G
48	5	934	C
48	5	936	C
48	5	938	C
48	5	939	G
48	5	941	C
48	5	943	A
48	5	944	A
48	5	945	U
48	5	955	G
48	5	956	A
48	5	959	G
48	5	960	A
48	5	961	G
48	5	962	C
48	5	965	G
48	5	966	A
48	5	967	C
48	5	968	C

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Mol	Chain	Res	Type
48	5	969	C
48	5	972	C
48	5	979	C
48	5	983	C
48	5	990	C
48	5	1072	C
48	5	1073	G
48	5	1075	G
48	5	1076	C
48	5	1078	A
48	5	1079	C
48	5	1082	C
48	5	1174	G
48	5	1177	U
48	5	1179	U
48	5	1195	G
48	5	1209	U
48	5	1210	C
48	5	1211	G
48	5	1212	G
48	5	1214	C
48	5	1215	C
48	5	1234	G
48	5	1235	G
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1239	C
48	5	1272	C
48	5	1273	G
48	5	1274	A
48	5	1275	G
48	5	1276	C
48	5	1280	C
48	5	1284	G
48	5	1287	G
48	5	1288	G
48	5	1291	G
48	5	1292	C
48	5	1293	G
48	5	1295	U
48	5	1296	G

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Mol	Chain	Res	Type
48	5	1301	C
48	5	1303	A
48	5	1304	C
48	5	1313	C
48	5	1326	A
48	5	1329	G
48	5	1330	A
48	5	1337	A
48	5	1353	G
48	5	1354	A
48	5	1359	G
48	5	1364	U
48	5	1370	G
48	5	1371	A
48	5	1377	G
48	5	1378	C
48	5	1380	G
48	5	1381	U
48	5	1387	A
48	5	1394	G
48	5	1397	A
48	5	1398	A
48	5	1401	C
48	5	1411(B)	C
48	5	1411(C)	C
48	5	1412	G
48	5	1416	G
48	5	1419	G
48	5	1420	A
48	5	1421	G
48	5	1422	G
48	5	1429	C
48	5	1432	G
48	5	1433	A
48	5	1435	G
48	5	1436	C
48	5	1437	C
48	5	1438	U
48	5	1441	C
48	5	1442	C
48	5	1445	U
48	5	1446	C

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Mol	Chain	Res	Type
48	5	1453	G
48	5	1455	G
48	5	1456	C
48	5	1457	G
48	5	1458	C
48	5	1465	G
48	5	1478	C
48	5	1482	G
48	5	1483	C
48	5	1484	G
48	5	1485	C
48	5	1486	C
48	5	1489	G
48	5	1497	A
48	5	1498	G
48	5	1502	G
48	5	1503	A
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	1525	A
48	5	1534	A
48	5	1535	C
48	5	1547	A
48	5	1554	A
48	5	1563	A
48	5	1564	A
48	5	1566	C
48	5	1568	C
48	5	1578	U
48	5	1586	G
48	5	1591	U
48	5	1596	U
48	5	1601	A
48	5	1602	U
48	5	1612	G
48	5	1613	A
48	5	1624	G
48	5	1625	G

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Mol	Chain	Res	Type
48	5	1631	A
48	5	1633	G
48	5	1634	A
48	5	1640	C
48	5	1641	G
48	5	1649	U
48	5	1652	U
48	5	1654	G
48	5	1656	U
48	5	1661	C
48	5	1676	C
48	5	1677	U
48	5	1679	A
48	5	1691	G
48	5	1694	C
48	5	1724	G
48	5	1729	A
48	5	1733	G
48	5	1734	G
48	5	1740	C
48	5	1741	G
48	5	1742	A
48	5	1750	G
48	5	1753	G
48	5	1755	C
48	5	1756	U
48	5	1757	U
48	5	1761	G
48	5	1763	C
48	5	1764	G
48	5	1768	C
48	5	1770	A
48	5	1772	C
48	5	1773	U
48	5	1776	A
48	5	1781	U
48	5	1785	C
48	5	1787	A
48	5	1799	G
48	5	1803	G
48	5	1804	A
48	5	1805	A

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Mol	Chain	Res	Type
48	5	1819	G
48	5	1821	G
48	5	1822	U
48	5	1828	C
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1836	G
48	5	1837	A
48	5	1842	G
48	5	1855	G
48	5	1869	G
48	5	1882	U
48	5	1890	G
48	5	1893	C
48	5	1897	A
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	1938	C
48	5	1948	G
48	5	1951	G
48	5	1952	G
48	5	1961	G
48	5	1962	A
48	5	1963	C
48	5	1966	C
48	5	1967	A
48	5	1976	G
48	5	1977	C
48	5	1978	C
48	5	1980	U
48	5	1982	G
48	5	1983	A
48	5	1984	A
48	5	1986	U
48	5	1987	C

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Mol	Chain	Res	Type
48	5	1991	A
48	5	1992	U
48	5	1993	C
48	5	1997	U
48	5	2001	G
48	5	2002	A
48	5	2003	G
48	5	2004	U
48	5	2005	G
48	5	2008	U
48	5	2011	C
48	5	2017	A
48	5	2024	G
48	5	2025	A
48	5	2026	A
48	5	2044	U
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	2069	A
48	5	2072	C
48	5	2084	U
48	5	2085	G
48	5	2089	G
48	5	2090	U
48	5	2092	G
48	5	2093	G
48	5	2094	C
48	5	2095	A
48	5	2097	A
48	5	2098	G
48	5	2100	G
48	5	2101	A
48	5	2102	G
48	5	2104	A
48	5	2105	A
48	5	2106	G
48	5	2107	A

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Mol	Chain	Res	Type
48	5	2108	G
48	5	2110	G
48	5	2259	G
48	5	2260	C
48	5	2262	G
48	5	2266	C
48	5	2267	U
48	5	2268	A
48	5	2269	C
48	5	2270	G
48	5	2274	C
48	5	2275	G
48	5	2279	A
48	5	2280	G
48	5	2289	C
48	5	2294	G
48	5	2300	A
48	5	2301	G
48	5	2313	A
48	5	2314	G
48	5	2325	C
48	5	2332	A
48	5	2333	G
48	5	2348	G
48	5	2351	C
48	5	2360	A
48	5	2364	G
48	5	2366	A
48	5	2395	A
48	5	2396	A
48	5	2399	G
48	5	2402	G
48	5	2416	G
48	5	2417	A
48	5	2421	G
48	5	2422	C
48	5	2424	G
48	5	2425	U
48	5	2433	G
48	5	2441	C
48	5	2447	U
48	5	2450	G

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Mol	Chain	Res	Type
48	5	2469	C
48	5	2471	G
48	5	2475	G
48	5	2479	G
48	5	2483	G
48	5	2488	C
48	5	2489	C
48	5	2490	U
48	5	2491	C
48	5	2493	G
48	5	2495	U
48	5	2503	G
48	5	2504	C
48	5	2505	C
48	5	2506	G
48	5	2511	A
48	5	2513	A
48	5	2514	G
48	5	2521	G
48	5	2530	U
48	5	2537	A
48	5	2546	G
48	5	2547	G
48	5	2549	G
48	5	2553	A
48	5	2554	U
48	5	2555	G
48	5	2564	G
48	5	2566	G
48	5	2575	U
48	5	2583	C
48	5	2587	A
48	5	2601	A
48	5	2611	A
48	5	2620	G
48	5	2627	C
48	5	2638	G
48	5	2647	A
48	5	2660	A
48	5	2662	G
48	5	2663	G
48	5	2669	C

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Mol	Chain	Res	Type
48	5	2670	C
48	5	2676	A
48	5	2681	G
48	5	2686	G
48	5	2687	U
48	5	2695	A
48	5	2696	A
48	5	2704	C
48	5	2707	U
48	5	2708	U
48	5	2709	C
48	5	2710	C
48	5	2711	G
48	5	2712	G
48	5	2714	G
48	5	2716	C
48	5	2719	C
48	5	2721	G
48	5	2725	A
48	5	2726	G
48	5	2735	G
48	5	2740	U
48	5	2743	A
48	5	2744	A
48	5	2754	G
48	5	2760	G
48	5	2761	U
48	5	2763	U
48	5	2764	A
48	5	2769	U
48	5	2787	A
48	5	2788	U
48	5	2790	U
48	5	2796	G
48	5	2798	A
48	5	2806	A
48	5	2807	A
48	5	2814	C
48	5	2826	U
48	5	2827	G
48	5	2828	U
48	5	2829	U

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Mol	Chain	Res	Type
48	5	2835	A
48	5	2838	G
48	5	2839	U
48	5	2842	G
48	5	2844	A
48	5	2855	G
48	5	2884	G
48	5	2896	G
48	5	2897	G
48	5	3598	C
48	5	3604	A
48	5	3605	C
48	5	3606	U
48	5	3615	G
48	5	3618	C
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	3667	C
48	5	3671	G
48	5	3673	C
48	5	3674	G
48	5	3692	A
48	5	3696	C
48	5	3698	G
48	5	3711	A
48	5	3712	A
48	5	3722	G
48	5	3729	U
48	5	3740	G
48	5	3748	A
48	5	3750	G
48	5	3753	G
48	5	3759	A
48	5	3760	A
48	5	3761	C
48	5	3765	G
48	5	3766	A

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Mol	Chain	Res	Type
48	5	3773	U
48	5	3774	A
48	5	3776	G
48	5	3777	G
48	5	3778	U
48	5	3780	G
48	5	3784	A
48	5	3785	A
48	5	3786	U
48	5	3798	U
48	5	3799	A
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	3824	A
48	5	3831	U
48	5	3838	U
48	5	3839	G
48	5	3840	U
48	5	3843	C
48	5	3859	G
48	5	3867	A
48	5	3874	G
48	5	3876	A
48	5	3877	A
48	5	3878	C
48	5	3879	G
48	5	3888	G
48	5	3889	G
48	5	3892	U
48	5	3897	G
48	5	3898	G
48	5	3901	A
48	5	3905	A
48	5	3906	A
48	5	3907	G
48	5	3915	U

