Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 02:40 PM EST

PDB ID	:	3JCS
EMDB ID	:	EMD-6583
Title	:	2.8 Angstrom cryo-EM structure of the large ribosomal subunit from the eukaryotic parasite Leishmania
Authors	:	Shalev-Benami, M.; Zhang, Y.; Matzov, D.; Halfon, Y.; Zackay, A.; Rozenberg, H.; Zimmerman, E.; Bashan, A.; Jaffe, C.L.; Yonath, A.; Skiniotis, G.
Deposited on	:	2016-01-21
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

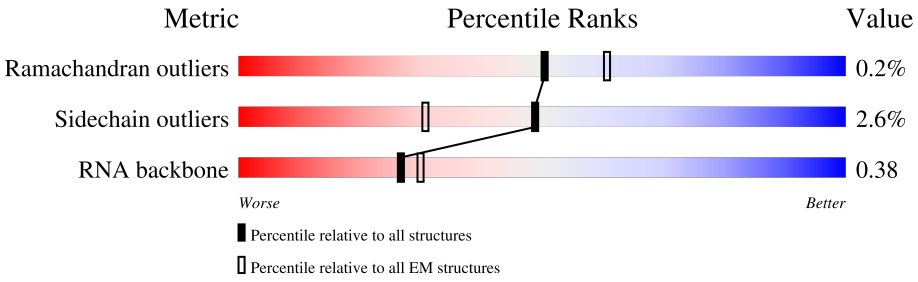
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1	1782	8% 52% 33% · 13%
2	2	1527	11% 43% 29% · 27%
3	3	213	17% 45% 41% 14%
4	4	183	9% 55% 26% · 19%
5	5	133	· 36% 23% · 40%
6	6	76	17% 16% 59% 5% 20%
7	7	171	· 60% 29% · 10%
8	8	121	· 53% 45% ·

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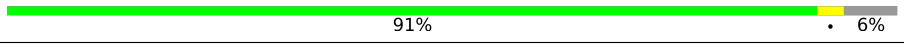
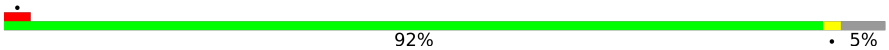
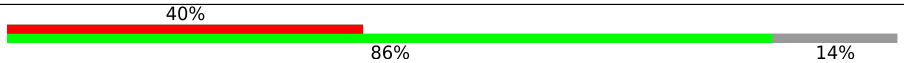
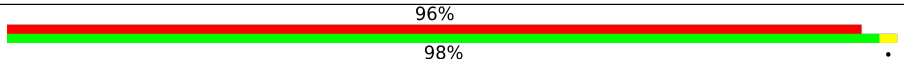
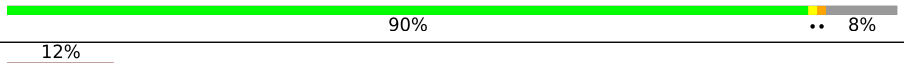
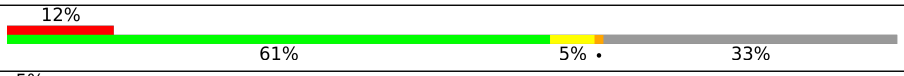
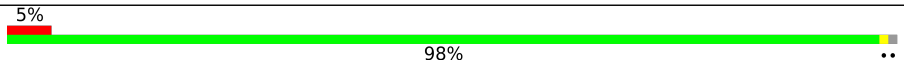
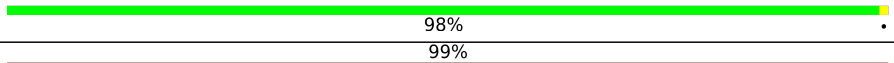
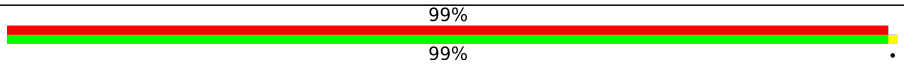
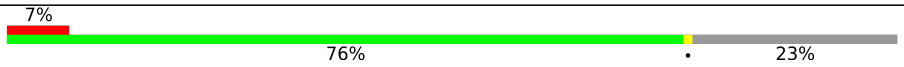
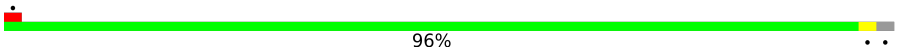
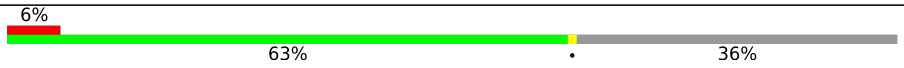
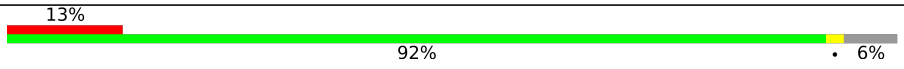
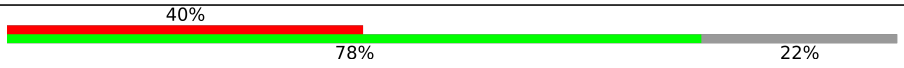
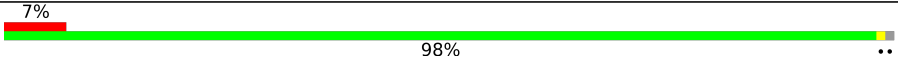
Mol	Chain	Length	Quality of chain
9	A	260	
10	B	419	
11	C	373	
12	D	188	
13	E	190	
14	F	195	
15	G	348	
16	H	222	
17	I	220	
18	J	139	
19	K	233	
20	L	145	
21	M	204	
22	N	213	
23	O	305	
24	P	198	
25	Q	245	
26	R	179	
27	S	159	
28	T	166	
29	U	129	
30	V	145	
31	W	143	
32	X	124	
33	Y	134	

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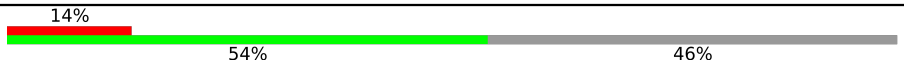
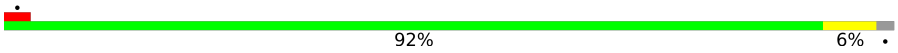
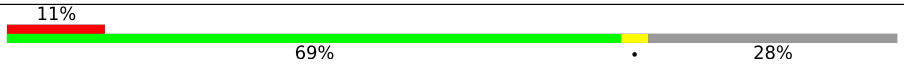
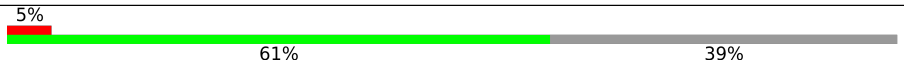
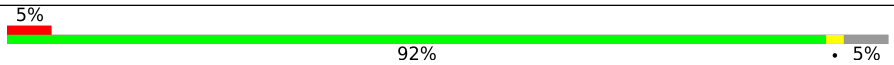
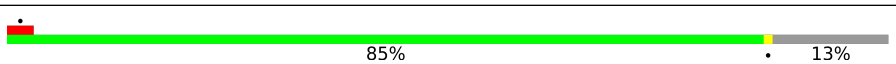
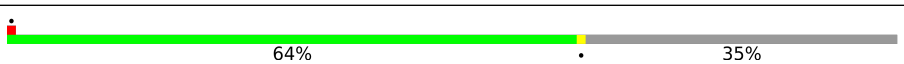
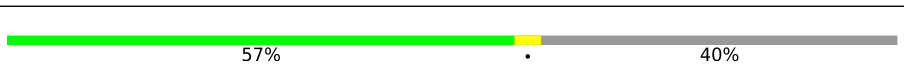
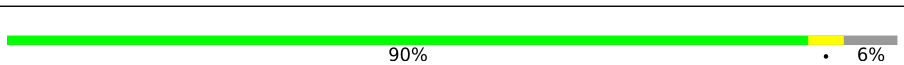
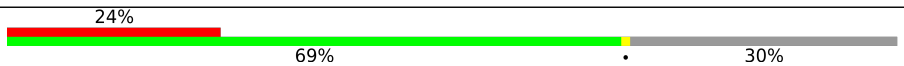
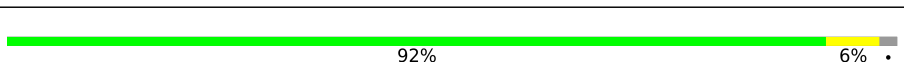
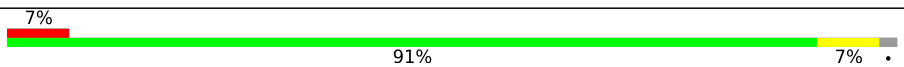
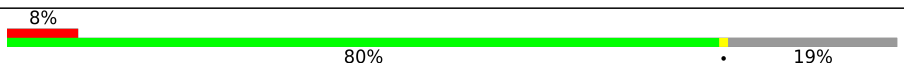
Mol	Chain	Length	Quality of chain
34	Z	147	
35	a	127	
36	b	70	
37	c	252	
38	d	104	
39	e	183	
40	f	133	
41	g	144	
42	h	168	
43	i	105	
44	j	83	
45	k	83	
46	l	51	
47	m	92	
48	n	106	

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 117257 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 RNA chain called 26S alpha ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	1554	33313	14886	6081	10792	1554	0	0

- Molecule 2 is a RNA chain called 26S delta ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	1119	23926	10702	4308	7797	1119	0	0

- Molecule 3 is a RNA chain called 26S gamma ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	3	184	3893	1740	662	1307	184	0	0

- Molecule 4 is a RNA chain called 26S delta ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	4	149	3177	1418	570	1040	149	0	0

- Molecule 5 is a RNA chain called 26S epsilon ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	5	80	1708	763	310	555	80	0	0

- Molecule 6 is a RNA chain called 26S zeta ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	6	61	1288	577	225	425	61	0	0

- Molecule 7 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	154	Total	C	N	O	P	0	0
			3280	1469	584	1074	153		

- Molecule 8 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	119	Total	C	N	O	P	0	0
			2531	1132	450	830	119		

- Molecule 9 is a protein called ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	245	Total	C	N	O	S	2	0
			1859	1158	384	307	10		

- Molecule 10 is a protein called ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	396	Total	C	N	O	S	2	0
			3020	1908	592	508	12		

- Molecule 11 is a protein called ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	301	Total	C	N	O	S	1	0
			2237	1413	428	384	12		

- Molecule 12 is a protein called ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	D	161	Total	C	N	O	0	0
			799	476	161	162		

- Molecule 13 is a protein called ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	190	Total	C	N	O	S	0	0
			1509	953	276	272	8		

- Molecule 14 is a protein called ribosomal protein L6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	137	Total	C	N	O	S	1	0
			1002	641	192	167	2		

- Molecule 15 is a protein called ribosomal protein L8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	226	Total	C	N	O	S	1	0
			1772	1113	353	299	7		

- Molecule 16 is a protein called ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	202	Total	C	N	O	S	0	0
			1596	1019	307	263	7		

- Molecule 17 is a protein called ribosomal protein L13e.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	132	Total	C	N	O	S	0	0
			1061	666	221	169	5		

- Molecule 18 is a protein called ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	128	Total	C	N	O	S	0	0
			924	588	171	160	5		

- Molecule 19 is a protein called ribosomal protein L14e.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	156	Total	C	N	O	S	0	0
			1061	661	212	184	4		

- Molecule 20 is a protein called ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	144	Total	C	N	O	S	0	0
			1096	691	223	177	5		

- Molecule 21 is a protein called ribosomal protein L15e.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	203	Total	C	N	O	S	0	0
			1714	1080	362	264	8		

- Molecule 22 is a protein called ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	213	Total	C	N	O	S	0	0
			1714	1077	340	281	16		

- Molecule 23 is a protein called ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	235	Total	C	N	O	S	0	0
			1557	986	300	268	3		

- Molecule 24 is a protein called ribosomal protein L18e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	195	Total	C	N	O	S	1	0
			1494	942	299	247	6		

- Molecule 25 is a protein called ribosomal protein L19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	156	Total	C	N	O	S	0	0
			1162	730	243	186	3		

- Molecule 26 is a protein called ribosomal protein L20e.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	131	Total	C	N	O	S	1	0
			1019	651	197	167	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	158	ILE	LEU	VARIANT	UNP E9BRT7

- Molecule 27 is a protein called ribosomal protein L21e.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	149	Total	C	N	O	S	2	0
			1112	704	218	187	3		

- Molecule 28 is a protein called ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	154	Total	C	N	O	S	2	0
			1221	763	241	206	11		

- Molecule 29 is a protein called ribosomal protein L22e.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	U	100	Total	C	N	O	0	0
			541	331	101	109		

- Molecule 30 is a protein called ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	118	Total	C	N	O	S	0	0
			892	566	171	153	2		

- Molecule 31 is a protein called ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	117	Total	C	N	O	S	1	0
			896	562	187	144	3		

- Molecule 32 is a protein called ribosomal protein L24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	X	64	Total	C	N	O	S	0	0
			508	333	96	76	3		

- Molecule 33 is a protein called ribosomal protein L27e.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Y	132	Total	C	N	O	0	0
			914	589	174	151		

- Molecule 34 is a protein called ribosomal protein L28e.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Z	79	Total	C	N	O	S	0	0
			538	329	111	95	3		

- Molecule 35 is a protein called ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	124	Total	C	N	O	S	0	0
			982	613	203	163	3		

- Molecule 36 is a protein called ribosomal protein L29e.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	65	Total	C	N	O	S	0	0
			503	309	113	80	1		

- Molecule 37 is a protein called ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	222	Total	C	N	O	S	0	0
			1732	1105	327	289	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	49	ALA	GLY	VARIANT	UNP E9BI29

- Molecule 38 is a protein called ribosomal protein L30e.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	75	Total	C	N	O	S	0	0
			518	325	93	97	3		

- Molecule 39 is a protein called ribosomal protein L31e.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	112	Total	C	N	O	S	1	0
			824	531	155	136	2		

- Molecule 40 is a protein called ribosomal protein L32e.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f	126	Total	C	N	O	S	0	0
			982	616	195	167	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	105	LYS	THR	VARIANT	UNP E9BFJ5

- Molecule 41 is a protein called ribosomal protein L33e.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	g	125	Total	C	N	O	S	0	0
			983	612	205	161	5		

- Molecule 42 is a protein called ribosomal protein L34e.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h	109	Total	C	N	O	S	0	0
			856	529	182	140	5		

- Molecule 43 is a protein called ribosomal protein L36e.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i	63	Total	C	N	O	S	1	0
			494	316	100	76	2		

- Molecule 44 is a protein called ribosomal protein L37e.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	78	Total	C	N	O	S	0	0
			639	385	149	99	6		

- Molecule 45 is a protein called ribosomal protein L38e.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	58	Total	C	N	O	S	0	0
			373	234	71	66	2		

- Molecule 46 is a protein called ribosomal protein L39e.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	l	50	Total	C	N	O	S	1	0
			457	294	98	64	1		

- Molecule 47 is a protein called ribosomal protein L43e.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	m	90	Total	C	N	O	S	0	0
			668	414	135	113	6		

- Molecule 48 is a protein called ribosomal protein L44e.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	n	86	Total	C	N	O	S	0	0
			659	418	129	110	2		

- Molecule 49 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
49	1	51	Total	Mg	0
			51	51	
49	2	25	Total	Mg	0
			25	25	
49	3	3	Total	Mg	0
			3	3	
49	4	2	Total	Mg	0
			2	2	
49	5	4	Total	Mg	0
			4	4	
49	7	9	Total	Mg	0
			9	9	
49	C	1	Total	Mg	0
			1	1	
49	K	1	Total	Mg	0
			1	1	
49	M	3	Total	Mg	0
			3	3	
49	V	1	Total	Mg	0
			1	1	
49	a	1	Total	Mg	0
			1	1	
49	f	2	Total	Mg	0
			2	2	

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Mol	Chain	Residues	Atoms	AltConf
49	g	1	Total Mg 1 1	0
49	h	1	Total Mg 1 1	0
49	j	4	Total Mg 4 4	0

- Molecule 50 is water.