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Mol	Chain	Res	Type
48	5	3916	G
48	5	3917	A
48	5	3927	U
48	5	3939	G
48	5	3941	G
48	5	3943	A
48	5	4067	U
48	5	4069	U
48	5	4071	U
48	5	4073	A
48	5	4076	G
48	5	4084	G
48	5	4085	A
48	5	4086	G
48	5	4088	C
48	5	4092	G
48	5	4099	G
48	5	4100	C
48	5	4116	C
48	5	4117	U
48	5	4118	U
48	5	4119	C
48	5	4120	U
48	5	4121	G
48	5	4122	G
48	5	4125	C
48	5	4127	A
48	5	4138	C
48	5	4162	C
48	5	4163	U
48	5	4164	C
48	5	4165	C
48	5	4166	G
48	5	4171	C
48	5	4183	G
48	5	4184	G
48	5	4191	G
48	5	4201	G
48	5	4203	A
48	5	4212	A
48	5	4218	U
48	5	4221	C

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Mol	Chain	Res	Type
48	5	4222	G
48	5	4229	U
48	5	4232	U
48	5	4233	A
48	5	4237	C
48	5	4251	A
48	5	4255	A
48	5	4257	A
48	5	4258	C
48	5	4265	U
48	5	4266	G
48	5	4267	G
48	5	4268	A
48	5	4271	A
48	5	4273	A
48	5	4281	A
48	5	4291	G
48	5	4297	G
48	5	4304	A
48	5	4305	G
48	5	4306	U
48	5	4314	C
48	5	4317	A
48	5	4318	C
48	5	4319	C
48	5	4329	G
48	5	4330	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	4368	G
48	5	4373	G
48	5	4377	G
48	5	4378	A
48	5	4379	A
48	5	4380	A
48	5	4387	C
48	5	4391	G

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Mol	Chain	Res	Type
48	5	4393	G
48	5	4394	A
48	5	4395	U
48	5	4396	A
48	5	4398	C
48	5	4401	G
48	5	4415	A
48	5	4419	U
48	5	4421	C
48	5	4422	A
48	5	4440	G
48	5	4444	C
48	5	4448	G
48	5	4449	A
48	5	4450	U
48	5	4453	C
48	5	4464	A
48	5	4472	G
48	5	4474	A
48	5	4475	G
48	5	4476	C
48	5	4488	A
48	5	4495	G
48	5	4500	U
48	5	4510	A
48	5	4511	A
48	5	4512	U
48	5	4513	A
48	5	4515	G
48	5	4519	C
48	5	4520	G
48	5	4524	G
48	5	4531	U
48	5	4548	A
48	5	4549	G
48	5	4560	C
48	5	4561	C
48	5	4567	G
48	5	4570	G
48	5	4572	U
48	5	4573	G
48	5	4575	G

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Mol	Chain	Res	Type
48	5	4584	A
48	5	4585	U
48	5	4586	G
48	5	4590	A
48	5	4599	A
48	5	4606	G
48	5	4618	G
48	5	4620	U
48	5	4636	U
48	5	4637	G
48	5	4652	G
48	5	4656	A
48	5	4661	G
48	5	4670	C
48	5	4672	A
48	5	4677	U
48	5	4678	G
48	5	4700	A
48	5	4701	A
48	5	4703	U
48	5	4709	U
48	5	4719	G
48	5	4720	C
48	5	4721	G
48	5	4728	U
48	5	4729	A
48	5	4736	C
48	5	4737	G
48	5	4745	G
48	5	4751	G
48	5	4754	G
48	5	4755	G
48	5	4756	C
48	5	4757	C
48	5	4759	C
48	5	4761	G
48	5	4765	G
48	5	4771	C
48	5	4772	C
48	5	4868	G
48	5	4870	G
48	5	4871	C

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Mol	Chain	Res	Type
48	5	4872	G
48	5	4873	G
48	5	4874	A
48	5	4875	G
48	5	4876	A
48	5	4877	G
48	5	4881	U
48	5	4882	U
48	5	4883	C
48	5	4885	U
48	5	4887	C
48	5	4891	G
48	5	4895	C
48	5	4897	G
48	5	4910	A
48	5	4912	G
48	5	4913	G
48	5	4914	G
48	5	4915	G
48	5	4919	G
48	5	4921	C
48	5	4924	C
48	5	4926	C
48	5	4927	G
48	5	4928	C
48	5	4931	G
48	5	4935	C
48	5	4937	C
48	5	4938	A
48	5	4940	C
48	5	4942	C
48	5	4943	A
48	5	4944	C
48	5	4945	G
48	5	4947	U
48	5	4948	C
48	5	4949	G
48	5	4950	U
48	5	4951	G
48	5	4956	A
48	5	4957	C
48	5	4958	C

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Mol	Chain	Res	Type
48	5	4964	C
48	5	4965	U
48	5	4966	A
48	5	4967	A
48	5	4976	U
48	5	4981	G
48	5	4985	U
48	5	4988	U
48	5	4989	U
48	5	4990	C
48	5	4991	U
48	5	4994	G
48	5	4997	G
48	5	4999	G
48	5	5014	A
48	5	5017	G
48	5	5040	U
48	5	5041	G
48	5	5047	C
48	5	5050	C
48	5	5053	U
48	5	5054	C
48	5	5056	A
48	5	5058	A
48	5	5061	A
48	5	5062	G
48	5	5066	U
49	7	7	G
49	7	22	A
49	7	25	G
49	7	33	U
49	7	53	U
49	7	54	A
49	7	64	G
49	7	76	U
49	7	97	G
49	7	100	A
49	7	110	G
49	7	111	C
49	7	120	U
50	8	2	G
50	8	3	A

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Mol	Chain	Res	Type
50	8	21	C
50	8	32	C
50	8	34	U
50	8	35	C
50	8	49	G
50	8	51	U
50	8	52	A
50	8	59	A
50	8	62	A
50	8	63	U
50	8	75	G
50	8	79	G
50	8	86	U
50	8	87	G
50	8	90	C
50	8	94	G
50	8	95	A
50	8	103	A
50	8	104	A
50	8	105	C
50	8	107	C
50	8	109	C
50	8	110	U
50	8	111	U
50	8	112	G
50	8	114	G
50	8	121	G
50	8	123	U
50	8	124	U
50	8	125	C
50	8	126	C
50	8	127	U
50	8	137	A
50	8	143	G
50	8	153	C
50	8	156	U
51	9	2	A
51	9	3	C
51	9	4	C
51	9	17	C
51	9	25	A
51	9	26	U

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Mol	Chain	Res	Type
51	9	33	G
51	9	37	C
51	9	44	U
51	9	45	A
51	9	46	A
51	9	56	G
51	9	58	C
51	9	60	A
51	9	64	A
51	9	65	C
51	9	67	C
51	9	68	A
51	9	70	G
51	9	71	G
51	9	73	C
51	9	74	G
51	9	75	G
51	9	77	A
51	9	79	A
51	9	99	A
51	9	100	U
51	9	103	A
51	9	104	A
51	9	110	U
51	9	111	A
51	9	113	G
51	9	115	U
51	9	116	U
51	9	124	U
51	9	126	G
51	9	127	C
51	9	128	U
51	9	129	C
51	9	130	G
51	9	141	A
51	9	142	C
51	9	143	U
51	9	147	A
51	9	155	G
51	9	158	A
51	9	161	U
51	9	162	C

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Mol	Chain	Res	Type
51	9	163	U
51	9	167	G
51	9	168	C
51	9	173	A
51	9	175	A
51	9	182	C
51	9	183	G
51	9	184	G
51	9	188	C
51	9	189	U
51	9	191	A
51	9	192	C
51	9	200	G
51	9	202	G
51	9	206	G
51	9	213	G
51	9	215	G
51	9	292	A
51	9	302	A
51	9	304	C
51	9	307	G
51	9	308	G
51	9	309	G
51	9	312	G
51	9	313	A
51	9	314	U
51	9	317	C
51	9	318	A
51	9	319	C
51	9	322	C
51	9	331	C
51	9	332	G
51	9	335	G
51	9	340	C
51	9	347	G
51	9	351	G
51	9	360	A
51	9	362	C
51	9	364	A
51	9	368	U
51	9	370	G
51	9	372	U

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Mol	Chain	Res	Type
51	9	379	C
51	9	381	C
51	9	382	C
51	9	385	G
51	9	386	C
51	9	400	C
51	9	407	G
51	9	409	C
51	9	417	C
51	9	418	A
51	9	434	G
51	9	435	A
51	9	438	G
51	9	441	C
51	9	448	A
51	9	449	A
51	9	450	C
51	9	453	C
51	9	459	C
51	9	460	A
51	9	462	C
51	9	463	C
51	9	464	A
51	9	465	A
51	9	466	G
51	9	468	A
51	9	472	C
51	9	473	A
51	9	474	G
51	9	476	A
51	9	482	G
51	9	487	U
51	9	492	C
51	9	496	C
51	9	501	C
51	9	523	A
51	9	525	A
51	9	531	A
51	9	532	C
51	9	533	A
51	9	544	G
51	9	545	A

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Mol	Chain	Res	Type
51	9	546	G
51	9	548	C
51	9	549	C
51	9	550	C
51	9	551	U
51	9	554	A
51	9	555	A
51	9	556	U
51	9	559	G
51	9	562	U
51	9	563	G
51	9	564	A
51	9	568	C
51	9	576	A
51	9	583	A
51	9	587	A
51	9	588	G
51	9	589	G
51	9	590	A
51	9	591	U
51	9	592	C
51	9	595	U
51	9	597	G
51	9	604	A
51	9	606	G
51	9	607	U
51	9	608	C
51	9	613	G
51	9	614	C
51	9	615	C
51	9	616	A
51	9	617	G
51	9	620	G
51	9	625	G
51	9	626	G
51	9	627	U
51	9	628	A
51	9	629	A
51	9	630	U
51	9	631	U
51	9	632	C
51	9	637	U

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Mol	Chain	Res	Type
51	9	643	A
51	9	644	G
51	9	646	G
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	670	A
51	9	671	A
51	9	672	A
51	9	684	G
51	9	688	U
51	9	689	U
51	9	733	C
51	9	752	G
51	9	753	C
51	9	754	G
51	9	798	G
51	9	811	A
51	9	812	A
51	9	821	G
51	9	822	U
51	9	830	A
51	9	834	C
51	9	844	U
51	9	847	A
51	9	861	A
51	9	869	A
51	9	870	A
51	9	871	U
51	9	872	A
51	9	873	G
51	9	874	G
51	9	875	A
51	9	876	C
51	9	877	C
51	9	878	G
51	9	885	U
51	9	887	U
51	9	890	U

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Mol	Chain	Res	Type
51	9	892	U
51	9	913	A
51	9	914	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	943	U
51	9	971	G
51	9	981	A
51	9	985	G
51	9	990	A
51	9	992	A
51	9	999	G
51	9	1002	U
51	9	1016	U
51	9	1017	U
51	9	1023	A
51	9	1041	G
51	9	1055	A
51	9	1060	A
51	9	1061	U
51	9	1062	A
51	9	1067	C
51	9	1078	C
51	9	1083	A
51	9	1085	C
51	9	1100	A
51	9	1114	U
51	9	1115	U
51	9	1116	C
51	9	1117	C
51	9	1118	C
51	9	1121	G
51	9	1131	G
51	9	1138	C
51	9	1139	C
51	9	1144	A
51	9	1148	A

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Mol	Chain	Res	Type
51	9	1149	A
51	9	1153	C
51	9	1154	U
51	9	1161	U
51	9	1165	G
51	9	1166	G
51	9	1195	A
51	9	1196	A
51	9	1207	G
51	9	1208	A
51	9	1211	G
51	9	1215	C
51	9	1221	G
51	9	1224	G
51	9	1227	G
51	9	1230	C
51	9	1240	A
51	9	1242	U
51	9	1251	A
51	9	1253	A
51	9	1254	C
51	9	1256	G
51	9	1257	G
51	9	1259	A
51	9	1260	A
51	9	1265	A
51	9	1266	C
51	9	1271	C
51	9	1274	G
51	9	1275	G
51	9	1280	G
51	9	1281	G
51	9	1284	A
51	9	1285	G
51	9	1286	G
51	9	1287	A
51	9	1289	U
51	9	1293	A
51	9	1298	G
51	9	1299	A
51	9	1300	U
51	9	1301	A

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Mol	Chain	Res	Type
51	9	1302	G
51	9	1303	C
51	9	1304	U
51	9	1307	U
51	9	1308	U
51	9	1313	A
51	9	1314	U
51	9	1316	C
51	9	1330	G
51	9	1331	C
51	9	1341	C
51	9	1342	U
51	9	1348	G
51	9	1369	A
51	9	1371	U
51	9	1372	U
51	9	1376	A
51	9	1378	A
51	9	1395	C
51	9	1396	A
51	9	1397	U
51	9	1401	A
51	9	1402	A
51	9	1404	U
51	9	1405	A
51	9	1412	C
51	9	1424	G
51	9	1428	G
51	9	1439	A
51	9	1449	G
51	9	1454	A
51	9	1455	A
51	9	1459	G
51	9	1462	U
51	9	1463	U
51	9	1466	G
51	9	1473	G
51	9	1476	A
51	9	1477	U
51	9	1487	A
51	9	1490	G
51	9	1494	U

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Mol	Chain	Res	Type
51	9	1498	A
51	9	1509	U
51	9	1510	G
51	9	1519	U
51	9	1521	C
51	9	1522	A
51	9	1523	C
51	9	1531	A
51	9	1533	A
51	9	1536	G
51	9	1539	U
51	9	1544	C
51	9	1545	A
51	9	1548	G
51	9	1552	G
51	9	1553	C
51	9	1555	U
51	9	1556	A
51	9	1557	C
51	9	1560	U
51	9	1570	G
51	9	1574	C
51	9	1575	G
51	9	1580	A
51	9	1581	C
51	9	1585	U
51	9	1587	G
51	9	1588	A
51	9	1600	G
51	9	1601	A
51	9	1602	U
51	9	1604	G
51	9	1621	U
51	9	1622	U
51	9	1623	A
51	9	1624	U
51	9	1625	U
51	9	1637	A
51	9	1638	G
51	9	1641	A
51	9	1647	A
51	9	1648	G

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Mol	Chain	Res	Type
51	9	1654	G
51	9	1664	A
51	9	1665	G
51	9	1671	G
51	9	1680	G
51	9	1683	C
51	9	1686	G
51	9	1695	A
51	9	1698	C
51	9	1703	C
51	9	1715	A
51	9	1721	U
51	9	1722	G
51	9	1726	G
51	9	1728	U
51	9	1729	U
51	9	1730	U
51	9	1732	G
51	9	1744	G
51	9	1745	A
51	9	1748	G
51	9	1753	C
51	9	1758	G
51	9	1760	G
51	9	1772	C
51	9	1783	C
51	9	1785	C
51	9	1800	A
51	9	1801	A
51	9	1805	G
51	9	1822	A
51	9	1823	A
51	9	1824	A
51	9	1825	A
51	9	1826	G
51	9	1829	G
51	9	1831	A
51	9	1835	A
51	9	1836	G
51	9	1838	U
51	9	1849	G
51	9	1851	A

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Mol	Chain	Res	Type
51	9	1852	C
51	9	1861	G
51	9	1862	G
51	9	1863	A
51	9	1865	C
51	9	1866	A
51	9	1867	U
51	9	1868	U
51	9	1869	A
85	hh	42	C
85	hh	43	A
85	hh	45	A
85	hh	46	G

All (275) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
47	3	74	C
48	5	12	A
48	5	20	U
48	5	47	A
48	5	48	G
48	5	64	A
48	5	119	G
48	5	125	C
48	5	134	G
48	5	143	C
48	5	159	C
48	5	217	C
48	5	224	U
48	5	226	G
48	5	245	C
48	5	265	C
48	5	275	C
48	5	278	G
48	5	315	G
48	5	385	A
48	5	387	G
48	5	406	C
48	5	408	A
48	5	409	G
48	5	417	G

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Mol	Chain	Res	Type
48	5	449	C
48	5	453	G
48	5	466	A
48	5	484	U
48	5	485	C
48	5	492	U
48	5	497	G
48	5	498	C
48	5	504	G
48	5	696	C
48	5	729	G
48	5	738(A)	C
48	5	747	A
48	5	916	C
48	5	922	C
48	5	922(B)	C
48	5	930	G
48	5	933	G
48	5	935(A)	G
48	5	936	C
48	5	955	G
48	5	956	A
48	5	959	G
48	5	966	A
48	5	968	C
48	5	969	C
48	5	971(A)	G
48	5	1072	C
48	5	1209	U
48	5	1211	G
48	5	1214	C
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1287	G
48	5	1291	G
48	5	1295	U
48	5	1329	G
48	5	1358	G
48	5	1370	G
48	5	1378	C
48	5	1380	G

*Continued on next page...*

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Mol	Chain	Res	Type
48	5	1432	G
48	5	1440	U
48	5	1445	U
48	5	1455	G
48	5	1477	C
48	5	1481	C
48	5	1485	C
48	5	1497	A
48	5	1523	A
48	5	1533	A
48	5	1625	G
48	5	1633	G
48	5	1654	G
48	5	1678	C
48	5	1733	G
48	5	1740	C
48	5	1804	A
48	5	1818	G
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1892	A
48	5	1919	G
48	5	1921	C
48	5	1935	C
48	5	1947	U
48	5	1983	A
48	5	1986	U
48	5	2001	G
48	5	2046	G
48	5	2068	C
48	5	2088	A
48	5	2089	G
48	5	2100	G
48	5	2265	G
48	5	2266	C
48	5	2278	G
48	5	2313	A
48	5	2333	G
48	5	2398	U
48	5	2428	A
48	5	2467	U

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Mol	Chain	Res	Type
48	5	2468	U
48	5	2474	G
48	5	2475	G
48	5	2490	U
48	5	2502	A
48	5	2513	A
48	5	2529	A
48	5	2530	U
48	5	2546	G
48	5	2553	A
48	5	2587	A
48	5	2661	U
48	5	2695	A
48	5	2724	G
48	5	2739	C
48	5	2754	G
48	5	2794	C
48	5	2806	A
48	5	2845	A
48	5	2874	U
48	5	3603	G
48	5	3625	G
48	5	3673	C
48	5	3697	U
48	5	3710	G
48	5	3759	A
48	5	3760	A
48	5	3765	G
48	5	3784	A
48	5	3785	A
48	5	3809	G
48	5	3876	A
48	5	3888	G
48	5	3904	G
48	5	3938	G
48	5	4075	U
48	5	4076	G
48	5	4084	G
48	5	4116	C
48	5	4119	C
48	5	4121	G
48	5	4124	G

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Mol	Chain	Res	Type
48	5	4162	C
48	5	4170	A
48	5	4221	C
48	5	4232	U
48	5	4254	G
48	5	4257	A
48	5	4266	G
48	5	4291	G
48	5	4378	A
48	5	4379	A
48	5	4395	U
48	5	4404	U
48	5	4448	G
48	5	4449	A
48	5	4463	U
48	5	4510	A
48	5	4527	G
48	5	4572	U
48	5	4699	U
48	5	4719	G
48	5	4753	U
48	5	4756	C
48	5	4872	G
48	5	4884	G
48	5	4925	U
48	5	4936	G
48	5	4942	C
48	5	4944	C
48	5	4947	U
48	5	4965	U
48	5	5013	C
48	5	5047	C
49	7	109	U
50	8	2	G
50	8	51	U
50	8	86	U
50	8	94	G
50	8	110	U
50	8	124	U
51	9	2	A
51	9	3	C
51	9	72	C

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Mol	Chain	Res	Type
51	9	110	U
51	9	126	G
51	9	128	U
51	9	141	A
51	9	142	C
51	9	160	U
51	9	182	C
51	9	214	U
51	9	293	C
51	9	312	G
51	9	360	A
51	9	363	A
51	9	369	C
51	9	434	G
51	9	465	A
51	9	492	C
51	9	500	A
51	9	532	C
51	9	550	C
51	9	553	U
51	9	555	A
51	9	559	G
51	9	563	G
51	9	587	A
51	9	591	U
51	9	594	A
51	9	606	G
51	9	613	G
51	9	615	C
51	9	620	G
51	9	625	G
51	9	626	G
51	9	627	U
51	9	628	A
51	9	629	A
51	9	642	U
51	9	656	G
51	9	670	A
51	9	688	U
51	9	752	G
51	9	821	G
51	9	869	A

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Mol	Chain	Res	Type
51	9	870	A
51	9	872	A
51	9	874	G
51	9	875	A
51	9	1016	U
51	9	1087	A
51	9	1114	U
51	9	1130	G
51	9	1137	U
51	9	1165	G
51	9	1253	A
51	9	1264	C
51	9	1274	G
51	9	1285	G
51	9	1313	A
51	9	1330	G
51	9	1394	G
51	9	1395	C
51	9	1396	A
51	9	1438	A
51	9	1476	A
51	9	1489	A
51	9	1493	C
51	9	1519	U
51	9	1520	G
51	9	1581	C
51	9	1621	U
51	9	1636	G
51	9	1637	A
51	9	1646	C
51	9	1663	A
51	9	1664	A
51	9	1679	A
51	9	1721	U
51	9	1744	G
51	9	1824	A
51	9	1825	A
51	9	1835	A
51	9	1867	U
51	9	1868	U