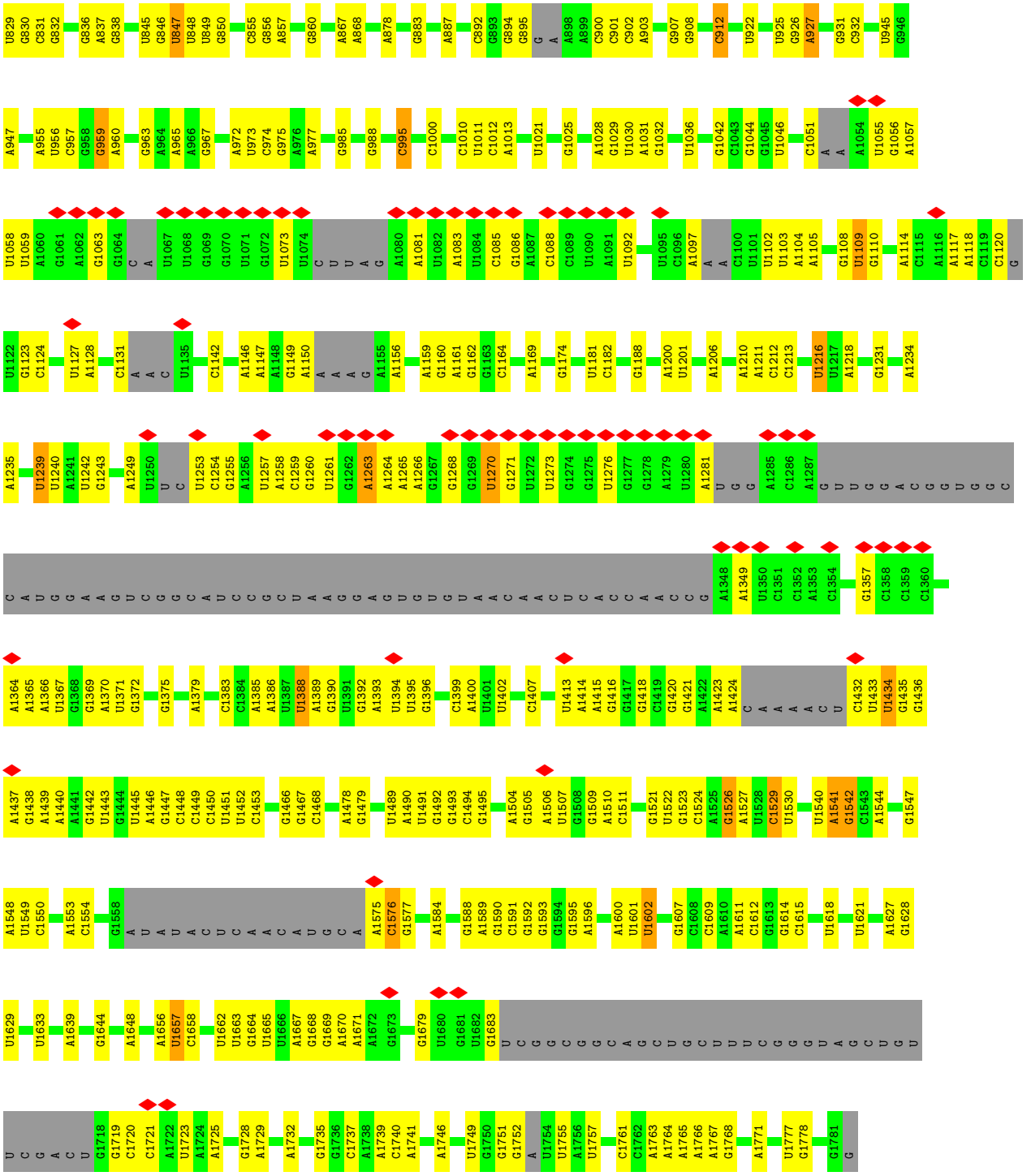
Mol	Chain	Residues	Atoms	AltConf
50	1	72	Total O 72 72	0
50	2	40	Total O 40 40	0
50	4	4	Total O 4 4	0
50	5	4	Total O 4 4	0
50	7	16	Total O 16 16	0
50	8	1	Total O 1 1	0
50	A	2	Total O 2 2	0
50	G	1	Total O 1 1	0
50	M	2	Total O 2 2	0
50	i	1	Total O 1 1	0
50	j	1	Total O 1 1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

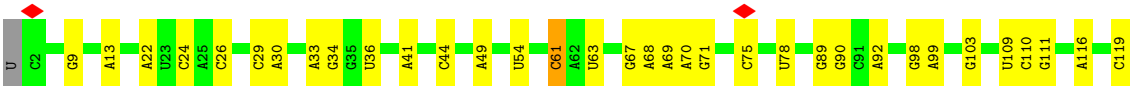
- Molecule 1: 26S alpha ribosomal RNA

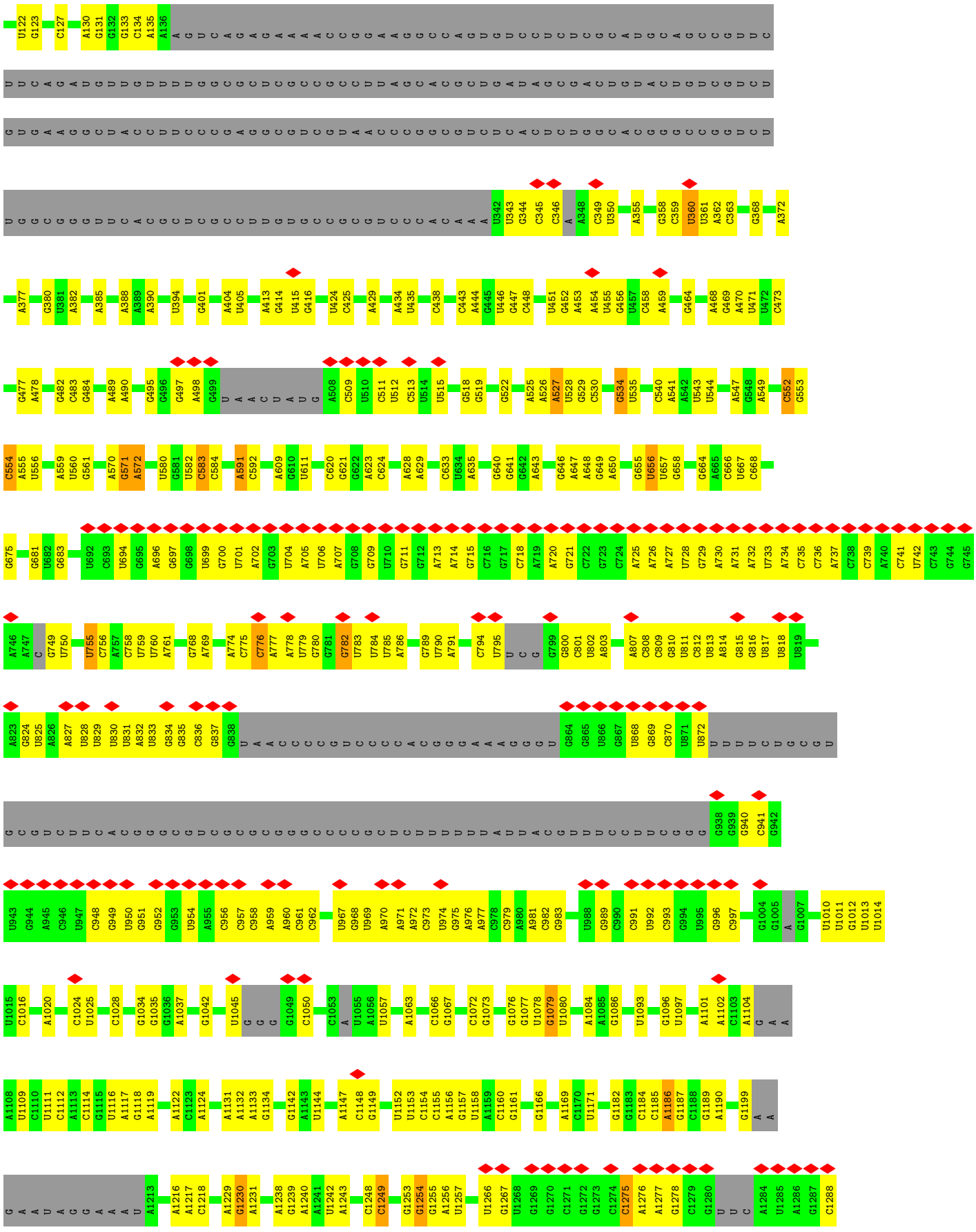
Chain 1:

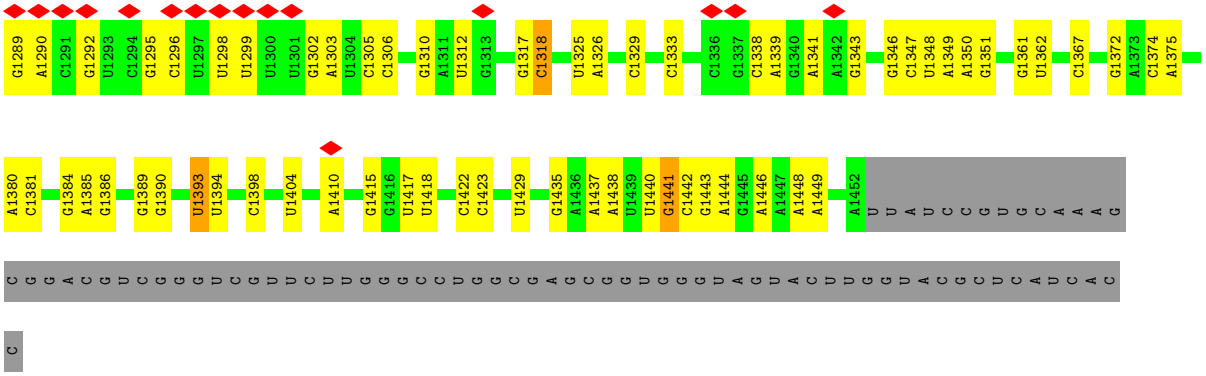


• Molecule 2: 26S delta ribosomal RNA

Chain 2:

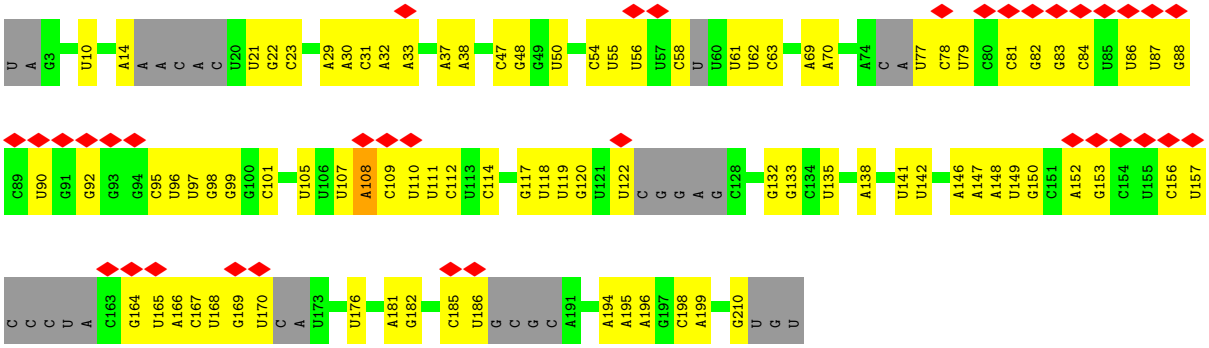






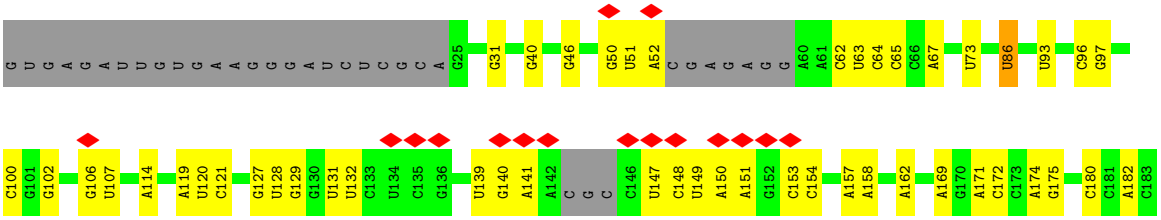
• Molecule 3: 26S gamma ribosomal RNA

Chain 3:



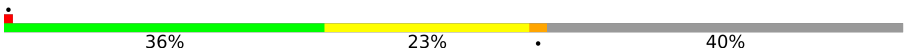
• Molecule 4: 26S delta ribosomal RNA

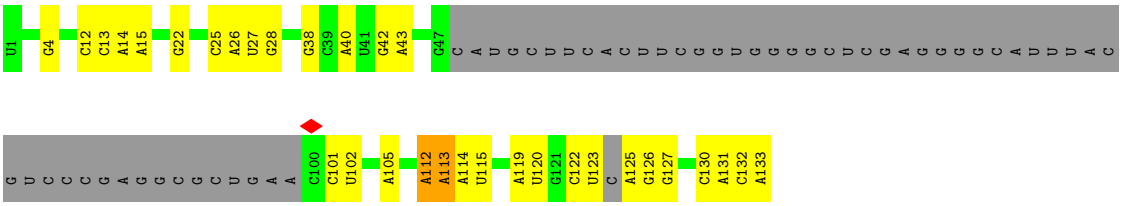
Chain 4:



• Molecule 5: 26S epsilon ribosomal RNA

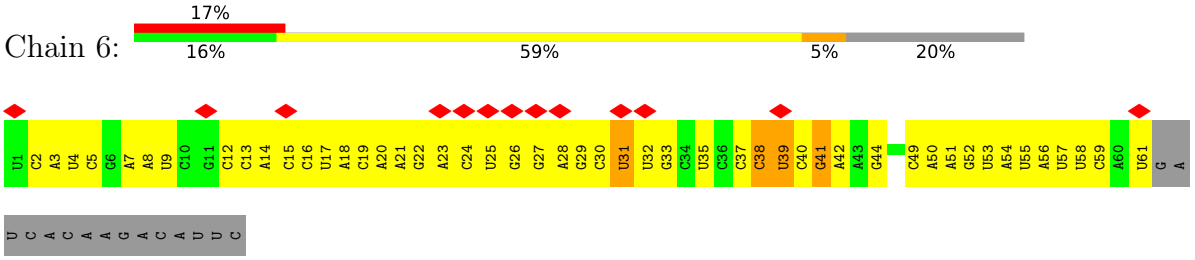
Chain 5:





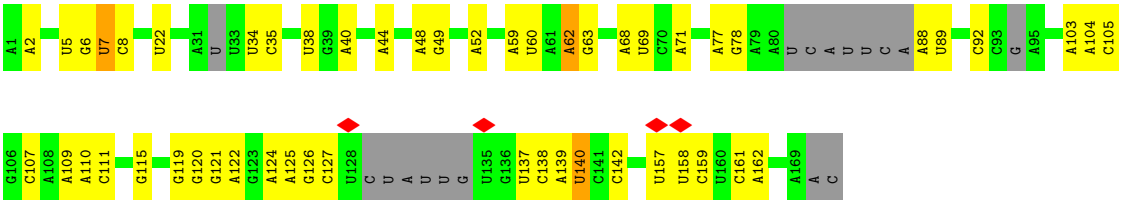
• Molecule 6: 26S zeta ribosomal RNA

Chain 6:



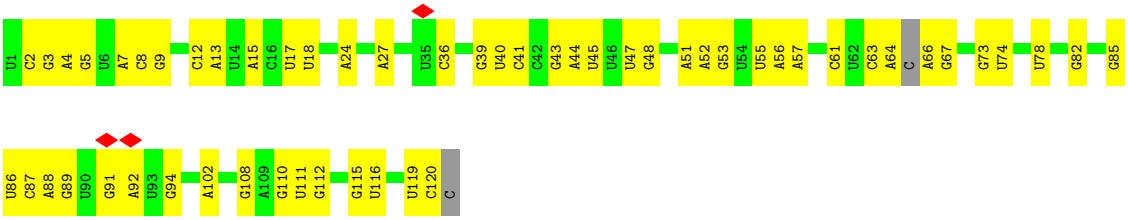
• Molecule 7: 5.8S ribosomal RNA

Chain 7:



• Molecule 8: 5S ribosomal RNA

Chain 8:

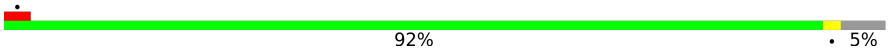


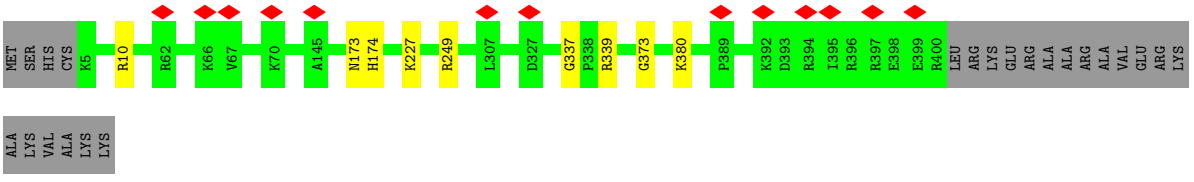
• Molecule 9: ribosomal protein L2

Chain A:

• Molecule 10: ribosomal protein L3

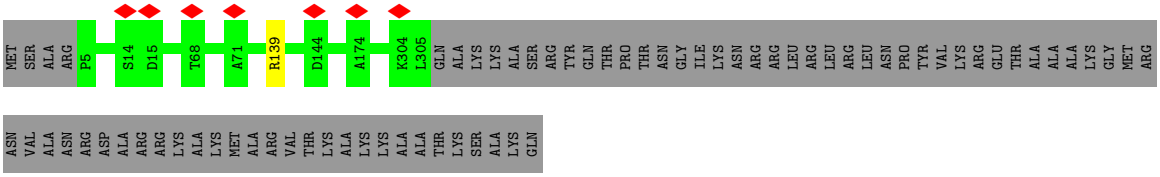
Chain B:





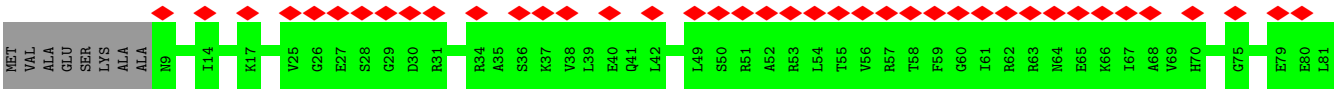
• Molecule 11: ribosomal protein L4

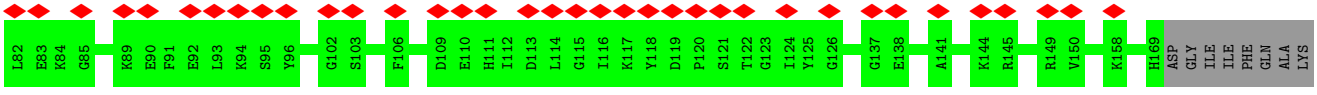
Chain C:



• Molecule 12: ribosomal protein L5

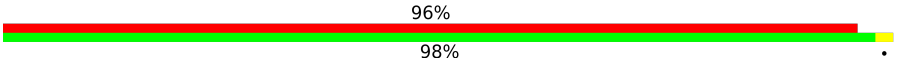
Chain D:

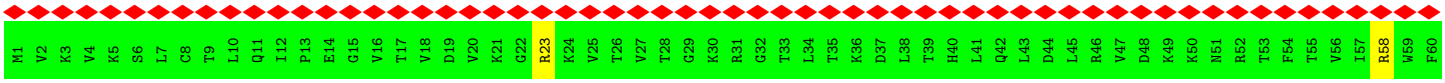


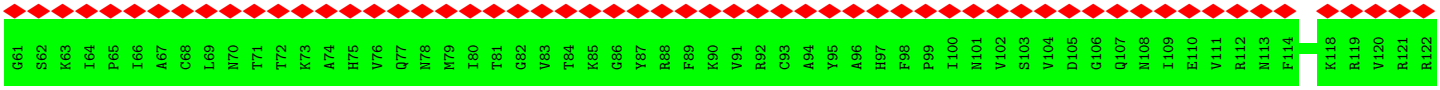


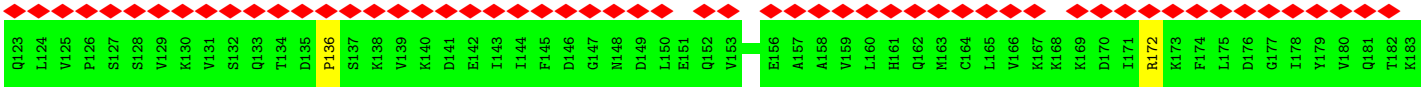
• Molecule 13: ribosomal protein L6

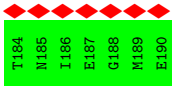
Chain E:





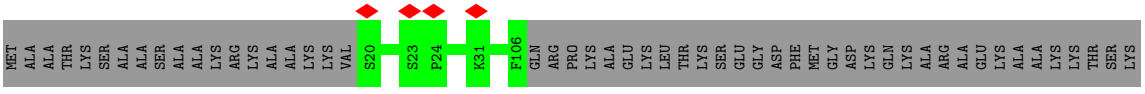


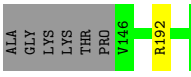




• Molecule 14: ribosomal protein L6e

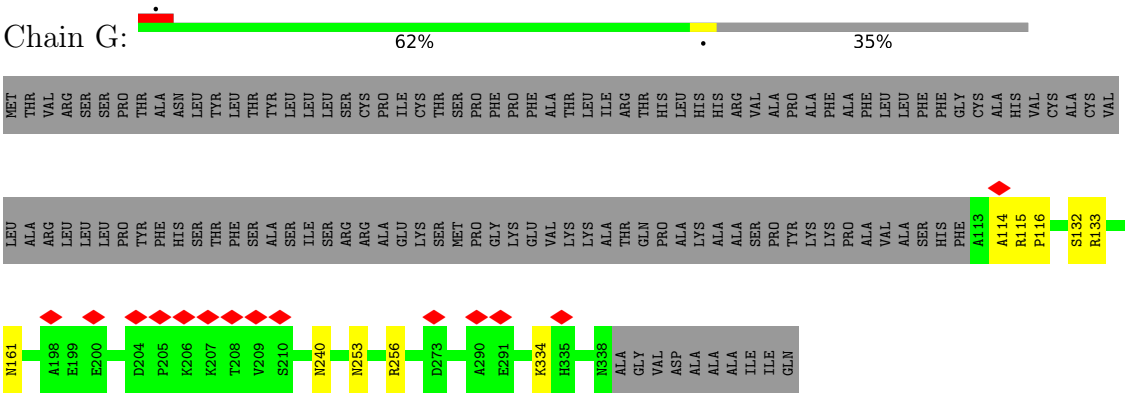
Chain F:





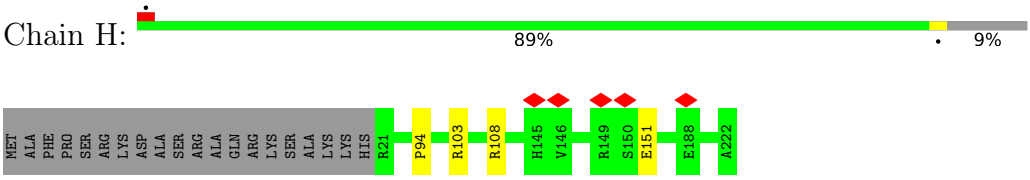
• Molecule 15: ribosomal protein L8e

Chain G:



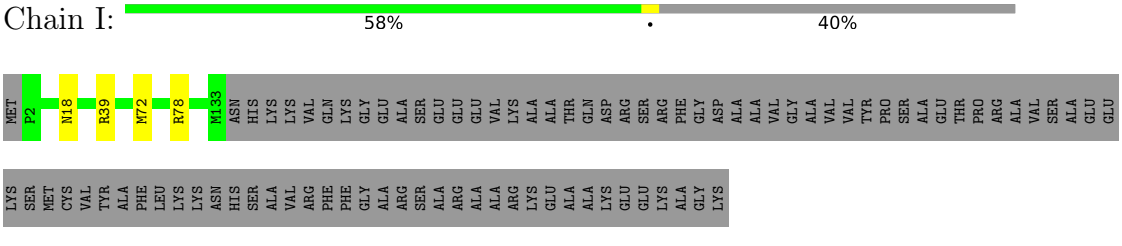
• Molecule 16: ribosomal protein L13

Chain H:



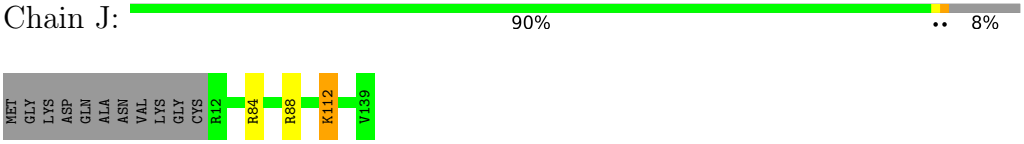
• Molecule 17: ribosomal protein L13e

Chain I:



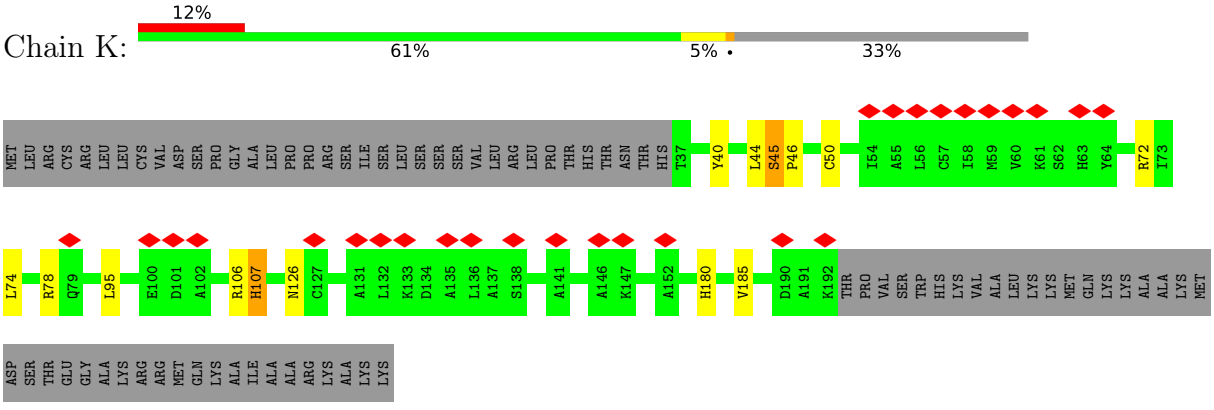
• Molecule 18: ribosomal protein L14

Chain J:



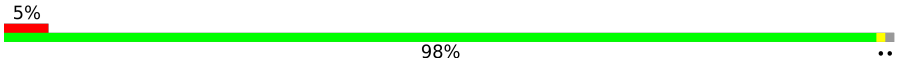
• Molecule 19: ribosomal protein L14e

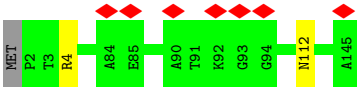
Chain K:



• Molecule 20: ribosomal protein L15

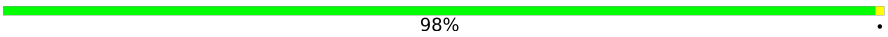
Chain L:

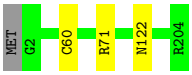




• Molecule 21: ribosomal protein L15e

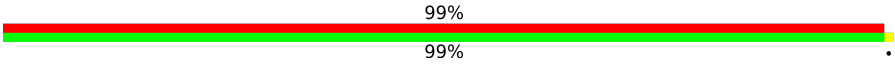
Chain M:

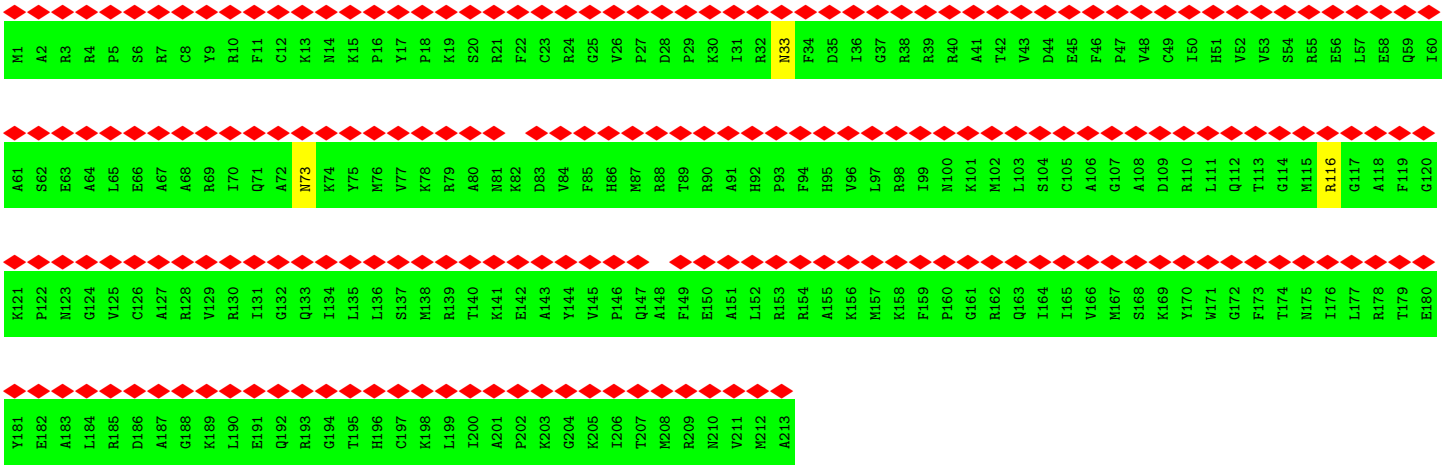




• Molecule 22: ribosomal protein L16

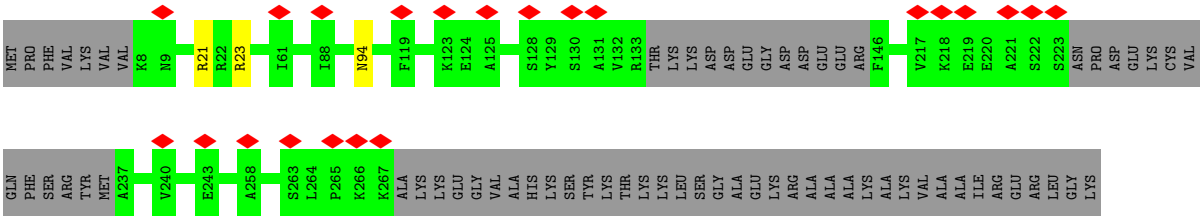
Chain N:





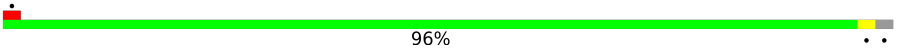
• Molecule 23: ribosomal protein L18

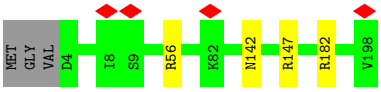
Chain O:



• Molecule 24: ribosomal protein L18e

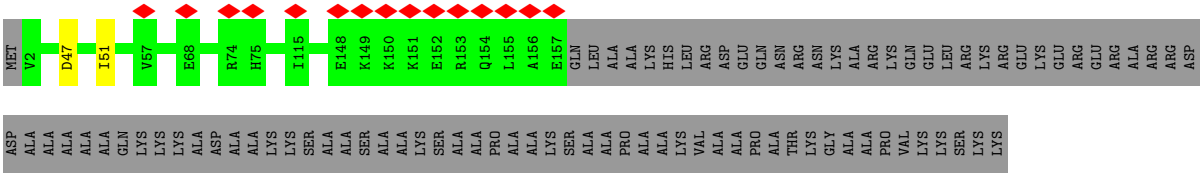
Chain P:





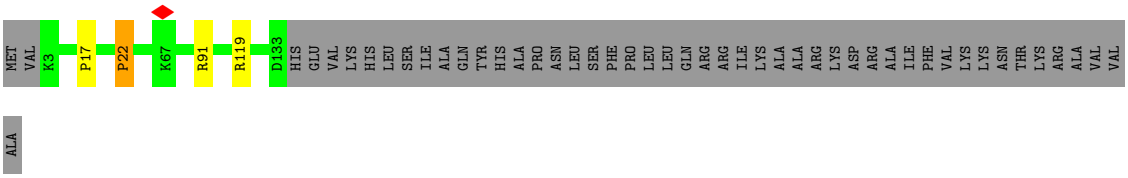
• Molecule 25: ribosomal protein L19e

Chain Q:



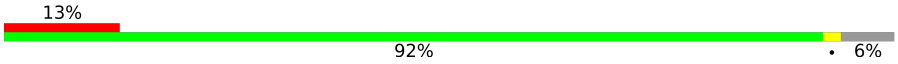
• Molecule 26: ribosomal protein L20e

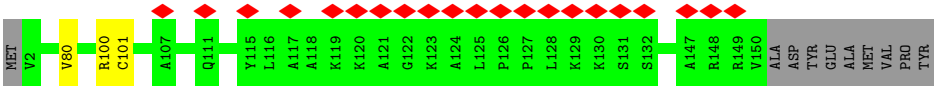
Chain R:



• Molecule 27: ribosomal protein L21e

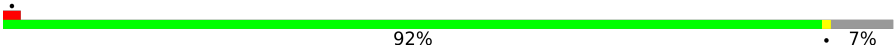
Chain S:

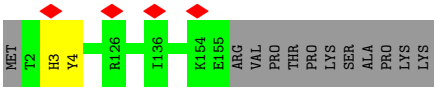




• Molecule 28: ribosomal protein L22

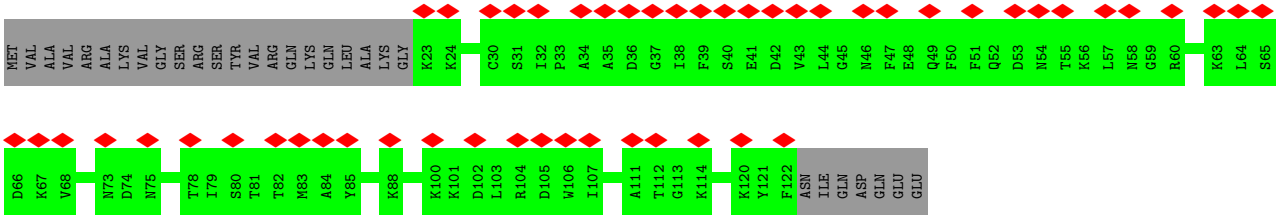
Chain T:





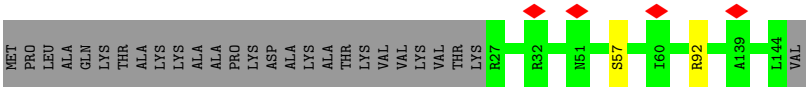
• Molecule 29: ribosomal protein L22e

Chain U:



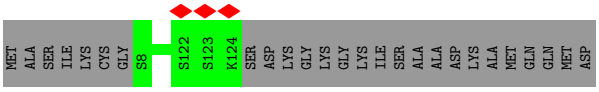
• Molecule 30: ribosomal protein L23

Chain V:



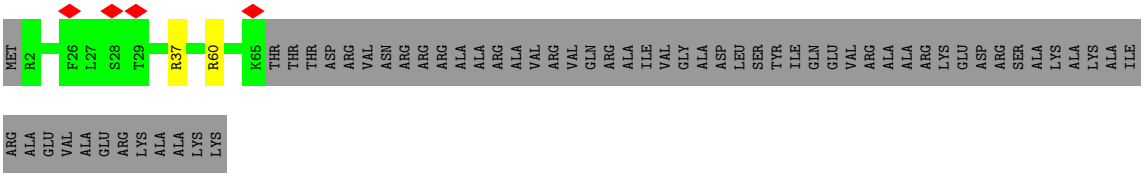
• Molecule 31: ribosomal protein L24

Chain W:



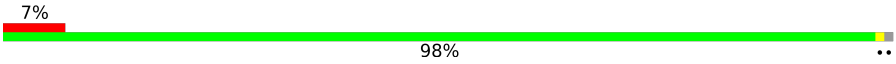
• Molecule 32: ribosomal protein L24e

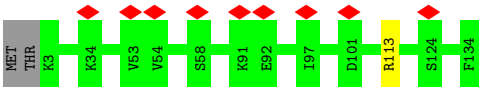
Chain X:



• Molecule 33: ribosomal protein L27e

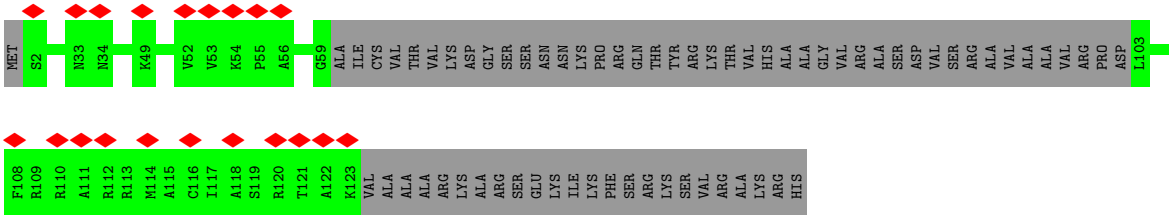
Chain Y:





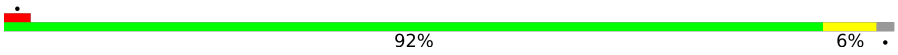
• Molecule 34: ribosomal protein L28e

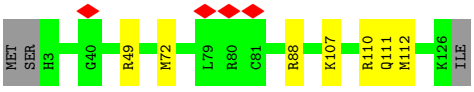
Chain Z:



• Molecule 35: ribosomal protein L29

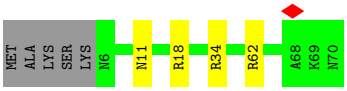
Chain a:





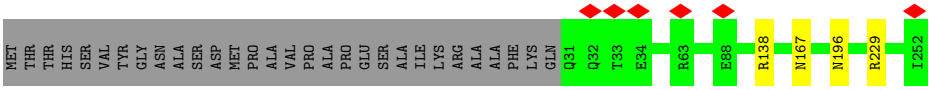
• Molecule 36: ribosomal protein L29e

Chain b:



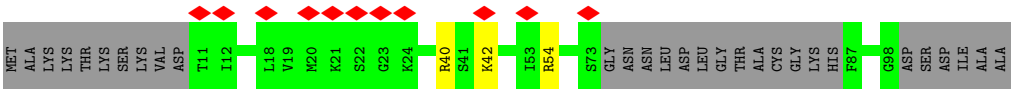
• Molecule 37: ribosomal protein L30

Chain c:



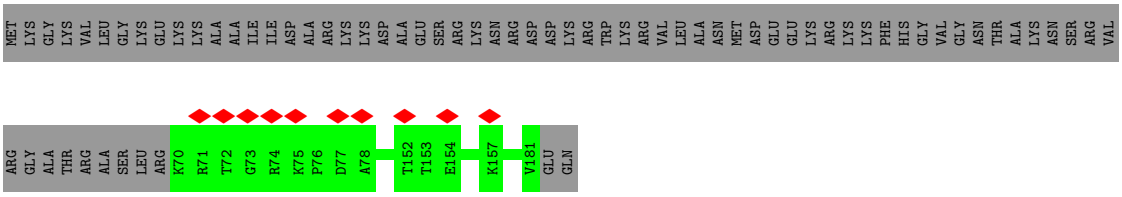
• Molecule 38: ribosomal protein L30e

Chain d:



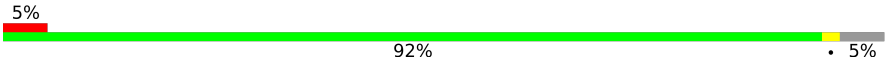
• Molecule 39: ribosomal protein L31e

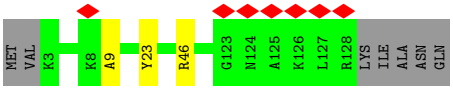
Chain e:



• Molecule 40: ribosomal protein L32e

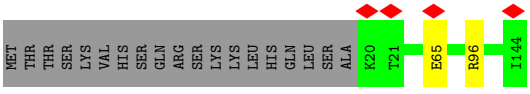
Chain f:





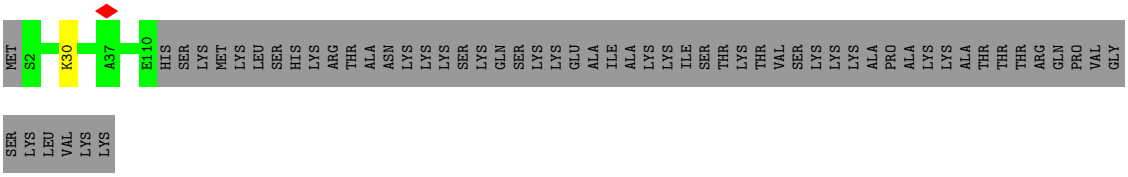
• Molecule 41: ribosomal protein L33e

Chain g:



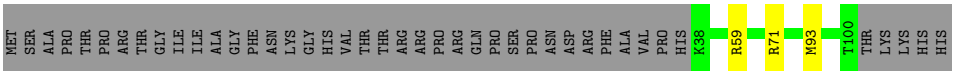
• Molecule 42: ribosomal protein L34e

Chain h:



• Molecule 43: ribosomal protein L36e

Chain i:

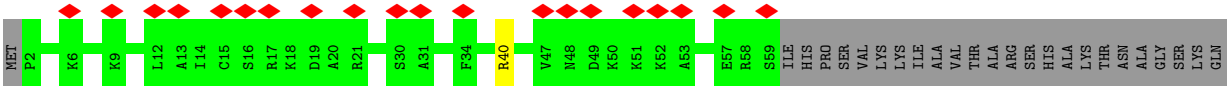


• Molecule 44: ribosomal protein L37e

Chain j:

• Molecule 45: ribosomal protein L38e

Chain k:

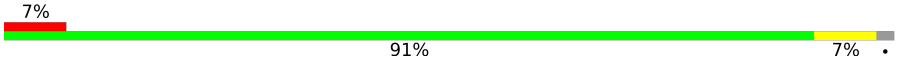


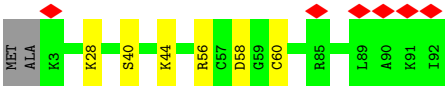
• Molecule 46: ribosomal protein L39e

Chain l:

• Molecule 47: ribosomal protein L43e

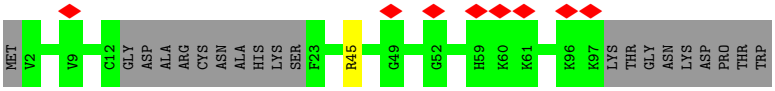
Chain m:





• Molecule 48: ribosomal protein L44e

Chain n:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	107134	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	25000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.231	Depositor
Minimum map value	-0.118	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	384.0, 384.0, 384.0	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, H2U, OMU, OMG, MG, A2M

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	1	0.75	8/36881 (0.0%)	0.90	48/57466 (0.1%)
2	2	0.60	0/26109	0.86	28/40668 (0.1%)
3	3	0.48	0/4337	0.84	1/6734 (0.0%)
4	4	0.69	0/3549	0.88	3/5525 (0.1%)
5	5	0.69	0/1908	0.91	3/2967 (0.1%)
6	6	0.39	2/1437 (0.1%)	0.79	4/2234 (0.2%)
7	7	0.76	0/3615	0.87	2/5622 (0.0%)
8	8	0.47	0/2828	0.82	0/4401
9	A	0.47	0/1903	0.56	0/2559
10	B	0.44	0/3086	0.55	0/4176
11	C	0.45	0/2284	0.60	0/3092
12	D	0.25	0/800	0.49	0/1111
13	E	0.29	0/1529	0.56	0/2056
14	F	0.40	0/1023	0.56	0/1390
15	G	0.38	0/1798	0.59	1/2423 (0.0%)
16	H	0.42	0/1628	0.60	0/2194
17	I	0.40	0/1084	0.57	0/1454
18	J	0.39	0/941	0.61	2/1277 (0.2%)
19	K	0.27	0/1077	0.59	1/1475 (0.1%)
20	L	0.43	0/1123	0.56	0/1505
21	M	0.49	0/1754	0.57	0/2342
22	N	0.27	0/1747	0.54	0/2338
23	O	0.32	0/1583	0.50	0/2157
24	P	0.42	0/1519	0.57	0/2040
25	Q	0.35	0/1179	0.53	0/1588
26	R	0.42	0/1044	0.59	1/1415 (0.1%)
27	S	0.43	0/1142	0.60	0/1547
28	T	0.45	0/1249	0.65	1/1679 (0.1%)
29	U	0.26	0/545	0.49	0/754
30	V	0.42	0/907	0.51	0/1227
31	W	0.37	0/910	0.56	0/1224
32	X	0.40	0/527	0.53	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
33	Y	0.37	0/934	0.51	0/1274
34	Z	0.28	0/545	0.52	0/739
35	a	0.32	0/992	0.53	0/1326
36	b	0.34	0/514	0.50	0/690
37	c	0.42	0/1763	0.52	0/2374
38	d	0.31	0/525	0.50	0/719
39	e	0.37	0/838	0.57	0/1131
40	f	0.46	0/1002	0.55	0/1346
41	g	0.49	0/1003	0.53	0/1352
42	h	0.38	0/868	0.55	0/1160
43	i	0.38	0/499	0.56	0/662
44	j	0.50	0/651	0.61	0/869
45	k	0.30	0/378	0.57	0/518
46	l	0.43	0/470	0.51	0/627
47	m	0.43	0/680	0.53	0/913
48	n	0.34	0/667	0.56	0/889
All	All	0.59	10/125375 (0.0%)	0.79	95/185945 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	A	0	1
10	B	0	2
13	E	0	1
15	G	0	1
16	H	0	1
19	K	0	3
26	R	0	1
27	S	0	1
28	T	0	1
40	f	0	1
All	All	0	13

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	634	G	C1'-N9	-6.69	1.37	1.46
1	1	159	U	C1'-N1	6.17	1.58	1.48
1	1	568	U	C1'-N1	6.06	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	564	U	C1'-N1	5.95	1.57	1.48
1	1	565	U	C1'-N1	5.91	1.57	1.48
1	1	562	U	C1'-N1	5.88	1.57	1.48
6	6	31	U	C1'-N1	5.28	1.56	1.48
1	1	692	A	N9-C4	-5.23	1.34	1.37
6	6	39	U	C1'-N1	5.16	1.56	1.48
1	1	170	U	C1'-N1	5.09	1.56	1.48