## 5.4 Non-standard residues in protein, DNA, RNA chains [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 273 ligands modelled in this entry, 272 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
90	GCP	jj	700	88	27,34,34	1.60	7 (25%)	34,54,54	1.80	7 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	GCP	jj	700	88	-	3/15/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	jj	700	GCP	C5-C6	4.38	1.48	1.41
90	jj	700	GCP	PG-O3G	3.02	1.61	1.54
90	jj	700	GCP	PG-O2G	2.85	1.61	1.54
90	jj	700	GCP	C5-C4	2.66	1.48	1.40
90	jj	700	GCP	PB-O3A	2.60	1.61	1.58
90	jj	700	GCP	PB-O2B	2.33	1.61	1.56
90	jj	700	GCP	O4'-C1'	2.11	1.44	1.41



All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	jj	700	GCP	C2-N3-C4	4.66	120.68	115.36
90	jj	700	GCP	C5-C6-N1	-4.06	117.88	123.43
90	jj	700	GCP	C2-N1-C6	3.90	122.12	115.93
90	jj	700	GCP	C4-C5-C6	-3.46	117.49	120.80
90	jj	700	GCP	N3-C2-N1	-3.12	123.06	127.22
90	jj	700	GCP	C4-C5-N7	-2.91	106.37	109.40
90	jj	700	GCP	PB-O3A-PA	-2.74	123.88	132.56

There are no chirality outliers.

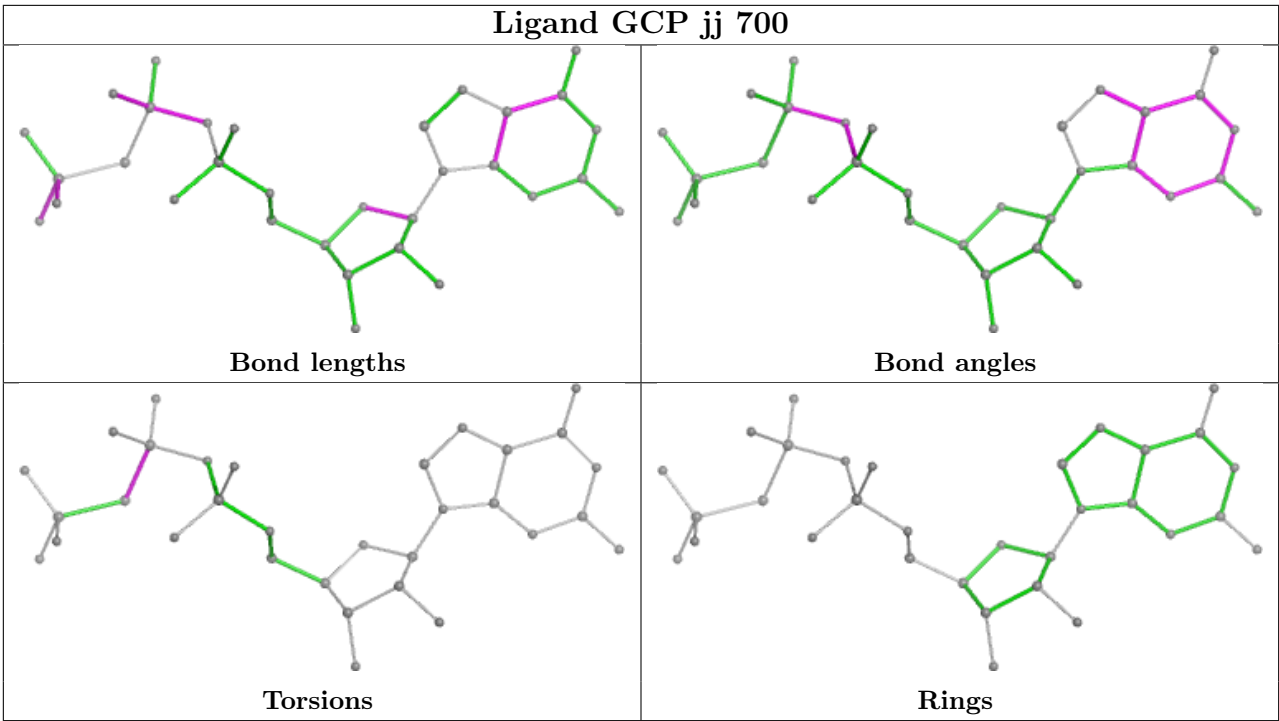
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
90	jj	700	GCP	PG-C3B-PB-O1B
90	jj	700	GCP	PG-C3B-PB-O3A
90	jj	700	GCP	PG-C3B-PB-O2B

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	42
51	9	8
47	3	2
46	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	40.91
1	5	1252:C	O3'	1271:G	P	36.05
1	5	1405:C	O3'	1406:G	P	23.79
1	5	1219:G	O3'	1233:G	P	22.30
1	5	1406:G	O3'	1406(A):G	P	20.51
1	5	3948:C	O3'	4065:G	P	19.69
1	5	990:C	O3'	1064:G	P	18.04

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	523:C	O3'	638:G	P	18.03
1	5	4138:C	O3'	4146:G	P	18.02
1	5	4101:C	O3'	4107:G	P	17.30
1	5	4777:C	O3'	4859:C	P	16.29
1	5	5022:U	O3'	5028:G	P	15.23
1	5	760:G	O3'	904:C	P	14.93
1	5	1696:C	O3'	1720:C	P	14.86
1	5	1364:U	O3'	1368:A	P	14.43
1	5	182:G	O3'	189:G	P	14.08
1	5	1406(C):G	O3'	1411:C	P	13.56
1	5	2901:G	O3'	3597:G	P	13.16
1	5	1411:C	O3'	1411(A):G	P	13.03
1	5	921:C	O3'	922:C	P	12.78
1	5	481:G	O3'	481(A):C	P	12.48
1	5	934:C	O3'	935:A	P	10.82
1	5	970:G	O3'	971:U	P	10.67
1	5	737:C	O3'	738:C	P	9.93
1	5	4729:A	O3'	4735:G	P	9.81
1	5	512:U	O3'	515:C	P	9.70
1	5	971:U	O3'	971(A):G	P	9.68
1	5	1180:C	O3'	1183:C	P	9.47
1	5	500:G	O3'	504:G	P	6.88
1	5	1100:U	O3'	1168:G	P	5.94
1	3	19:G	O3'	20:U	P	5.60
1	5	480:C	O3'	481:G	P	5.46
1	3	16:C	O3'	18:U	P	5.24
1	5	4740:G	O3'	4743:G	P	5.13
1	9	322:C	O3'	323:C	P	5.02
1	9	798:G	O3'	799:U	P	4.84
1	5	1239:C	O3'	1244:G	P	4.76
1	2	16:C	O3'	18:G	P	4.39
1	9	304:C	O3'	305:U	P	4.29
1	5	935:A	O3'	935(A):G	P	4.26
1	9	309:G	O3'	310:C	P	4.26
1	5	170:C	O3'	171:U	P	3.83
1	5	738:C	O3'	738(A):C	P	3.67
1	5	1438:U	O3'	1440:U	P	3.47
1	5	4899:G	O3'	4902:C	P	3.40
1	9	902:G	O3'	903:A	P	3.37
1	9	903:A	O3'	904:A	P	3.27
1	9	1295:A	O3'	1296:U	P	3.25
1	5	267:G	O3'	268:G	P	3.08

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	5020:G	O3'	5021:C	P	3.05
1	5	751:G	O3'	752:G	P	2.99
1	9	593:C	O3'	594:A	P	2.98
1	5	2031:C	O3'	2032:U	P	2.33

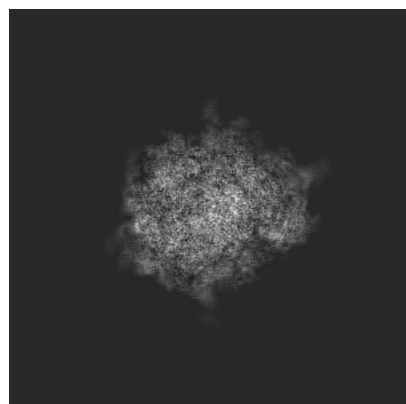
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4137. These allow visual inspection of the internal detail of the map and identification of artifacts.

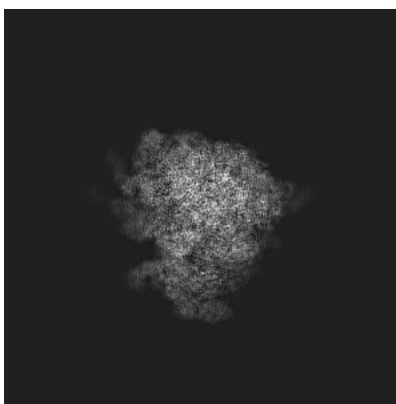
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

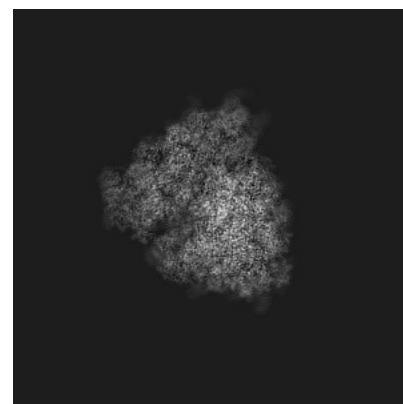
#### 6.1.1 Primary map



X

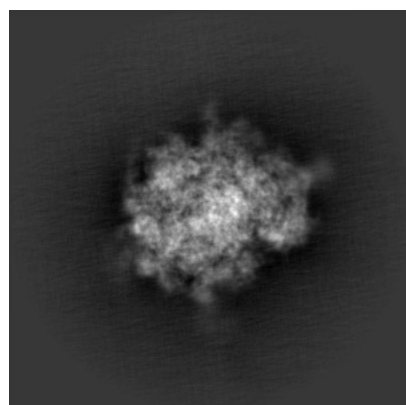


Y

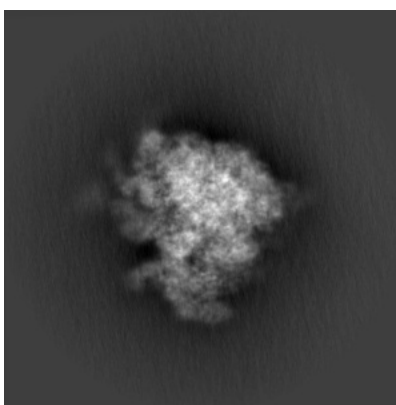


Z

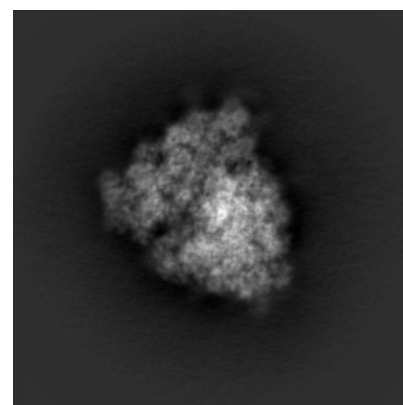
#### 6.1.2 Raw map



X



Y

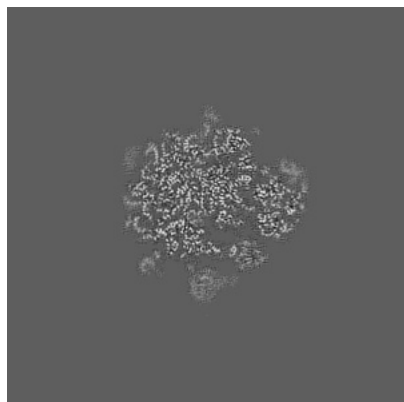


Z

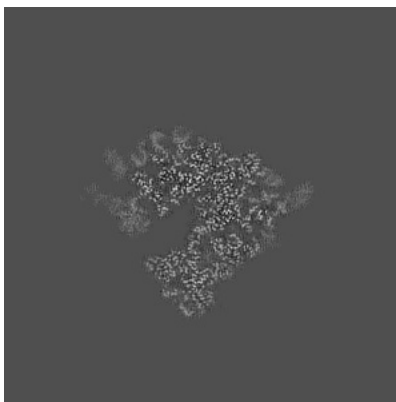
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

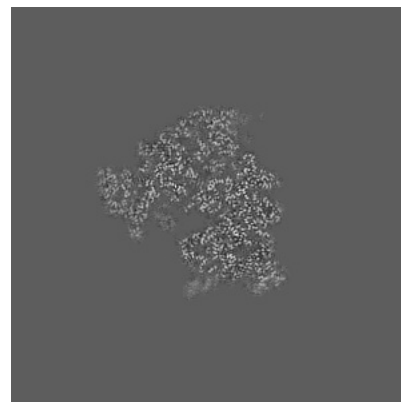
### 6.2.1 Primary map



X Index: 210

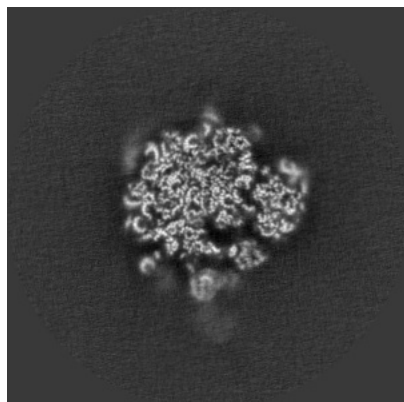


Y Index: 210

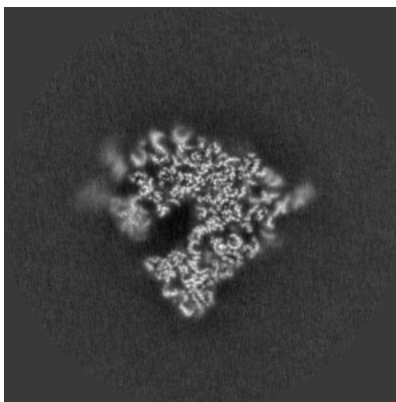


Z Index: 210

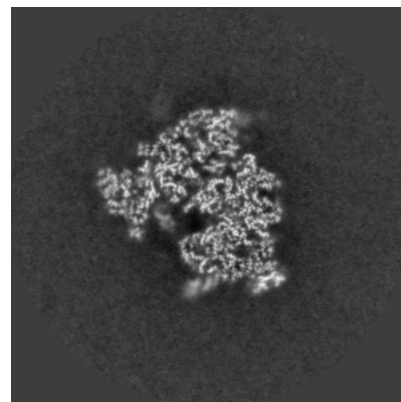
### 6.2.2 Raw map



X Index: 210



Y Index: 210

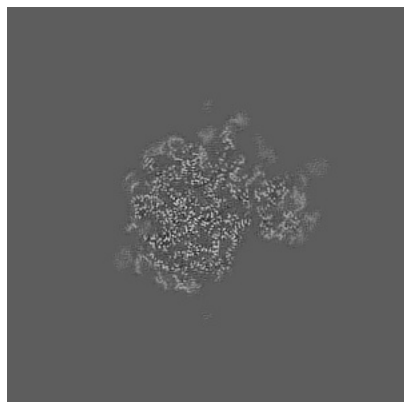


Z Index: 210

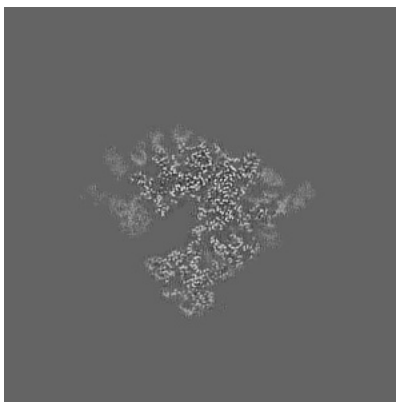
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

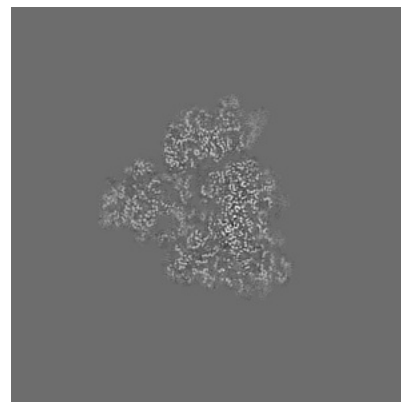
### 6.3.1 Primary map



X Index: 233

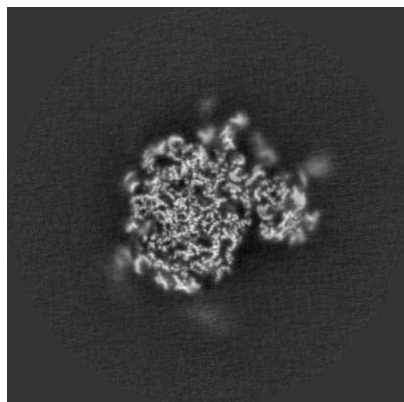


Y Index: 211

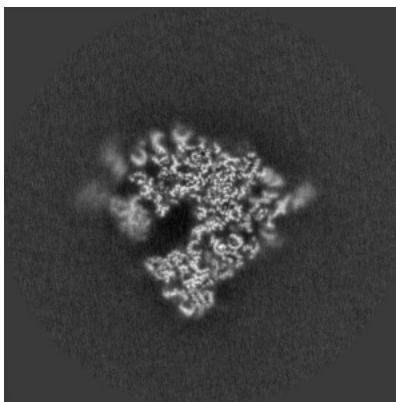


Z Index: 195

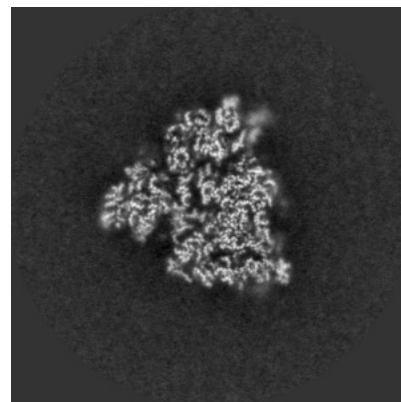
### 6.3.2 Raw map



X Index: 233



Y Index: 211

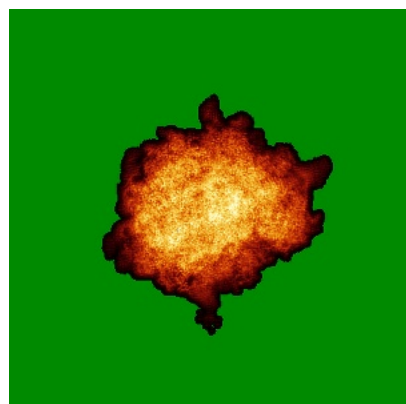


Z Index: 198

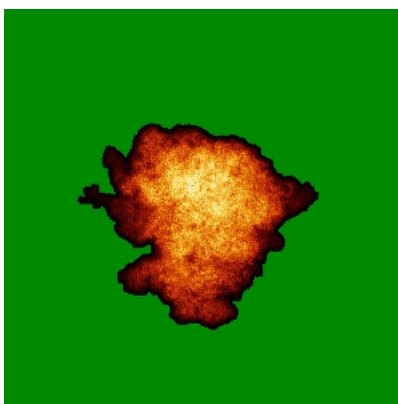
The images above show the largest variance slices of the map in three orthogonal directions.