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	K	45	SER	C-N-CD	-11.87	94.48	120.60
1	1	1575	A	OP1-P-O3'	-11.81	79.22	105.20
1	1	1757	U	C2-N1-C1'	8.96	128.45	117.70
2	2	776	C	N1-C2-O2	8.91	124.25	118.90
2	2	776	C	C2-N1-C1'	8.72	128.39	118.80
2	2	24	C	C2-N1-C1'	8.09	127.70	118.80
1	1	1575	A	OP2-P-O3'	-8.07	87.44	105.20
1	1	1216	U	C2-N1-C1'	8.01	127.32	117.70
2	2	1275	C	N1-C2-O2	7.88	123.63	118.90
1	1	1270	U	N1-C2-O2	7.83	128.28	122.80
26	R	22	PRO	N-CA-CB	7.49	112.29	103.30
1	1	1270	U	C2-N1-C1'	7.48	126.68	117.70
1	1	1216	U	N1-C2-O2	7.48	128.03	122.80
2	2	24	C	N1-C2-O2	7.32	123.29	118.90
1	1	1216	U	N3-C2-O2	-7.12	117.22	122.20
6	6	38	C	P-O3'-C3'	7.06	128.18	119.70
2	2	776	C	N3-C2-O2	-7.05	116.97	121.90
2	2	540	C	C2-N1-C1'	6.94	126.43	118.80
1	1	1270	U	N3-C2-O2	-6.94	117.34	122.20
1	1	1576	C	OP1-P-OP2	6.93	129.99	119.60
2	2	1275	C	C2-N1-C1'	6.89	126.38	118.80
1	1	973	U	C2-N1-C1'	6.86	125.93	117.70
2	2	1275	C	N3-C2-O2	-6.76	117.17	121.90
1	1	1757	U	N1-C2-O2	6.72	127.50	122.80
18	J	112	LYS	CB-CA-C	-6.67	97.06	110.40
2	2	552	C	N1-C2-O2	6.67	122.90	118.90
2	2	552	C	C2-N1-C1'	6.65	126.11	118.80
1	1	1109	U	C2-N1-C1'	6.62	125.64	117.70
1	1	1602	U	C4-C5-C6	6.58	123.65	119.70
1	1	1602	U	C5-C6-N1	-6.54	119.43	122.70
4	4	86	U	N1-C2-O2	6.47	127.33	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	J	112	LYS	N-CA-C	6.45	128.41	111.00
1	1	1757	U	N3-C2-O2	-6.36	117.75	122.20
2	2	360	U	OP2-P-O3'	6.33	119.13	105.20
28	T	4	TYR	N-CA-C	6.17	127.67	111.00
2	2	776	C	C6-N1-C1'	-6.17	113.40	120.80
4	4	86	U	C2-N1-C1'	6.16	125.09	117.70
15	G	115	ARG	C-N-CD	-6.10	107.18	120.60
7	7	62	A	C2-N3-C4	-6.09	107.56	110.60
1	1	1757	U	C6-N1-C1'	-6.07	112.70	121.20
6	6	31	U	C2'-C3'-O3'	6.04	123.37	113.70
1	1	1618	U	C2-N1-C1'	5.99	124.89	117.70
1	1	912	C	C2-N1-C1'	5.96	125.36	118.80
2	2	1404	H2U	P-O3'-C3'	-5.94	112.58	119.70
2	2	24	C	N3-C2-O2	-5.93	117.75	121.90
2	2	61	C	C2-N1-C1'	5.78	125.16	118.80
4	4	86	U	N3-C2-O2	-5.78	118.16	122.20
2	2	24	C	C6-N1-C1'	-5.77	113.87	120.80
1	1	170	U	OP1-P-O3'	5.76	117.87	105.20
5	5	112	A	N7-C8-N9	5.72	116.66	113.80
2	2	1441	G	O4'-C1'-N9	5.65	112.72	108.20
1	1	665	C	O4'-C1'-N1	5.61	112.69	108.20
2	2	782	G	OP1-P-O3'	5.61	117.54	105.20
2	2	1289	G	C4-N9-C1'	5.59	133.77	126.50
1	1	205	A	OP1-P-O3'	5.58	117.49	105.20
1	1	912	C	N3-C2-O2	-5.51	118.04	121.90
1	1	1012	C	N1-C2-O2	5.49	122.20	118.90
2	2	540	C	C6-N1-C1'	-5.47	114.24	120.80
1	1	912	C	N1-C2-O2	5.42	122.15	118.90
2	2	776	C	C6-N1-C2	-5.42	118.13	120.30
1	1	1657	U	O4'-C1'-N1	5.40	112.52	108.20
1	1	1012	C	C2-N1-C1'	5.39	124.73	118.80
1	1	1618	U	N3-C2-O2	-5.38	118.43	122.20
6	6	41	G	C2'-C3'-O3'	5.38	122.30	113.70
6	6	39	U	O5'-P-OP1	-5.37	100.87	105.70
1	1	995	C	C2-N1-C1'	5.35	124.69	118.80
1	1	301	A	O4'-C1'-N9	5.34	112.48	108.20
3	3	108	A	P-O3'-C3'	5.34	126.11	119.70
1	1	458	A	O4'-C1'-N9	5.26	112.41	108.20
2	2	540	C	N1-C2-O2	5.20	122.02	118.90
5	5	112	A	C8-N9-C4	-5.20	103.72	105.80
1	1	824	U	C2-N1-C1'	5.19	123.93	117.70
1	1	1434	U	C2-N1-C1'	5.17	123.91	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1155	C	N3-C2-O2	-5.17	118.28	121.90
1	1	229	C	P-O3'-C3'	5.16	125.89	119.70
2	2	360	U	P-O3'-C3'	5.16	125.89	119.70
1	1	1263	A	P-O3'-C3'	5.13	125.86	119.70
1	1	1596	A	O5'-P-OP1	-5.12	101.09	105.70
2	2	1393	U	P-O3'-C3'	5.12	125.85	119.70
1	1	141	U	P-O3'-C3'	5.12	125.85	119.70
1	1	1388	U	P-O3'-C3'	5.12	125.85	119.70
1	1	1600	A	O4'-C1'-N9	5.12	112.30	108.20
1	1	1618	U	N1-C2-O2	5.12	126.38	122.80
1	1	136	G	OP1-P-O3'	5.12	116.46	105.20
1	1	1239	U	P-O3'-C3'	5.11	125.83	119.70
5	5	113	A	P-O3'-C3'	5.09	125.80	119.70
1	1	542	C	P-O3'-C3'	5.08	125.80	119.70
1	1	1493	G	O4'-C1'-N9	5.08	112.27	108.20
1	1	1216	U	C6-N1-C1'	-5.06	114.12	121.20
1	1	1602	U	N1-C2-N3	5.05	117.93	114.90
2	2	755	U	P-O3'-C3'	5.04	125.75	119.70
7	7	140	U	C2-N1-C1'	5.03	123.74	117.70
1	1	205	A	P-O3'-C3'	5.02	125.73	119.70
2	2	552	C	C6-N1-C1'	-5.01	114.78	120.80
1	1	1216	U	C5-C6-N1	5.01	125.20	122.70

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	A	60[B]	ARG	Mainchain
10	B	337	GLY	Peptide
10	B	373	GLY	Peptide
13	E	136	PRO	Peptide
15	G	114	ALA	Peptide
16	H	151	GLU	Peptide
19	K	107	HIS	Peptide
19	K	126	ASN	Peptide
19	K	40	TYR	Peptide
26	R	17	PRO	Peptide
27	S	100[B]	ARG	Mainchain
28	T	3	HIS	Peptide
40	f	9	ALA	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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	
9	A	245/260 (94%)	220 (90%)	25 (10%)	0	100	100
10	B	396/419 (94%)	352 (89%)	43 (11%)	1 (0%)	41	72
11	C	300/373 (80%)	269 (90%)	31 (10%)	0	100	100
12	D	159/188 (85%)	136 (86%)	23 (14%)	0	100	100
13	E	188/190 (99%)	160 (85%)	28 (15%)	0	100	100
14	F	134/195 (69%)	112 (84%)	22 (16%)	0	100	100
15	G	225/348 (65%)	205 (91%)	18 (8%)	2 (1%)	17	46
16	H	200/222 (90%)	175 (88%)	24 (12%)	1 (0%)	29	61
17	I	130/220 (59%)	120 (92%)	10 (8%)	0	100	100
18	J	126/139 (91%)	115 (91%)	11 (9%)	0	100	100
19	K	154/233 (66%)	136 (88%)	17 (11%)	1 (1%)	25	56
20	L	142/145 (98%)	127 (89%)	15 (11%)	0	100	100
21	M	201/204 (98%)	187 (93%)	14 (7%)	0	100	100
22	N	211/213 (99%)	186 (88%)	25 (12%)	0	100	100
23	O	229/305 (75%)	205 (90%)	24 (10%)	0	100	100
24	P	194/198 (98%)	179 (92%)	15 (8%)	0	100	100
25	Q	154/245 (63%)	141 (92%)	13 (8%)	0	100	100
26	R	130/179 (73%)	104 (80%)	25 (19%)	1 (1%)	19	49
27	S	149/159 (94%)	125 (84%)	22 (15%)	2 (1%)	12	36
28	T	154/166 (93%)	127 (82%)	27 (18%)	0	100	100
29	U	98/129 (76%)	81 (83%)	17 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	V	116/145 (80%)	99 (85%)	17 (15%)	0	100	100
31	W	116/143 (81%)	106 (91%)	10 (9%)	0	100	100
32	X	62/124 (50%)	59 (95%)	3 (5%)	0	100	100
33	Y	130/134 (97%)	111 (85%)	19 (15%)	0	100	100
34	Z	75/147 (51%)	65 (87%)	10 (13%)	0	100	100
35	a	122/127 (96%)	105 (86%)	17 (14%)	0	100	100
36	b	63/70 (90%)	53 (84%)	10 (16%)	0	100	100
37	c	220/252 (87%)	190 (86%)	30 (14%)	0	100	100
38	d	71/104 (68%)	63 (89%)	8 (11%)	0	100	100
39	e	111/183 (61%)	92 (83%)	19 (17%)	0	100	100
40	f	124/133 (93%)	110 (89%)	14 (11%)	0	100	100
41	g	123/144 (85%)	112 (91%)	11 (9%)	0	100	100
42	h	106/168 (63%)	91 (86%)	15 (14%)	0	100	100
43	i	62/105 (59%)	57 (92%)	5 (8%)	0	100	100
44	j	76/83 (92%)	68 (90%)	8 (10%)	0	100	100
45	k	56/83 (68%)	52 (93%)	4 (7%)	0	100	100
46	l	49/51 (96%)	46 (94%)	2 (4%)	1 (2%)	7	24
47	m	88/92 (96%)	71 (81%)	16 (18%)	1 (1%)	14	41
48	n	82/106 (77%)	66 (80%)	16 (20%)	0	100	100
All	All	5771/7124 (81%)	5078 (88%)	683 (12%)	10 (0%)	50	78

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	G	132	SER
26	R	22	PRO
27	S	101	CYS
47	m	40	SER
10	B	380	LYS
46	l	46	ARG
19	K	46	PRO
15	G	116	PRO
27	S	80	VAL
16	H	94	PRO

5.3.2 Protein sidechains (i)

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
9	A	188/204 (92%)	181 (96%)	7 (4%)	34 68
10	B	296/352 (84%)	288 (97%)	8 (3%)	44 78
11	C	222/302 (74%)	221 (100%)	1 (0%)	88 96
12	D	4/163 (2%)	4 (100%)	0	100 100
13	E	172/172 (100%)	169 (98%)	3 (2%)	60 87
14	F	92/154 (60%)	91 (99%)	1 (1%)	73 92
15	G	179/292 (61%)	173 (97%)	6 (3%)	37 71
16	H	166/188 (88%)	164 (99%)	2 (1%)	71 92
17	I	114/181 (63%)	110 (96%)	4 (4%)	36 70
18	J	91/111 (82%)	88 (97%)	3 (3%)	38 72
19	K	79/195 (40%)	68 (86%)	11 (14%)	3 11
20	L	105/115 (91%)	103 (98%)	2 (2%)	57 85
21	M	179/180 (99%)	176 (98%)	3 (2%)	60 87
22	N	178/179 (99%)	175 (98%)	3 (2%)	60 87
23	O	103/242 (43%)	100 (97%)	3 (3%)	42 76
24	P	149/164 (91%)	145 (97%)	4 (3%)	44 78
25	Q	100/196 (51%)	98 (98%)	2 (2%)	55 84
26	R	98/158 (62%)	96 (98%)	2 (2%)	55 84
27	S	100/133 (75%)	100 (100%)	0	100 100
28	T	125/144 (87%)	125 (100%)	0	100 100
29	U	13/114 (11%)	13 (100%)	0	100 100
30	V	86/124 (69%)	84 (98%)	2 (2%)	50 82
31	W	87/122 (71%)	87 (100%)	0	100 100
32	X	48/104 (46%)	46 (96%)	2 (4%)	30 63
33	Y	70/115 (61%)	69 (99%)	1 (1%)	67 90
34	Z	44/119 (37%)	44 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
35	a	99/117 (85%)	92 (93%)	7 (7%)	14 39
36	b	48/58 (83%)	44 (92%)	4 (8%)	11 32
37	c	168/209 (80%)	164 (98%)	4 (2%)	49 81
38	d	47/90 (52%)	44 (94%)	3 (6%)	17 45
39	e	79/156 (51%)	79 (100%)	0	100 100
40	f	97/114 (85%)	95 (98%)	2 (2%)	53 84
41	g	98/121 (81%)	96 (98%)	2 (2%)	55 84
42	h	85/145 (59%)	84 (99%)	1 (1%)	71 92
43	i	47/89 (53%)	44 (94%)	3 (6%)	17 45
44	j	63/70 (90%)	60 (95%)	3 (5%)	25 58
45	k	26/74 (35%)	25 (96%)	1 (4%)	33 67
46	l	46/47 (98%)	44 (96%)	2 (4%)	29 62
47	m	63/74 (85%)	58 (92%)	5 (8%)	12 34
48	n	64/92 (70%)	63 (98%)	1 (2%)	62 88
All	All	4118/5979 (69%)	4010 (97%)	108 (3%)	49 79

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	A	16	TYR
9	A	30	ARG
9	A	42	ARG
9	A	73	LYS
9	A	115	ASN
9	A	190	ARG
9	A	193	ARG
10	B	10	ARG
10	B	173	ASN
10	B	174[A]	HIS
10	B	174[B]	HIS
10	B	227[A]	LYS
10	B	227[B]	LYS
10	B	249	ARG
10	B	339	ARG
11	C	139	ARG
13	E	23	ARG
13	E	58	ARG

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Mol	Chain	Res	Type
13	E	172	ARG
14	F	192	ARG
15	G	133	ARG
15	G	161	ASN
15	G	240	ASN
15	G	253	ASN
15	G	256	ARG
15	G	334	LYS
16	H	103	ARG
16	H	108	ARG
17	I	18	ASN
17	I	39	ARG
17	I	72	MET
17	I	78	ARG
18	J	84	ARG
18	J	88	ARG
18	J	112	LYS
19	K	44	LEU
19	K	45	SER
19	K	50	CYS
19	K	72	ARG
19	K	74	LEU
19	K	78	ARG
19	K	95	LEU
19	K	106	ARG
19	K	107	HIS
19	K	180	HIS
19	K	185	VAL
20	L	4	ARG
20	L	112	ASN
21	M	60	CYS
21	M	71	ARG
21	M	122	ASN
22	N	33	ASN
22	N	73	ASN
22	N	116	ARG
23	O	21	ARG
23	O	23	ARG
23	O	94	ASN
24	P	56	ARG
24	P	142	ASN
24	P	147	ARG

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Mol	Chain	Res	Type
24	P	182	ARG
25	Q	47	ASP
25	Q	51	ILE
26	R	91	ARG
26	R	119	ARG
30	V	57	SER
30	V	92	ARG
32	X	37	ARG
32	X	60	ARG
33	Y	113	ARG
35	a	49	ARG
35	a	72	MET
35	a	88	ARG
35	a	107	LYS
35	a	110	ARG
35	a	111	GLN
35	a	112	MET
36	b	11	ASN
36	b	18	ARG
36	b	34	ARG
36	b	62	ARG
37	c	138	ARG
37	c	167	ASN
37	c	196	ASN
37	c	229	ARG
38	d	40	ARG
38	d	42	LYS
38	d	54	ARG
40	f	23	TYR
40	f	46	ARG
41	g	65	GLU
41	g	96	ARG
42	h	30	LYS
43	i	59	ARG
43	i	71	ARG
43	i	93	MET
44	j	22	CYS
44	j	33	ARG
44	j	73	ARG
45	k	40	ARG
46	l	5	LYS
46	l	34	ARG

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Mol	Chain	Res	Type
47	m	28	LYS
47	m	44	LYS
47	m	56	ARG
47	m	58	ASP
47	m	60	CYS
48	n	45	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
9	A	19	HIS
9	A	21	HIS
9	A	65	HIS
9	A	92	GLN
9	A	115	ASN
9	A	140	ASN
9	A	194	ASN
9	A	205	ASN
10	B	55	HIS
10	B	109	HIS
10	B	165	HIS
10	B	173	ASN
10	B	279	HIS
10	B	282	GLN
10	B	326	ASN
10	B	378	GLN
11	C	49	GLN
11	C	197	ASN
11	C	237	HIS
13	E	42	GLN
13	E	51	ASN
13	E	70	ASN
13	E	78	ASN
13	E	97	HIS
13	E	123	GLN
13	E	161	HIS
14	F	72	ASN
14	F	154	GLN
15	G	161	ASN
15	G	222	GLN
16	H	74	GLN
16	H	90	HIS

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Mol	Chain	Res	Type
16	H	190	GLN
17	I	12	HIS
17	I	13	GLN
17	I	33	GLN
17	I	70	HIS
17	I	108	ASN
18	J	77	ASN
18	J	134	HIS
19	K	52	GLN
19	K	92	ASN
19	K	107	HIS
19	K	180	HIS
20	L	28	HIS
20	L	60	HIS
20	L	112	ASN
21	M	57	GLN
21	M	76	HIS
21	M	122	ASN
22	N	33	ASN
22	N	59	GLN
22	N	71	GLN
22	N	100	ASN
22	N	163	GLN
22	N	196	HIS
23	O	17	GLN
23	O	31	HIS
23	O	39	GLN
23	O	94	ASN
24	P	58	ASN
24	P	142	ASN
24	P	197	HIS
25	Q	58	HIS
25	Q	118	HIS
25	Q	130	ASN
25	Q	137	ASN
26	R	8	HIS
26	R	107	GLN
26	R	122	ASN
27	S	54	HIS
27	S	58	HIS
27	S	77	ASN
27	S	95	HIS