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

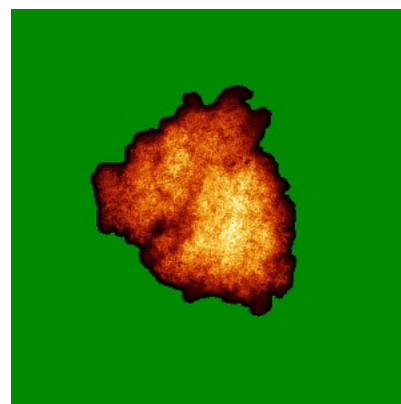
### 6.4.1 Primary map



X

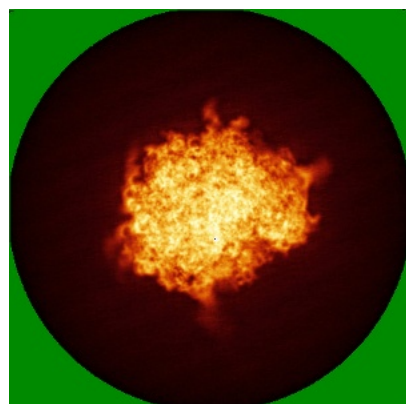


Y

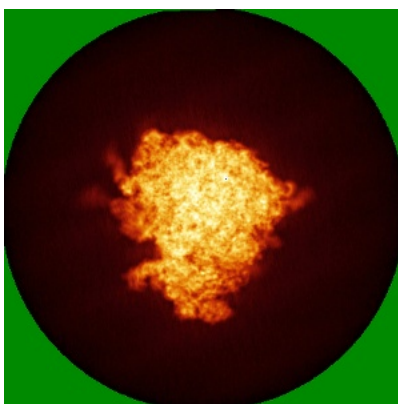


Z

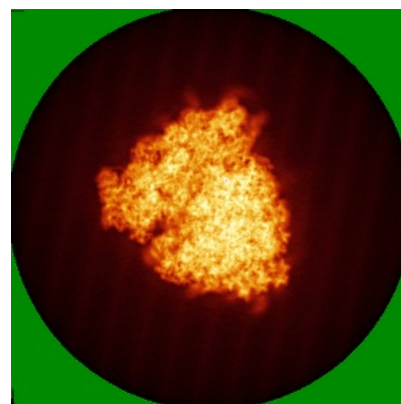
### 6.4.2 Raw map



X



Y



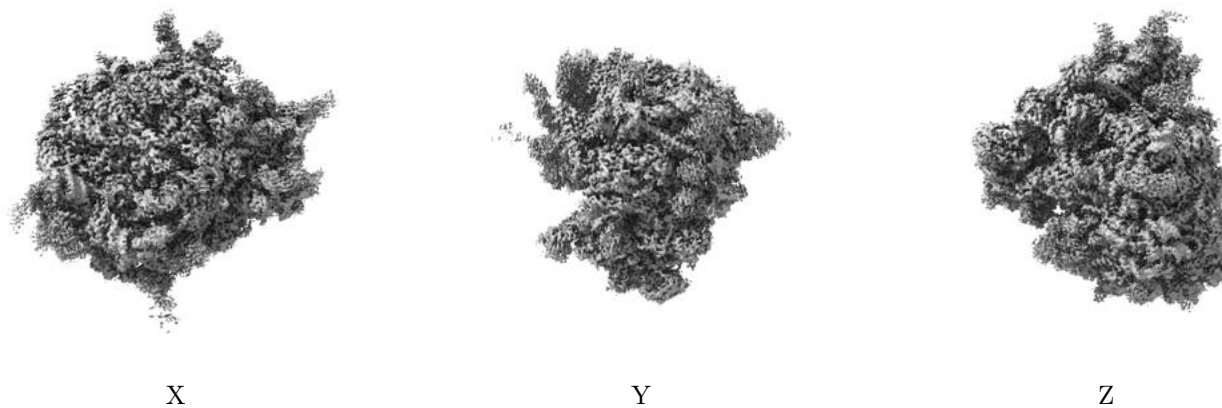
Z

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



## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

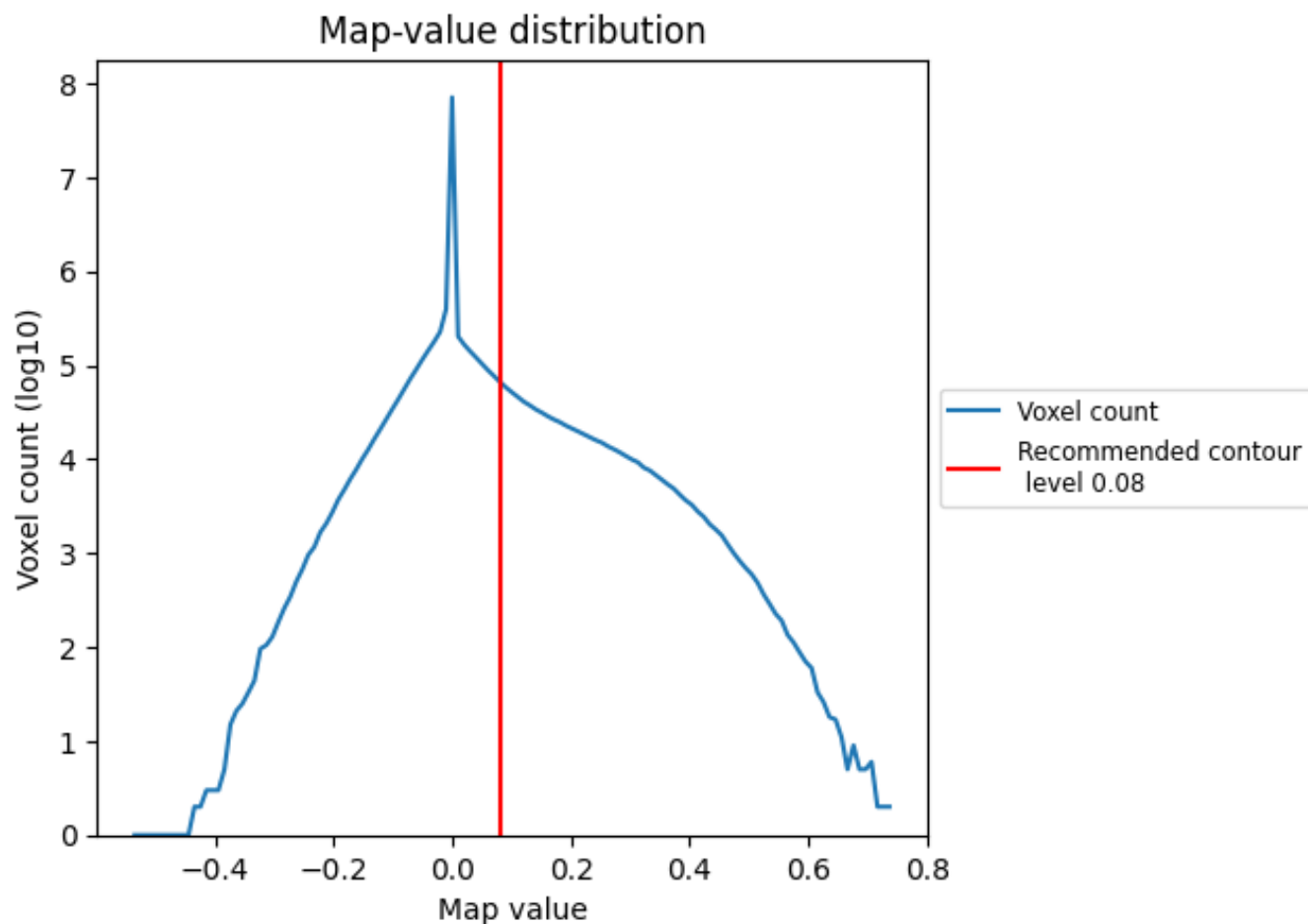
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

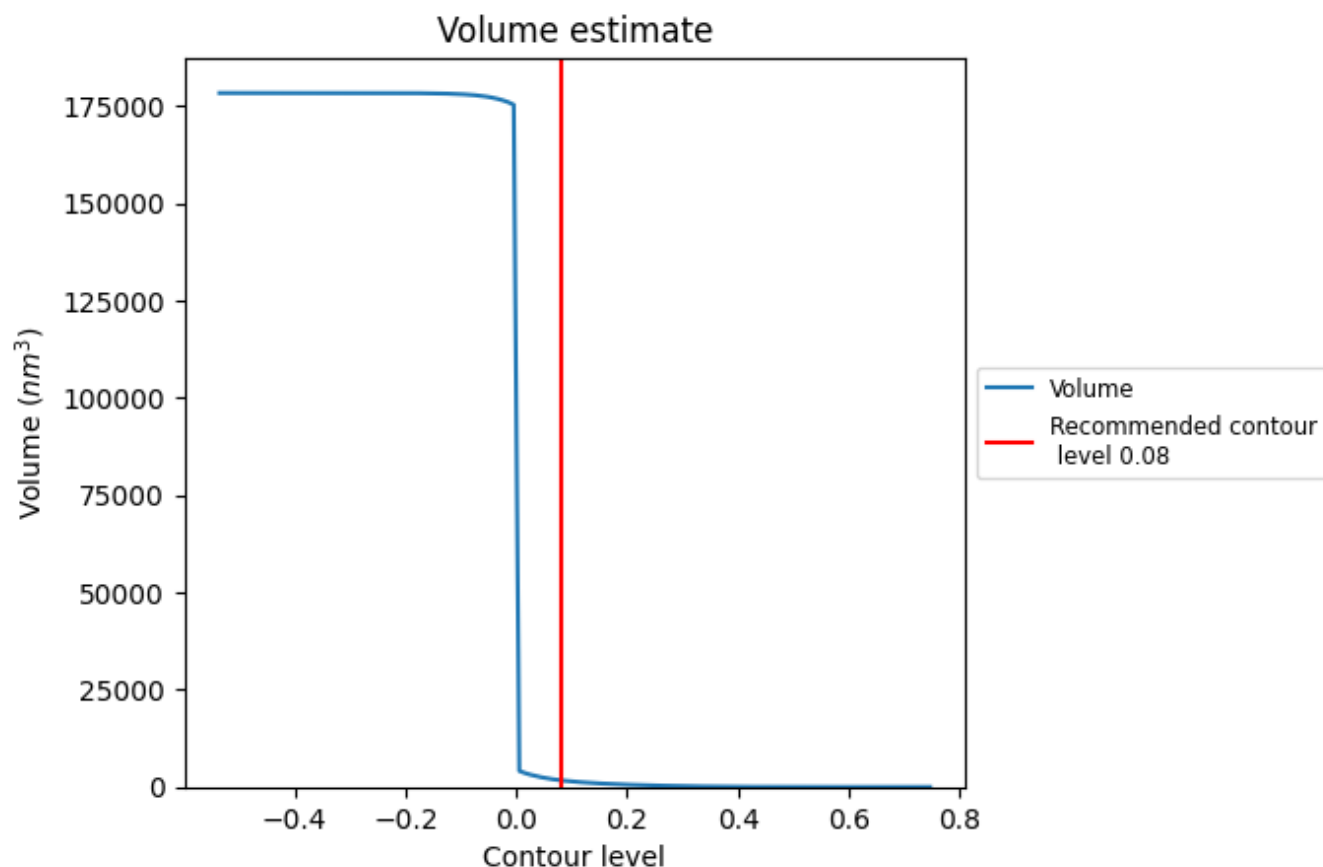
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