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Mol	Chain	Res	Type
28	T	3	HIS
28	T	78	GLN
28	T	97	ASN
28	T	110	ASN
30	V	34	GLN
30	V	114	ASN
30	V	133	HIS
31	W	18	GLN
31	W	110	HIS
33	Y	79	HIS
33	Y	86	ASN
33	Y	121	ASN
34	Z	3	HIS
34	Z	14	GLN
35	a	116	HIS
36	b	7	HIS
36	b	11	ASN
36	b	16	ASN
36	b	30	HIS
36	b	43	ASN
37	c	120	GLN
37	c	123	ASN
37	c	135	ASN
37	c	167	ASN
37	c	176	ASN
37	c	196	ASN
37	c	245	ASN
38	d	71	HIS
39	e	120	ASN
40	f	122	ASN
41	g	52	GLN
41	g	80	HIS
42	h	13	HIS
42	h	51	HIS
42	h	62	HIS
44	j	12	HIS
44	j	16	HIS
45	k	27	HIS
46	l	33	ASN
46	l	43	HIS
47	m	33	GLN
48	n	3	ASN

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Mol	Chain	Res	Type
48	n	82	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1535/1782 (86%)	588 (38%)	57 (3%)
2	2	1106/1527 (72%)	445 (40%)	28 (2%)
3	3	177/213 (83%)	83 (46%)	10 (5%)
4	4	146/183 (79%)	48 (32%)	5 (3%)
5	5	78/133 (58%)	30 (38%)	4 (5%)
6	6	60/76 (78%)	48 (80%)	15 (25%)
7	7	150/171 (87%)	50 (33%)	2 (1%)
8	8	118/121 (97%)	54 (45%)	5 (4%)
All	All	3370/4206 (80%)	1346 (39%)	126 (3%)

All (1346) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	4	G
1	1	10	A
1	1	13	G
1	1	23	U
1	1	24	A
1	1	32	A
1	1	36	OMU
1	1	38	A
1	1	41	A
1	1	47	C
1	1	48	OMU
1	1	49	C
1	1	51	G
1	1	54	G
1	1	57	G
1	1	58	A
1	1	64	A
1	1	66	A
1	1	83	A
1	1	85	U
1	1	86	G
1	1	87	A
1	1	91	G

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Mol	Chain	Res	Type
1	1	92	C
1	1	104	G
1	1	109	A
1	1	110	A
1	1	119	C
1	1	121	A
1	1	126	G
1	1	127	G
1	1	130	U
1	1	131	U
1	1	132	A
1	1	133	C
1	1	134	A
1	1	135	A
1	1	136	G
1	1	137	G
1	1	139	C
1	1	141	U
1	1	142	G
1	1	145	U
1	1	153	C
1	1	154	A
1	1	155	A
1	1	156	A
1	1	158	A
1	1	159	U
1	1	160	C
1	1	165	C
1	1	168	G
1	1	169	G
1	1	170	U
1	1	171	U
1	1	172	G
1	1	174	U
1	1	175	G
1	1	177	A
1	1	178	G
1	1	180	A
1	1	184	G
1	1	187	A
1	1	188	A
1	1	189	A

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Mol	Chain	Res	Type
1	1	191	U
1	1	192	C
1	1	193	A
1	1	195	G
1	1	196	C
1	1	197	G
1	1	198	C
1	1	199	A
1	1	202	G
1	1	204	A
1	1	206	A
1	1	207	C
1	1	209	C
1	1	210	G
1	1	211	U
1	1	214	C
1	1	216	G
1	1	217	A
1	1	218	A
1	1	221	C
1	1	222	A
1	1	227	U
1	1	228	U
1	1	230	A
1	1	231	U
1	1	232	G
1	1	233	U
1	1	236	G
1	1	237	U
1	1	239	U
1	1	240	U
1	1	242	A
1	1	243	G
1	1	248	A
1	1	249	G
1	1	250	A
1	1	251	A
1	1	252	G
1	1	255	G
1	1	256	U
1	1	260	C
1	1	261	C

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Mol	Chain	Res	Type
1	1	264	U
1	1	267	A
1	1	268	G
1	1	270	C
1	1	271	A
1	1	273	A
1	1	275	A
1	1	278	U
1	1	279	G
1	1	280	A
1	1	282	C
1	1	283	G
1	1	284	C
1	1	286	U
1	1	288	A
1	1	291	A
1	1	293	C
1	1	294	U
1	1	299	U
1	1	301	A
1	1	303	C
1	1	305	A
1	1	306	G
1	1	313	U
1	1	314	G
1	1	320	G
1	1	323	U
1	1	332	A
1	1	333	A
1	1	334	G
1	1	335	U
1	1	336	U
1	1	337	G
1	1	341	G
1	1	343	U
1	1	344	A
1	1	348	G
1	1	361	A
1	1	367	A
1	1	368	G
1	1	370	G
1	1	371	U

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Mol	Chain	Res	Type
1	1	374	G
1	1	377	G
1	1	378	A
1	1	380	C
1	1	383	U
1	1	409	U
1	1	410	U
1	1	411	U
1	1	416	A
1	1	417	G
1	1	428	A
1	1	431	G
1	1	438	A
1	1	440	A
1	1	442	A
1	1	443	A
1	1	444	C
1	1	448	A
1	1	454	U
1	1	455	G
1	1	458	A
1	1	459	A
1	1	460	A
1	1	462	A
1	1	463	C
1	1	464	A
1	1	475	C
1	1	476	U
1	1	477	C
1	1	478	C
1	1	483	C
1	1	484	A
1	1	486	C
1	1	487	G
1	1	490	C
1	1	494	A
1	1	495	C
1	1	498	G
1	1	500	C
1	1	501	C
1	1	502	U
1	1	505	U

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Mol	Chain	Res	Type
1	1	508	A
1	1	510	U
1	1	512	U
1	1	513	C
1	1	515	U
1	1	516	G
1	1	519	G
1	1	520	G
1	1	532	C
1	1	533	G
1	1	534	G
1	1	537	G
1	1	539	C
1	1	540	A
1	1	541	A
1	1	543	G
1	1	544	A
1	1	545	A
1	1	547	U
1	1	548	G
1	1	549	C
1	1	551	A
1	1	553	A
1	1	554	A
1	1	558	U
1	1	559	G
1	1	560	G
1	1	561	G
1	1	563	C
1	1	566	G
1	1	567	G
1	1	569	G
1	1	570	A
1	1	634	G
1	1	636	U
1	1	638	C
1	1	648	A
1	1	650	G
1	1	651	G
1	1	652	A
1	1	653	A
1	1	654	A

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Mol	Chain	Res	Type
1	1	658	G
1	1	659	G
1	1	665	C
1	1	666	C
1	1	669	C
1	1	670	C
1	1	677	A
1	1	679	A
1	1	680	C
1	1	681	A2M
1	1	693	G
1	1	694	U
1	1	695	OMC
1	1	696	A
1	1	698	A
1	1	709	A
1	1	713	A
1	1	728	C
1	1	729	A
1	1	730	G
1	1	735	U
1	1	737	U
1	1	741	G
1	1	742	U
1	1	750	G
1	1	753	A
1	1	767	U
1	1	768	C
1	1	769	U
1	1	770	G
1	1	771	U
1	1	779	A
1	1	780	C
1	1	782	C
1	1	783	G
1	1	785	C
1	1	787	A
1	1	788	A
1	1	789	U
1	1	790	C
1	1	793	U
1	1	795	U

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Mol	Chain	Res	Type
1	1	799	U
1	1	801	G
1	1	802	C
1	1	807	C
1	1	817	C
1	1	818	C
1	1	820	U
1	1	821	C
1	1	823	G
1	1	824	U
1	1	826	G
1	1	829	U
1	1	830	G
1	1	831	C
1	1	832	G
1	1	836	G
1	1	837	A
1	1	838	G
1	1	846	G
1	1	847	OMU
1	1	848	U
1	1	849	U
1	1	850	G
1	1	855	C
1	1	857	A
1	1	860	G
1	1	867	A
1	1	868	A
1	1	878	A
1	1	883	G
1	1	887	A
1	1	892	C
1	1	894	G
1	1	895	G
1	1	900	C
1	1	901	C
1	1	902	C
1	1	903	A
1	1	907	G
1	1	908	G
1	1	912	C
1	1	922	U

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Mol	Chain	Res	Type
1	1	925	U
1	1	926	G
1	1	927	A2M
1	1	931	G
1	1	932	C
1	1	945	U
1	1	947	A
1	1	956	U
1	1	957	C
1	1	959	OMG
1	1	960	A
1	1	963	G
1	1	965	A
1	1	967	G
1	1	972	A
1	1	974	C
1	1	975	G
1	1	977	A
1	1	985	G
1	1	988	G
1	1	995	C
1	1	1000	C
1	1	1010	C
1	1	1011	U
1	1	1013	A
1	1	1021	U
1	1	1025	G
1	1	1028	A
1	1	1029	G
1	1	1030	U
1	1	1031	A
1	1	1032	G
1	1	1036	U
1	1	1042	G
1	1	1044	G
1	1	1046	U
1	1	1051	C
1	1	1055	U
1	1	1056	G
1	1	1057	A
1	1	1058	U
1	1	1059	U

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Mol	Chain	Res	Type
1	1	1063	G
1	1	1073	U
1	1	1081	A
1	1	1083	A
1	1	1085	C
1	1	1086	G
1	1	1088	C
1	1	1092	U
1	1	1097	A
1	1	1102	U
1	1	1103	U
1	1	1104	A
1	1	1105	A
1	1	1108	G
1	1	1110	G
1	1	1114	A
1	1	1117	A
1	1	1118	A
1	1	1120	C
1	1	1123	G
1	1	1124	C
1	1	1127	U
1	1	1128	A
1	1	1131	C
1	1	1142	C
1	1	1146	A
1	1	1147	A
1	1	1149	G
1	1	1150	A
1	1	1156	A
1	1	1159	A
1	1	1160	G
1	1	1161	A
1	1	1162	G
1	1	1164	C
1	1	1169	A
1	1	1174	G
1	1	1181	U
1	1	1182	C
1	1	1188	G
1	1	1200	A
1	1	1201	U

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Mol	Chain	Res	Type
1	1	1206	A
1	1	1210	A
1	1	1211	A
1	1	1212	C
1	1	1213	C
1	1	1216	U
1	1	1218	A
1	1	1231	G
1	1	1234	A
1	1	1235	A
1	1	1239	U
1	1	1240	U
1	1	1242	U
1	1	1243	G
1	1	1249	A
1	1	1254	C
1	1	1255	G
1	1	1257	U
1	1	1258	A
1	1	1259	C
1	1	1260	G
1	1	1261	U
1	1	1263	A
1	1	1264	A
1	1	1265	A
1	1	1266	A
1	1	1268	G
1	1	1270	U
1	1	1271	G
1	1	1273	U
1	1	1276	U
1	1	1281	A
1	1	1349	A
1	1	1357	G
1	1	1364	A
1	1	1365	A
1	1	1366	A
1	1	1367	U
1	1	1369	G
1	1	1370	A
1	1	1371	U
1	1	1372	G

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Mol	Chain	Res	Type
1	1	1375	G
1	1	1379	A
1	1	1383	C
1	1	1385	A
1	1	1386	A
1	1	1389	A
1	1	1390	G
1	1	1392	G
1	1	1393	A
1	1	1394	U
1	1	1395	U
1	1	1396	G
1	1	1399	C
1	1	1400	A
1	1	1402	U
1	1	1407	C
1	1	1413	U
1	1	1414	A
1	1	1415	A
1	1	1416	G
1	1	1418	G
1	1	1420	G
1	1	1421	G
1	1	1423	A
1	1	1424	A
1	1	1433	U
1	1	1434	U
1	1	1435	G
1	1	1436	G
1	1	1437	A
1	1	1438	G
1	1	1439	A
1	1	1440	A
1	1	1443	U
1	1	1445	U
1	1	1446	A
1	1	1447	G
1	1	1448	C
1	1	1449	C
1	1	1450	C
1	1	1451	U
1	1	1452	U

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Mol	Chain	Res	Type
1	1	1453	C
1	1	1466	G
1	1	1467	G
1	1	1468	C
1	1	1478	A
1	1	1479	G
1	1	1489	U
1	1	1490	A
1	1	1491	U
1	1	1492	G
1	1	1494	C
1	1	1495	G
1	1	1504	A
1	1	1505	G
1	1	1506	A
1	1	1507	U
1	1	1509	G
1	1	1510	A
1	1	1511	C
1	1	1521	G
1	1	1522	U
1	1	1523	G
1	1	1524	C
1	1	1526	OMG
1	1	1527	A
1	1	1529	OMC
1	1	1530	U
1	1	1540	U
1	1	1541	A2M
1	1	1542	OMG
1	1	1544	A
1	1	1547	G
1	1	1548	A
1	1	1549	U
1	1	1550	C
1	1	1553	A
1	1	1554	C
1	1	1576	C
1	1	1577	G
1	1	1584	A
1	1	1588	G
1	1	1589	A

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Mol	Chain	Res	Type
1	1	1590	G
1	1	1591	C
1	1	1592	G
1	1	1593	G
1	1	1595	G
1	1	1601	U
1	1	1602	U
1	1	1607	G
1	1	1609	C
1	1	1611	A
1	1	1612	C
1	1	1614	G
1	1	1615	C
1	1	1621	U
1	1	1627	A
1	1	1629	U
1	1	1633	U
1	1	1639	A
1	1	1644	G
1	1	1648	A
1	1	1656	A
1	1	1657	U
1	1	1658	C
1	1	1662	U
1	1	1663	U
1	1	1664	G
1	1	1665	U
1	1	1667	A
1	1	1668	G
1	1	1669	G
1	1	1670	A
1	1	1671	A
1	1	1679	G
1	1	1683	G
1	1	1719	G
1	1	1720	C
1	1	1721	C
1	1	1723	U
1	1	1725	A
1	1	1728	G
1	1	1729	A
1	1	1732	A

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Mol	Chain	Res	Type
1	1	1735	G
1	1	1737	C
1	1	1739	A
1	1	1740	C
1	1	1741	A
1	1	1746	A
1	1	1749	U
1	1	1752	G
1	1	1755	U
1	1	1761	C
1	1	1763	A
1	1	1764	A
1	1	1765	A
1	1	1766	A
1	1	1767	A
1	1	1768	G
1	1	1771	A
1	1	1777	U
1	1	1778	G
2	2	9	G
2	2	13	A
2	2	22	A
2	2	26	C
2	2	29	C
2	2	30	A
2	2	33	A
2	2	34	G
2	2	36	U
2	2	41	A
2	2	44	C
2	2	49	A
2	2	54	U
2	2	61	C
2	2	63	U
2	2	67	G
2	2	68	A
2	2	69	A
2	2	70	A
2	2	75	C
2	2	78	U
2	2	89	G
2	2	90	G

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Mol	Chain	Res	Type
2	2	92	A
2	2	98	G
2	2	99	A
2	2	103	G
2	2	109	U
2	2	110	C
2	2	111	G
2	2	116	A
2	2	119	C
2	2	122	U
2	2	123	G
2	2	127	C
2	2	130	A
2	2	131	G
2	2	133	G
2	2	134	C
2	2	135	A
2	2	343	U
2	2	344	G
2	2	345	C
2	2	346	C
2	2	349	C
2	2	350	U
2	2	355	A
2	2	358	G
2	2	359	C
2	2	360	U
2	2	361	U
2	2	362	A
2	2	363	C
2	2	368	G
2	2	372	A
2	2	377	A
2	2	380	G
2	2	385	A
2	2	388	A
2	2	390	A
2	2	394	U
2	2	401	G
2	2	404	A
2	2	405	U
2	2	413	A

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Mol	Chain	Res	Type
2	2	414	G
2	2	415	U
2	2	416	G
2	2	424	U
2	2	425	C
2	2	429	A
2	2	434	A
2	2	435	U
2	2	438	C
2	2	444	A
2	2	446	U
2	2	447	G
2	2	448	C
2	2	451	U
2	2	452	G
2	2	453	A
2	2	454	A
2	2	455	U
2	2	456	G
2	2	458	C
2	2	459	A
2	2	464	G
2	2	469	G
2	2	470	A
2	2	471	U
2	2	473	C
2	2	477	G
2	2	478	A
2	2	482	G
2	2	483	C
2	2	484	G
2	2	489	A
2	2	490	A
2	2	495	G
2	2	497	G
2	2	498	A
2	2	509	C
2	2	511	C
2	2	512	U
2	2	513	C
2	2	515	U
2	2	518	G

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Mol	Chain	Res	Type
2	2	519	G
2	2	522	G
2	2	525	A
2	2	526	A
2	2	527	A2M
2	2	528	U
2	2	529	G
2	2	530	C
2	2	534	OMG
2	2	535	U
2	2	541	A
2	2	543	U
2	2	544	U
2	2	547	A
2	2	549	A
2	2	553	G
2	2	554	OMC
2	2	555	A
2	2	556	U
2	2	559	A
2	2	560	U
2	2	561	G
2	2	570	A
2	2	571	OMG
2	2	572	A2M
2	2	580	U
2	2	582	U
2	2	583	OMC
2	2	584	C
2	2	591	A2M
2	2	592	C
2	2	609	A
2	2	611	U
2	2	620	C
2	2	621	G
2	2	623	A
2	2	624	C
2	2	629	A
2	2	633	C
2	2	635	A
2	2	640	G
2	2	643	A

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Mol	Chain	Res	Type
2	2	647	A
2	2	648	A
2	2	649	G
2	2	650	A
2	2	656	OMU
2	2	657	U
2	2	658	G
2	2	664	G
2	2	666	C
2	2	668	C
2	2	675	G
2	2	681	G
2	2	683	G
2	2	694	U
2	2	696	A
2	2	697	G
2	2	699	U
2	2	700	G
2	2	701	U
2	2	702	A
2	2	704	U
2	2	705	A
2	2	706	U
2	2	707	A
2	2	709	G
2	2	711	G
2	2	713	A
2	2	714	A
2	2	715	G
2	2	718	C
2	2	720	A
2	2	721	G
2	2	725	A
2	2	726	A
2	2	727	A
2	2	728	U
2	2	729	G
2	2	730	A
2	2	731	A
2	2	732	A
2	2	733	U
2	2	734	A

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Mol	Chain	Res	Type
2	2	735	C
2	2	736	C
2	2	737	A
2	2	739	C
2	2	741	C
2	2	742	U
2	2	750	U
2	2	756	C
2	2	758	C
2	2	759	U
2	2	760	U
2	2	761	A
2	2	768	G
2	2	769	A
2	2	774	A
2	2	775	C
2	2	776	C
2	2	777	A
2	2	778	A
2	2	779	U
2	2	780	G
2	2	782	G
2	2	783	U
2	2	784	U
2	2	785	U
2	2	786	A
2	2	789	G
2	2	790	U
2	2	791	A
2	2	794	C
2	2	795	U
2	2	800	G
2	2	801	C
2	2	802	U
2	2	803	A
2	2	807	A
2	2	808	C
2	2	809	C
2	2	810	G
2	2	811	U
2	2	812	C
2	2	813	U

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Mol	Chain	Res	Type
2	2	814	A
2	2	816	G
2	2	817	U
2	2	818	U
2	2	824	G
2	2	825	U
2	2	827	A
2	2	828	U
2	2	829	U
2	2	830	U
2	2	831	U
2	2	833	U
2	2	834	G
2	2	835	G
2	2	836	C
2	2	837	G
2	2	868	U
2	2	869	G
2	2	870	C
2	2	872	U
2	2	940	G
2	2	941	C
2	2	948	C
2	2	949	G
2	2	950	U
2	2	951	G
2	2	952	G
2	2	954	U
2	2	956	C
2	2	957	C
2	2	958	C
2	2	959	A
2	2	960	A
2	2	961	C
2	2	962	C
2	2	967	U
2	2	968	G
2	2	969	U
2	2	970	A
2	2	971	A
2	2	972	A
2	2	973	C

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Mol	Chain	Res	Type
2	2	974	U
2	2	975	G
2	2	976	A
2	2	977	A
2	2	979	C
2	2	981	A
2	2	982	C
2	2	983	G
2	2	989	G
2	2	991	C
2	2	992	U
2	2	993	C
2	2	996	G
2	2	997	C
2	2	1010	U
2	2	1011	U
2	2	1012	G
2	2	1013	U
2	2	1014	U
2	2	1016	C
2	2	1020	A
2	2	1024	C
2	2	1025	U
2	2	1028	C
2	2	1034	G
2	2	1035	G
2	2	1037	A
2	2	1042	G
2	2	1045	U
2	2	1050	C
2	2	1057	U
2	2	1063	A
2	2	1066	C
2	2	1067	G
2	2	1072	C
2	2	1073	G
2	2	1076	G
2	2	1077	G
2	2	1079	OMG
2	2	1080	U
2	2	1084	A
2	2	1086	G

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Mol	Chain	Res	Type
2	2	1093	U
2	2	1096	G
2	2	1097	U
2	2	1101	A
2	2	1102	A
2	2	1104	A
2	2	1109	U
2	2	1111	U
2	2	1112	C
2	2	1114	C
2	2	1116	U
2	2	1117	A
2	2	1118	G
2	2	1119	A
2	2	1122	A
2	2	1124	A
2	2	1131	A
2	2	1132	A
2	2	1133	A
2	2	1134	G
2	2	1142	G
2	2	1144	U
2	2	1147	A
2	2	1148	C
2	2	1149	G
2	2	1152	U
2	2	1154	C
2	2	1156	A
2	2	1157	G
2	2	1158	U
2	2	1161	G
2	2	1166	G
2	2	1169	A
2	2	1171	U
2	2	1182	G
2	2	1184	C
2	2	1185	C
2	2	1186	A2M
2	2	1187	G
2	2	1189	G
2	2	1190	A
2	2	1199	G

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Mol	Chain	Res	Type
2	2	1216	A
2	2	1217	A
2	2	1218	C
2	2	1229	A
2	2	1230	OMG
2	2	1231	A
2	2	1238	A
2	2	1239	G
2	2	1240	A
2	2	1242	U
2	2	1243	A
2	2	1248	C
2	2	1249	OMC
2	2	1253	G
2	2	1254	OMG
2	2	1255	G
2	2	1256	A
2	2	1257	U
2	2	1266	U
2	2	1267	G
2	2	1275	C
2	2	1276	A
2	2	1277	A
2	2	1278	G
2	2	1288	C
2	2	1290	A
2	2	1292	G
2	2	1295	G
2	2	1296	C
2	2	1298	U
2	2	1299	U
2	2	1302	G
2	2	1303	A
2	2	1305	C
2	2	1306	C
2	2	1310	G
2	2	1312	U
2	2	1317	G
2	2	1318	OMC
2	2	1325	U
2	2	1326	A
2	2	1329	C

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Mol	Chain	Res	Type
2	2	1333	C
2	2	1338	C
2	2	1339	A
2	2	1341	A
2	2	1343	G
2	2	1346	G
2	2	1347	C
2	2	1348	U
2	2	1349	A
2	2	1350	A
2	2	1351	G
2	2	1361	G
2	2	1362	U
2	2	1367	C
2	2	1372	G
2	2	1374	C
2	2	1375	A
2	2	1380	A
2	2	1381	C
2	2	1384	G
2	2	1385	A
2	2	1386	G
2	2	1389	G
2	2	1390	G
2	2	1393	U
2	2	1394	U
2	2	1410	A
2	2	1415	G
2	2	1417	U
2	2	1418	U
2	2	1422	C
2	2	1423	C
2	2	1429	U
2	2	1435	G
2	2	1437	A
2	2	1438	A
2	2	1440	U
2	2	1441	G
2	2	1442	C
2	2	1443	G
2	2	1444	A
2	2	1446	A

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Mol	Chain	Res	Type
2	2	1448	A
2	2	1449	A
3	3	10	U
3	3	14	A
3	3	21	U
3	3	22	G
3	3	23	C
3	3	29	A
3	3	30	A
3	3	32	A
3	3	33	A
3	3	37	A
3	3	38	A
3	3	47	C
3	3	48	G
3	3	50	U
3	3	54	C
3	3	55	U
3	3	56	U
3	3	58	C
3	3	61	U
3	3	62	U
3	3	63	C
3	3	69	A
3	3	70	A
3	3	78	C
3	3	79	U
3	3	81	C
3	3	82	G
3	3	83	G
3	3	84	C
3	3	86	U
3	3	87	U
3	3	88	G
3	3	90	U
3	3	92	G
3	3	95	C
3	3	96	U
3	3	97	U
3	3	98	G
3	3	99	G
3	3	101	C

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Mol	Chain	Res	Type
3	3	105	U
3	3	107	U
3	3	108	A
3	3	109	C
3	3	110	U
3	3	111	U
3	3	112	C
3	3	114	C
3	3	118	U
3	3	119	U
3	3	120	G
3	3	122	U
3	3	133	G
3	3	135	U
3	3	138	A
3	3	142	U
3	3	146	A
3	3	147	A
3	3	148	A
3	3	149	U
3	3	150	G
3	3	152	A
3	3	153	G
3	3	156	C
3	3	157	U
3	3	164	G
3	3	165	U
3	3	166	A
3	3	167	C
3	3	168	U
3	3	169	G
3	3	170	U
3	3	176	U
3	3	181	A
3	3	182	G
3	3	185	C
3	3	186	U
3	3	194	A
3	3	195	A
3	3	196	A
3	3	198	C
3	3	199	A

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Mol	Chain	Res	Type
3	3	210	G
4	4	31	G
4	4	40	G
4	4	46	G
4	4	50	G
4	4	51	U
4	4	52	A
4	4	62	C
4	4	63	U
4	4	64	C
4	4	65	C
4	4	67	A
4	4	73	U
4	4	86	U
4	4	93	U
4	4	96	C
4	4	97	G
4	4	100	C
4	4	102	G
4	4	106	G
4	4	107	U
4	4	114	A
4	4	119	A
4	4	120	U
4	4	121	C
4	4	127	G
4	4	128	U
4	4	129	G
4	4	131	U
4	4	132	U
4	4	139	U
4	4	140	G
4	4	141	A
4	4	147	U
4	4	148	C
4	4	150	A
4	4	151	A
4	4	153	C
4	4	154	C
4	4	157	A
4	4	158	A
4	4	162	A

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Mol	Chain	Res	Type
4	4	169	A
4	4	171	A
4	4	172	C
4	4	174	A
4	4	175	G
4	4	180	C
4	4	182	A
5	5	4	G
5	5	12	C
5	5	13	C
5	5	14	A
5	5	15	A
5	5	22	G
5	5	25	C
5	5	26	A
5	5	27	U
5	5	28	G
5	5	38	G
5	5	40	A
5	5	42	G
5	5	43	A
5	5	101	C
5	5	102	U
5	5	105	A
5	5	112	A
5	5	113	A
5	5	114	A
5	5	115	U
5	5	119	A
5	5	120	U
5	5	122	C
5	5	123	U
5	5	126	G
5	5	127	G
5	5	131	A
5	5	132	C
5	5	133	A
6	6	2	C
6	6	3	A
6	6	4	U
6	6	5	C
6	6	7	A

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Mol	Chain	Res	Type
6	6	8	A
6	6	9	U
6	6	12	C
6	6	13	C
6	6	14	A
6	6	15	C
6	6	16	C
6	6	17	U
6	6	18	A
6	6	19	C
6	6	20	A
6	6	21	A
6	6	22	G
6	6	23	A
6	6	24	C
6	6	25	U
6	6	26	G
6	6	27	G
6	6	28	A
6	6	29	G
6	6	30	C
6	6	31	U
6	6	32	U
6	6	33	G
6	6	35	U
6	6	37	C
6	6	39	U
6	6	40	C
6	6	41	G
6	6	42	A
6	6	44	G
6	6	49	C
6	6	50	A
6	6	51	A
6	6	52	G
6	6	53	U
6	6	54	A
6	6	55	U
6	6	56	A
6	6	57	U
6	6	58	U
6	6	59	C

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Mol	Chain	Res	Type
6	6	61	U
7	7	2	A
7	7	5	U
7	7	6	G
7	7	7	OMU
7	7	8	C
7	7	22	U
7	7	34	U
7	7	35	C
7	7	38	U
7	7	40	A
7	7	44	A
7	7	48	A
7	7	49	G
7	7	52	A
7	7	59	A
7	7	60	U
7	7	62	A
7	7	63	G
7	7	68	A
7	7	69	U
7	7	71	A
7	7	77	A
7	7	78	G
7	7	89	U
7	7	92	C
7	7	103	A
7	7	104	A
7	7	105	C
7	7	107	C
7	7	109	A
7	7	110	A
7	7	111	C
7	7	115	G
7	7	119	G
7	7	120	G
7	7	121	G
7	7	122	A
7	7	124	A
7	7	125	A
7	7	126	G
7	7	127	C

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Mol	Chain	Res	Type
7	7	137	U
7	7	138	C
7	7	139	A
7	7	140	U
7	7	142	C
7	7	157	U
7	7	158	U
7	7	159	C
7	7	161	C
8	8	2	C
8	8	3	G
8	8	4	A
8	8	5	G
8	8	7	A
8	8	8	C
8	8	9	G
8	8	12	C
8	8	13	A
8	8	15	A
8	8	17	U
8	8	18	U
8	8	24	A
8	8	27	A
8	8	36	C
8	8	39	G
8	8	40	U
8	8	41	C
8	8	43	G
8	8	44	A
8	8	45	U
8	8	47	U
8	8	48	G
8	8	51	A
8	8	52	A
8	8	53	G
8	8	55	U
8	8	56	A
8	8	57	A
8	8	61	C
8	8	63	C
8	8	64	A
8	8	67	G

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Mol	Chain	Res	Type
8	8	73	G
8	8	74	U
8	8	78	U
8	8	82	G
8	8	85	G
8	8	86	U
8	8	87	C
8	8	88	A
8	8	89	G
8	8	91	G
8	8	92	A
8	8	94	G
8	8	102	A
8	8	108	G
8	8	110	G
8	8	111	U
8	8	112	G
8	8	115	G
8	8	116	U
8	8	119	U
8	8	120	C

All (126) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	23	U
1	1	132	A
1	1	136	G
1	1	141	U
1	1	153	C
1	1	154	A
1	1	155	A
1	1	167	U
1	1	170	U
1	1	171	U
1	1	191	U
1	1	195	G
1	1	203	C
1	1	205	A
1	1	229	C
1	1	232	G
1	1	333	A

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Mol	Chain	Res	Type
1	1	334	G
1	1	367	A
1	1	409	U
1	1	415	A
1	1	477	C
1	1	559	G
1	1	560	G
1	1	669	C
1	1	693	G
1	1	786	A
1	1	822	C
1	1	959	OMG
1	1	1029	G
1	1	1109	U
1	1	1239	U
1	1	1253	U
1	1	1257	U
1	1	1263	A
1	1	1270	U
1	1	1369	G
1	1	1388	U
1	1	1389	A
1	1	1392	G
1	1	1413	U
1	1	1420	G
1	1	1423	A
1	1	1432	C
1	1	1436	G
1	1	1439	A
1	1	1442	G
1	1	1452	U
1	1	1466	G
1	1	1506	A
1	1	1526	OMG
1	1	1529	OMC
1	1	1542	OMG
1	1	1591	C
1	1	1662	U
1	1	1751	G
1	1	1763	A
2	2	29	C
2	2	68	A

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Mol	Chain	Res	Type
2	2	349	C
2	2	360	U
2	2	443	OMC
2	2	468	A
2	2	512	U
2	2	552	C
2	2	646	G
2	2	749	G
2	2	755	U
2	2	775	C
2	2	776	C
2	2	782	G
2	2	815	G
2	2	827	A
2	2	832	A
2	2	835	G
2	2	948	C
2	2	957	C
2	2	973	C
2	2	981	A
2	2	996	G
2	2	1184	C
2	2	1318	OMC
2	2	1393	U
2	2	1437	A
2	2	1443	G
3	3	22	G
3	3	31	C
3	3	32	A
3	3	77	U
3	3	78	C
3	3	108	A
3	3	117	G
3	3	132	G
3	3	141	U
3	3	195	A
4	4	50	G
4	4	64	C
4	4	149	U
4	4	157	A
4	4	174	A
5	5	113	A

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Mol	Chain	Res	Type
5	5	125	A
5	5	126	G
5	5	130	C
6	6	2	C
6	6	4	U
6	6	8	A
6	6	14	A
6	6	21	A
6	6	24	C
6	6	29	G
6	6	30	C
6	6	31	U
6	6	32	U
6	6	38	C
6	6	40	C
6	6	41	G
6	6	50	A
6	6	58	U
7	7	88	A
7	7	139	A
8	8	43	G
8	8	48	G
8	8	66	A
8	8	85	G
8	8	91	G