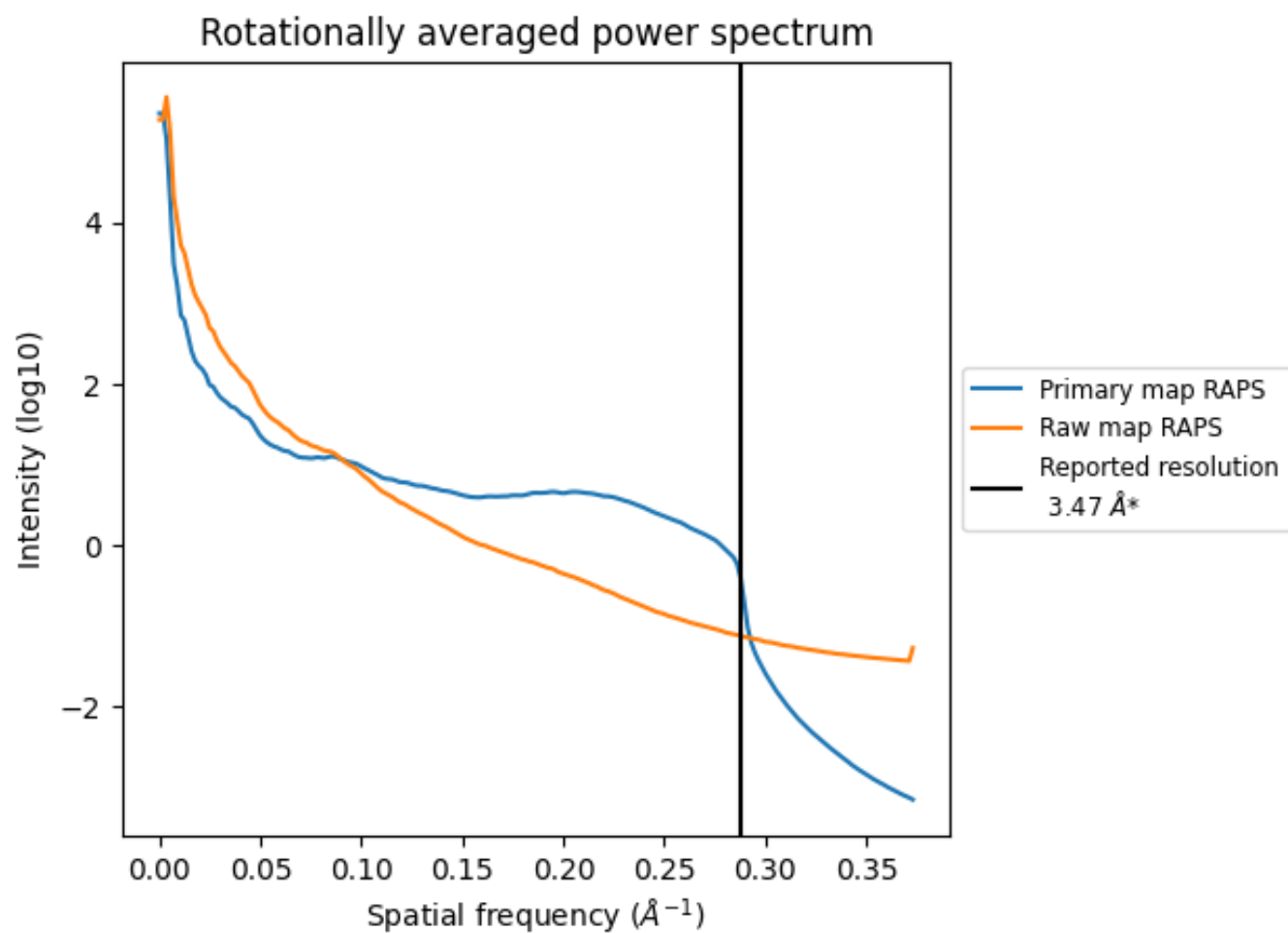
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1722 nm<sup>3</sup>; this corresponds to an approximate mass of 1556 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 ⓘ

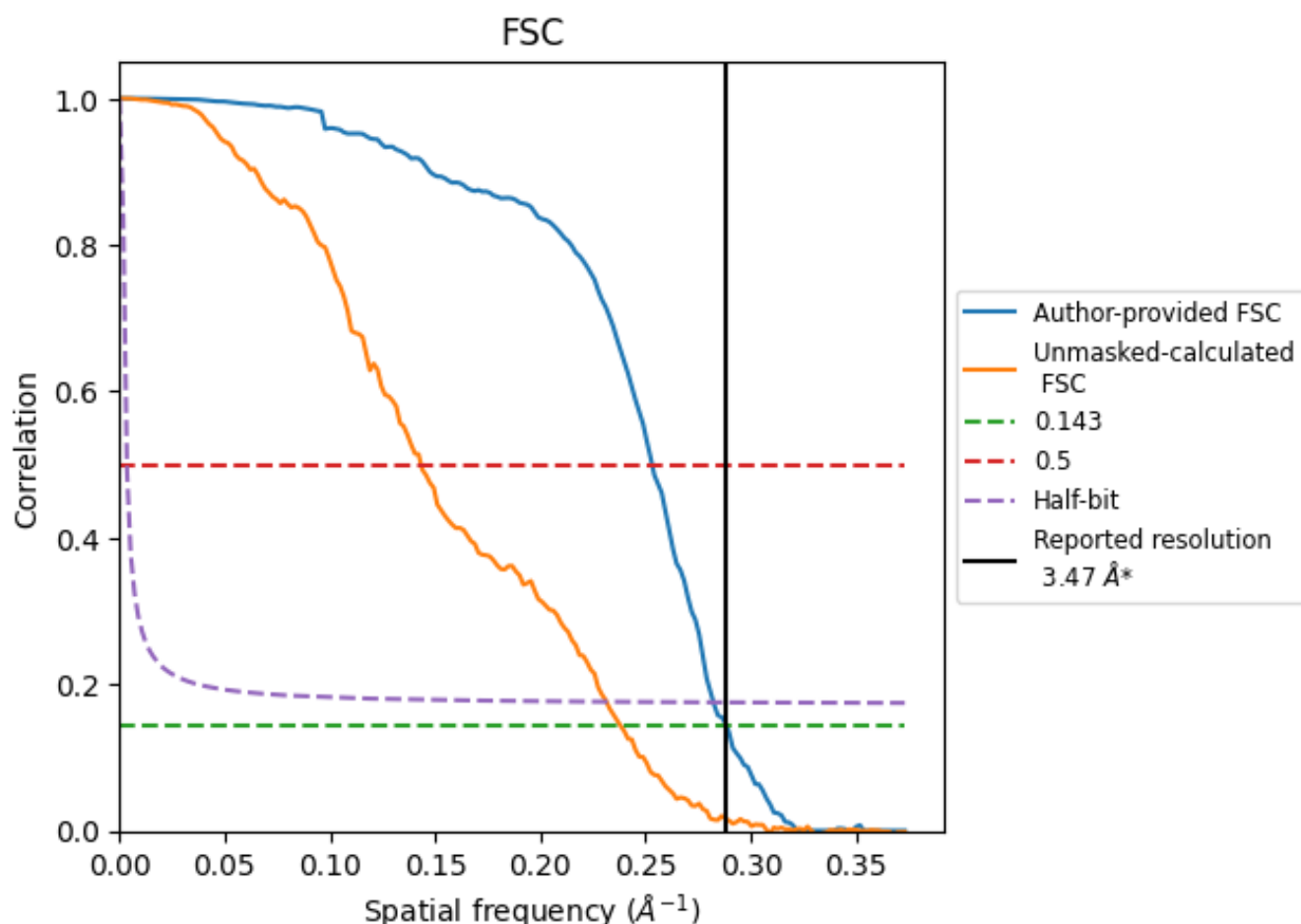


\*Reported resolution corresponds to spatial frequency of  $0.288 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.288 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

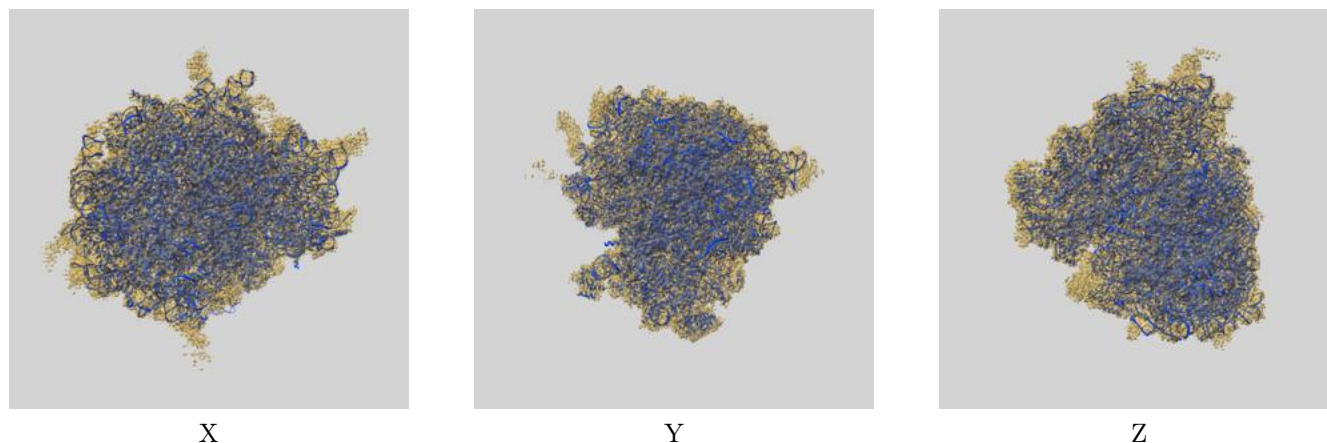
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	3.47	3.95	3.54
Unmasked-calculated*	4.20	6.98	4.32

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.20 differs from the reported value 3.47 by more than 10 %

## 9 Map-model fit [i](#)

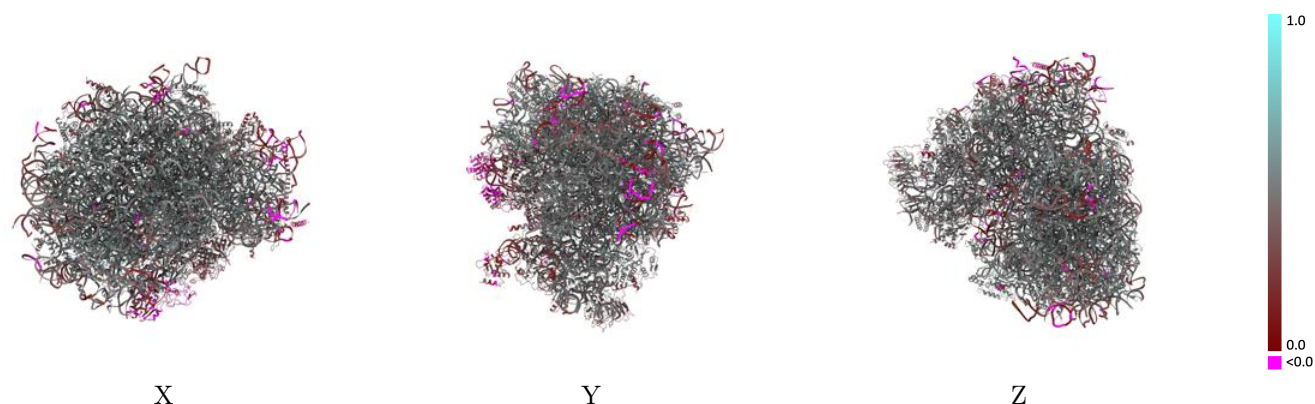
This section contains information regarding the fit between EMDB map EMD-4137 and PDB model 5LZZ. Per-residue inclusion information can be found in section [3](#) on page [24](#).

### 9.1 Map-model overlay [i](#)



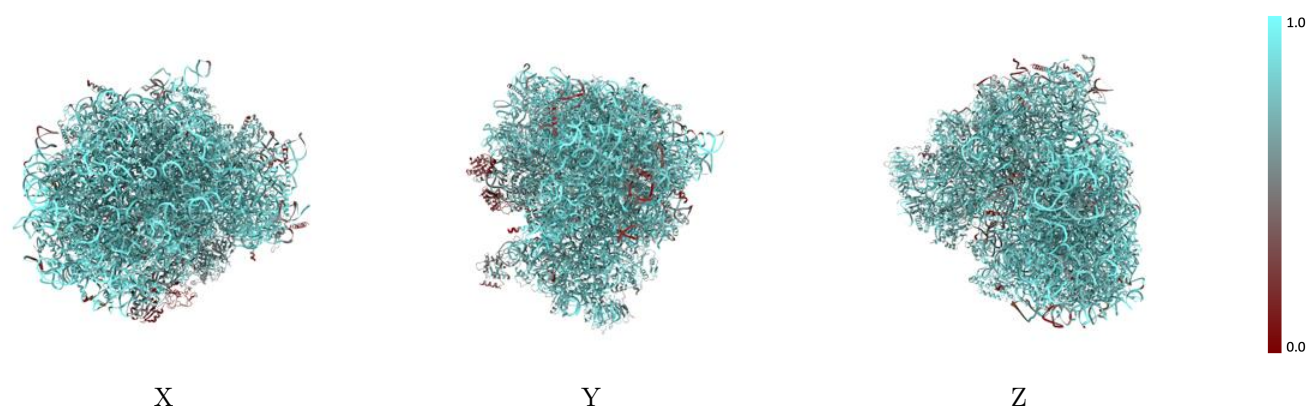
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

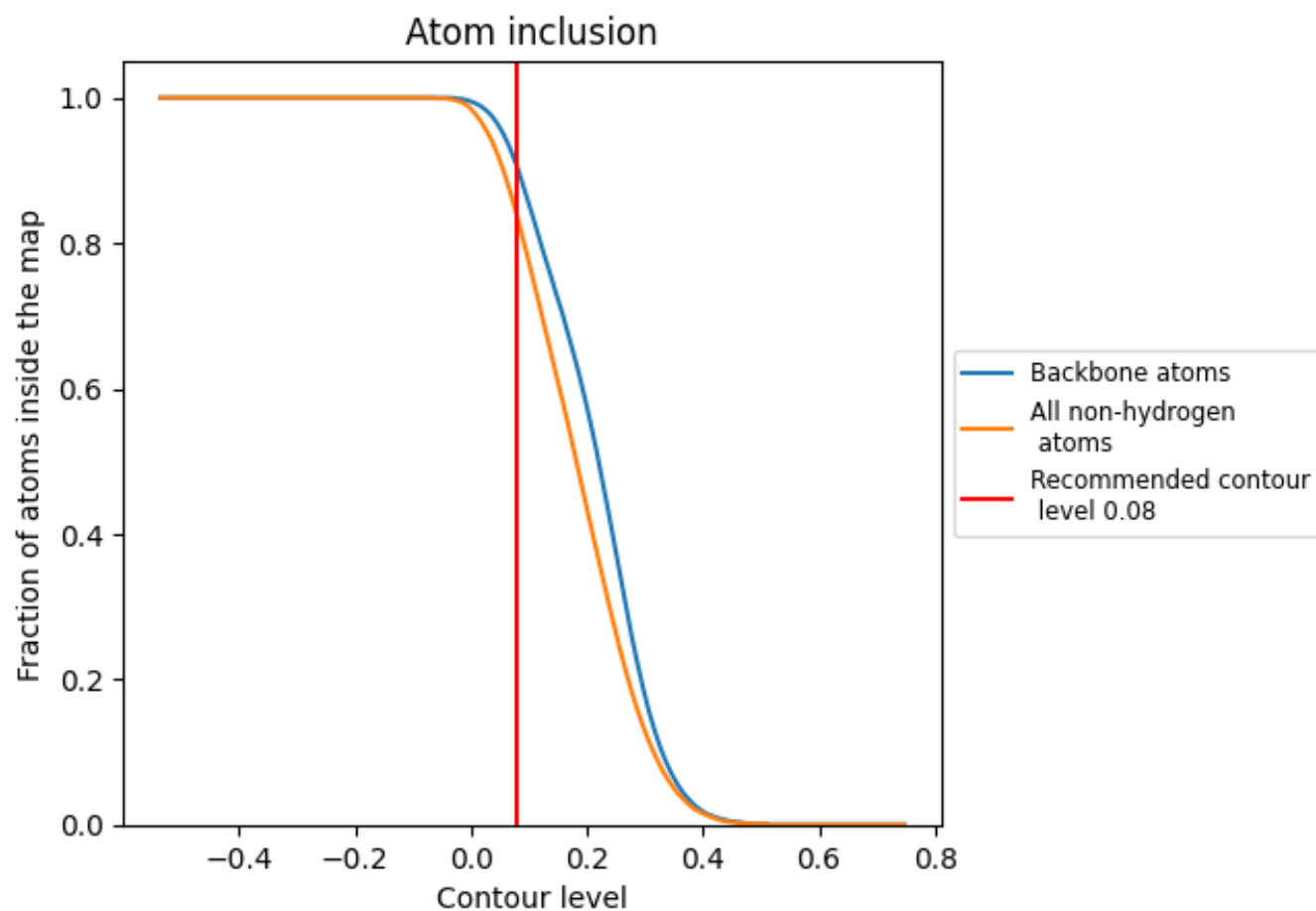
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.08).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 84% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8350	 0.4460
1	 0.4490	 0.3290
2	 0.8300	 0.4290
3	 0.5840	 0.2260
5	 0.8920	 0.4490
7	 0.9390	 0.4940
8	 0.8980	 0.4490
9	 0.8790	 0.4310
A	 0.8530	 0.5150
AA	 0.7930	 0.4570
B	 0.8560	 0.5110
BB	 0.7820	 0.4670
C	 0.8520	 0.5060
CC	 0.8060	 0.4810
D	 0.8370	 0.4780
DD	 0.7470	 0.4350
E	 0.8450	 0.4890
EE	 0.7990	 0.4750
F	 0.8520	 0.5180
FF	 0.7620	 0.4480
G	 0.7640	 0.4410
GG	 0.7380	 0.3920
H	 0.8260	 0.4940
HH	 0.7000	 0.4040
I	 0.8310	 0.5080
II	 0.7870	 0.4610
J	 0.8210	 0.4720
JJ	 0.8210	 0.4670
KK	 0.7630	 0.4020
L	 0.8150	 0.4760
LL	 0.8000	 0.4810
M	 0.8390	 0.4900
MM	 0.4840	 0.1950
N	 0.8500	 0.5180
NN	 0.8130	 0.4850

























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Chain	Atom inclusion	Q-score
O	 0.8500	 0.5100
OO	 0.8140	 0.4840
P	 0.8490	 0.5110
PP	 0.7380	 0.4060
Q	 0.8430	 0.5100
QQ	 0.7960	 0.4620
R	 0.7950	 0.4600
RR	 0.7580	 0.4370
S	 0.8620	 0.5210
SS	 0.7710	 0.4240
T	 0.8210	 0.4920
TT	 0.8100	 0.4360
U	 0.7940	 0.4370
UU	 0.7460	 0.4290
V	 0.8130	 0.5150
VV	 0.8100	 0.4750
W	 0.6790	 0.3720
WW	 0.8440	 0.5080
X	 0.8010	 0.4830
XX	 0.8010	 0.5020
Y	 0.8300	 0.4960
YY	 0.7960	 0.4470
Z	 0.8540	 0.4880
ZZ	 0.7020	 0.3930
a	 0.8460	 0.5160
aa	 0.8080	 0.4770
b	 0.7340	 0.4180
bb	 0.7500	 0.4340
c	 0.7940	 0.4640
cc	 0.7210	 0.4510
d	 0.8100	 0.4820
dd	 0.8460	 0.4950
e	 0.8470	 0.5140
ee	 0.7250	 0.4270
f	 0.8650	 0.5260
ff	 0.5620	 0.2600
g	 0.8120	 0.4920
gg	 0.7550	 0.4020
h	 0.8030	 0.4760
hh	 0.1480	 0.2260
i	 0.8100	 0.4640
ii	 0.6220	 0.3820

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Chain	Atom inclusion	Q-score
j	 0.8680	 0.5140
jj	 0.6420	 0.3630
k	 0.7500	 0.4310
l	 0.8410	 0.4970
m	 0.8490	 0.5040
n	 0.6740	 0.4700
o	 0.8090	 0.5040
p	 0.7980	 0.4900
r	 0.8750	 0.5190
s	 0.2300	 0.0810
t	 0.1440	 0.0370