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

44 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	OMG	2	1079	2	18,26,27	0.99	1 (5%)	19,38,41	1.13	2 (10%)
2	H2U	2	1404	2	18,21,22	1.10	2 (11%)	21,30,33	1.65	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	OMC	2	583	2	19,22,23	0.87	0	26,31,34	1.02	1 (3%)
2	A2M	2	591	2	18,25,26	0.98	1 (5%)	18,36,39	1.33	2 (11%)
1	A2M	1	1541	2,1	18,25,26	0.96	1 (5%)	18,36,39	1.21	2 (11%)
2	OMG	2	1254	2	18,26,27	1.04	1 (5%)	19,38,41	1.05	2 (10%)
1	OMC	1	1529	1	19,22,23	0.88	0	26,31,34	0.99	1 (3%)
1	OMG	1	1628	1	18,26,27	1.01	1 (5%)	19,38,41	1.18	2 (10%)
7	OMU	7	7	7,1	19,22,23	1.25	2 (10%)	26,31,34	2.12	6 (23%)
7	A2M	7	162	7,1	18,25,26	1.02	1 (5%)	18,36,39	1.22	2 (11%)
2	OMG	2	71	2	18,26,27	1.03	1 (5%)	19,38,41	1.05	2 (10%)
2	A2M	2	572	2	18,25,26	0.98	1 (5%)	18,36,39	1.19	2 (11%)
1	OMG	1	959	1	18,26,27	1.07	1 (5%)	19,38,41	1.25	2 (10%)
2	OMU	2	667	2	19,22,23	1.26	3 (15%)	26,31,34	1.83	6 (23%)
2	A2M	2	382	2	18,25,26	0.93	1 (5%)	18,36,39	1.20	2 (11%)
2	OMG	2	1230	2	18,26,27	1.03	1 (5%)	19,38,41	1.05	2 (10%)
2	A2M	2	628	2	18,25,26	0.93	1 (5%)	18,36,39	1.24	2 (11%)
1	OMU	1	847	1	19,22,23	1.25	3 (15%)	26,31,34	1.81	6 (23%)
2	OMG	2	534	2	18,26,27	1.01	1 (5%)	19,38,41	1.04	2 (10%)
2	OMC	2	554	2	19,22,23	0.85	0	26,31,34	1.01	1 (3%)
2	OMG	2	641	2	18,26,27	1.04	1 (5%)	19,38,41	1.03	2 (10%)
2	OMG	2	655	2	18,26,27	1.02	1 (5%)	19,38,41	1.13	2 (10%)
2	OMU	2	656	2	19,22,23	1.23	3 (15%)	26,31,34	1.97	6 (23%)
2	OMU	2	1153	2	19,22,23	1.30	3 (15%)	26,31,34	1.99	6 (23%)
2	OMC	2	1318	2	19,22,23	0.86	0	26,31,34	0.99	2 (7%)
2	OMG	2	571	2	18,26,27	0.98	1 (5%)	19,38,41	1.10	2 (10%)
1	A2M	1	955	1	18,25,26	0.96	1 (5%)	18,36,39	1.33	2 (11%)
1	A2M	1	681	1	18,25,26	0.93	1 (5%)	18,36,39	1.24	2 (11%)
1	A2M	1	927	1	18,25,26	1.02	1 (5%)	18,36,39	1.29	2 (11%)
2	OMC	2	443	2	19,22,23	0.85	0	26,31,34	0.87	0
1	OMU	1	48	1	19,22,23	1.36	3 (15%)	26,31,34	1.84	6 (23%)
1	OMG	1	1526	1	18,26,27	1.00	1 (5%)	19,38,41	1.21	2 (10%)
1	OMU	1	36	1	19,22,23	1.31	3 (15%)	26,31,34	1.85	6 (23%)
1	OMG	1	1542	2,1	18,26,27	1.00	1 (5%)	19,38,41	1.17	2 (10%)
2	OMC	2	1398	2	19,22,23	0.86	0	26,31,34	1.06	1 (3%)
1	OMC	1	695	1	19,22,23	0.92	1 (5%)	26,31,34	1.19	2 (7%)
1	OMU	1	845	1	19,22,23	1.32	4 (21%)	26,31,34	1.97	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	OMC	2	1249	2	19,22,23	0.85	0	26,31,34	1.00	1 (3%)
2	A2M	2	1186	2	18,25,26	0.95	1 (5%)	18,36,39	1.27	2 (11%)
1	A2M	1	678	2,1	18,25,26	0.97	1 (5%)	18,36,39	1.29	2 (11%)
1	OMG	1	856	1	18,26,27	1.01	1 (5%)	19,38,41	1.05	2 (10%)
2	A2M	2	527	2	18,25,26	0.95	1 (5%)	18,36,39	1.38	2 (11%)
2	OMU	2	1078	2	19,22,23	1.27	2 (10%)	26,31,34	1.81	6 (23%)
2	OMC	2	1160	2	19,22,23	0.86	0	26,31,34	0.97	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	2	1079	2	-	2/5/27/28	0/3/3/3
2	H2U	2	1404	2	-	3/7/38/39	0/2/2/2
2	OMC	2	583	2	-	2/9/27/28	0/2/2/2
2	A2M	2	591	2	-	3/5/27/28	0/3/3/3
1	A2M	1	1541	2,1	-	3/5/27/28	0/3/3/3
2	OMG	2	1254	2	-	4/5/27/28	0/3/3/3
1	OMC	1	1529	1	-	2/9/27/28	0/2/2/2
1	OMG	1	1628	1	-	0/5/27/28	0/3/3/3
7	OMU	7	7	7,1	-	4/9/27/28	0/2/2/2
7	A2M	7	162	7,1	-	1/5/27/28	0/3/3/3
2	OMG	2	71	2	-	2/5/27/28	0/3/3/3
2	A2M	2	572	2	-	2/5/27/28	0/3/3/3
1	OMG	1	959	1	-	0/5/27/28	0/3/3/3
2	OMU	2	667	2	-	3/9/27/28	0/2/2/2
2	A2M	2	382	2	-	1/5/27/28	0/3/3/3
2	OMG	2	1230	2	-	3/5/27/28	0/3/3/3
2	A2M	2	628	2	-	0/5/27/28	0/3/3/3
1	OMU	1	847	1	-	3/9/27/28	0/2/2/2
2	OMG	2	534	2	-	0/5/27/28	0/3/3/3
2	OMC	2	554	2	-	2/9/27/28	0/2/2/2
2	OMG	2	641	2	-	2/5/27/28	0/3/3/3
2	OMG	2	655	2	-	0/5/27/28	0/3/3/3
2	OMU	2	656	2	-	4/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMU	2	1153	2	-	2/9/27/28	0/2/2/2
2	OMC	2	1318	2	-	2/9/27/28	0/2/2/2
2	OMG	2	571	2	-	2/5/27/28	0/3/3/3
1	A2M	1	955	1	-	3/5/27/28	0/3/3/3
1	A2M	1	681	1	-	3/5/27/28	0/3/3/3
1	A2M	1	927	1	-	1/5/27/28	0/3/3/3
2	OMC	2	443	2	-	5/9/27/28	0/2/2/2
1	OMU	1	48	1	-	3/9/27/28	0/2/2/2
1	OMG	1	1526	1	-	1/5/27/28	0/3/3/3
1	OMU	1	36	1	-	2/9/27/28	0/2/2/2
1	OMG	1	1542	2,1	-	2/5/27/28	0/3/3/3
2	OMC	2	1398	2	-	0/9/27/28	0/2/2/2
1	OMC	1	695	1	-	0/9/27/28	0/2/2/2
1	OMU	1	845	1	-	0/9/27/28	0/2/2/2
2	OMC	2	1249	2	-	3/9/27/28	0/2/2/2
2	A2M	2	1186	2	-	3/5/27/28	0/3/3/3
1	A2M	1	678	2,1	-	4/5/27/28	0/3/3/3
1	OMG	1	856	1	-	0/5/27/28	0/3/3/3
2	A2M	2	527	2	-	1/5/27/28	0/3/3/3
2	OMU	2	1078	2	-	0/9/27/28	0/2/2/2
2	OMC	2	1160	2	-	0/9/27/28	0/2/2/2

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	36	OMU	C4-N3	-2.96	1.33	1.38
1	1	48	OMU	C4-N3	-2.95	1.33	1.38
1	1	845	OMU	C4-N3	-2.94	1.33	1.38
1	1	856	OMG	C6-N1	-2.89	1.33	1.37
2	2	1153	OMU	C4-N3	-2.83	1.33	1.38
2	2	71	OMG	C6-N1	-2.82	1.33	1.37
2	2	1254	OMG	C6-N1	-2.81	1.33	1.37
2	2	1078	OMU	C4-N3	-2.78	1.33	1.38
1	1	1542	OMG	C6-N1	-2.76	1.33	1.37
2	2	1230	OMG	C6-N1	-2.75	1.33	1.37
2	2	667	OMU	C4-N3	-2.74	1.33	1.38
2	2	641	OMG	C6-N1	-2.72	1.33	1.37
2	2	571	OMG	C6-N1	-2.71	1.33	1.37
2	2	655	OMG	C6-N1	-2.69	1.33	1.37
1	1	959	OMG	C6-N1	-2.68	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	847	OMU	C4-N3	-2.67	1.33	1.38
2	2	1404	H2U	C2-N3	-2.67	1.33	1.38
1	1	845	OMU	C2-N3	-2.65	1.33	1.38
1	1	1526	OMG	C6-N1	-2.64	1.33	1.37
7	7	7	OMU	C4-N3	-2.62	1.33	1.38
1	1	48	OMU	C2-N3	-2.60	1.33	1.38
2	2	656	OMU	C4-N3	-2.58	1.33	1.38
1	1	1628	OMG	C6-N1	-2.56	1.34	1.37
2	2	1404	H2U	C4-N3	-2.54	1.33	1.37
2	2	534	OMG	C6-N1	-2.53	1.34	1.37
1	1	36	OMU	C2-N3	-2.46	1.33	1.38
1	1	847	OMU	C2-N3	-2.46	1.33	1.38
7	7	162	A2M	C5-C4	2.46	1.47	1.40
2	2	1079	OMG	C6-N1	-2.44	1.34	1.37
2	2	1153	OMU	C2-N3	-2.42	1.33	1.38
2	2	572	A2M	C5-C4	2.36	1.47	1.40
2	2	667	OMU	C2-N3	-2.35	1.33	1.38
1	1	48	OMU	C5-C4	-2.34	1.38	1.43
2	2	1078	OMU	C2-N3	-2.32	1.33	1.38
2	2	1186	A2M	C5-C4	2.30	1.47	1.40
1	1	927	A2M	C5-C4	2.30	1.47	1.40
2	2	591	A2M	C5-C4	2.29	1.47	1.40
1	1	678	A2M	C5-C4	2.26	1.46	1.40
2	2	656	OMU	C2-N3	-2.24	1.34	1.38
2	2	628	A2M	C5-C4	2.24	1.46	1.40
7	7	7	OMU	C2-N3	-2.23	1.34	1.38
2	2	527	A2M	C5-C4	2.22	1.46	1.40
2	2	382	A2M	C5-C4	2.22	1.46	1.40
1	1	1541	A2M	C5-C4	2.22	1.46	1.40
1	1	847	OMU	C5-C4	-2.22	1.38	1.43
1	1	36	OMU	C5-C4	-2.21	1.38	1.43
1	1	845	OMU	C5-C4	-2.20	1.38	1.43
1	1	955	A2M	C5-C4	2.20	1.46	1.40
2	2	1153	OMU	C5-C4	-2.19	1.38	1.43
1	1	681	A2M	C5-C4	2.17	1.46	1.40
2	2	667	OMU	C5-C4	-2.13	1.38	1.43
1	1	695	OMC	C5-C4	-2.12	1.38	1.42
2	2	656	OMU	C5-C4	-2.11	1.39	1.43
1	1	845	OMU	C6-N1	-2.00	1.33	1.38

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1404	H2U	C4-N3-C2	-6.13	120.71	125.79
7	7	7	OMU	C2'-C1'-N1	-5.47	103.60	114.22
7	7	7	OMU	C4-N3-C2	-4.79	120.26	126.58
2	2	656	OMU	C4-N3-C2	-4.76	120.31	126.58
1	1	845	OMU	C4-N3-C2	-4.75	120.31	126.58
2	2	1078	OMU	C4-N3-C2	-4.70	120.37	126.58
1	1	36	OMU	C4-N3-C2	-4.69	120.39	126.58
2	2	1153	OMU	C4-N3-C2	-4.69	120.40	126.58
1	1	847	OMU	C4-N3-C2	-4.68	120.40	126.58
1	1	48	OMU	C4-N3-C2	-4.55	120.58	126.58
1	1	845	OMU	N3-C2-N1	4.48	120.84	114.89
7	7	7	OMU	N3-C2-N1	4.46	120.82	114.89
2	2	1078	OMU	N3-C2-N1	4.43	120.77	114.89
2	2	667	OMU	C4-N3-C2	-4.43	120.74	126.58
2	2	1153	OMU	N3-C2-N1	4.39	120.72	114.89
2	2	667	OMU	N3-C2-N1	4.37	120.69	114.89
1	1	847	OMU	N3-C2-N1	4.37	120.69	114.89
2	2	656	OMU	N3-C2-N1	4.37	120.69	114.89
1	1	48	OMU	N3-C2-N1	4.33	120.64	114.89
1	1	36	OMU	N3-C2-N1	4.22	120.50	114.89
1	1	845	OMU	C2'-C1'-N1	-4.12	106.23	114.22
2	2	1398	OMC	C2'-C1'-N1	-4.04	106.38	114.22
2	2	1153	OMU	C2'-C1'-N1	-4.01	106.43	114.22
2	2	656	OMU	C2'-C1'-N1	-4.01	106.43	114.22
1	1	36	OMU	C5-C4-N3	3.73	120.42	114.84
1	1	847	OMU	C5-C4-N3	3.67	120.33	114.84
1	1	845	OMU	C5-C4-N3	3.62	120.25	114.84
2	2	656	OMU	C5-C4-N3	3.61	120.24	114.84
1	1	48	OMU	C5-C4-N3	3.60	120.23	114.84
2	2	1078	OMU	C5-C4-N3	3.60	120.22	114.84
2	2	1153	OMU	C5-C4-N3	3.58	120.19	114.84
1	1	695	OMC	C2'-C1'-N1	-3.54	107.34	114.22
7	7	7	OMU	C5-C4-N3	3.54	120.14	114.84
2	2	667	OMU	C5-C4-N3	3.52	120.10	114.84
1	1	36	OMU	C2'-C1'-N1	-3.48	107.46	114.22
2	2	1249	OMC	C2'-C1'-N1	-3.41	107.61	114.22
1	1	927	A2M	N3-C2-N1	-3.39	123.37	128.68
1	1	678	A2M	N3-C2-N1	-3.36	123.43	128.68
1	1	955	A2M	N3-C2-N1	-3.33	123.47	128.68
2	2	628	A2M	N3-C2-N1	-3.31	123.50	128.68
2	2	583	OMC	C2'-C1'-N1	-3.31	107.80	114.22
2	2	591	A2M	N3-C2-N1	-3.26	123.59	128.68
1	1	681	A2M	N3-C2-N1	-3.25	123.60	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	656	OMU	O4-C4-C5	-3.22	119.49	125.16
1	1	1541	A2M	N3-C2-N1	-3.22	123.65	128.68
2	2	527	A2M	N3-C2-N1	-3.18	123.70	128.68
1	1	48	OMU	O4-C4-C5	-3.13	119.66	125.16
2	2	1186	A2M	N3-C2-N1	-3.10	123.83	128.68
1	1	847	OMU	O4-C4-C5	-3.10	119.72	125.16
7	7	162	A2M	N3-C2-N1	-3.06	123.89	128.68
2	2	382	A2M	N3-C2-N1	-3.06	123.89	128.68
1	1	36	OMU	O4-C4-C5	-3.04	119.82	125.16
2	2	667	OMU	C2'-C1'-N1	-3.01	108.38	114.22
2	2	572	A2M	N3-C2-N1	-3.00	123.99	128.68
2	2	1160	OMC	C2'-C1'-N1	-3.00	108.41	114.22
2	2	656	OMU	O2-C2-N1	-2.99	118.82	122.79
2	2	1153	OMU	O4-C4-C5	-2.97	119.94	125.16
1	1	678	A2M	C4-C5-N7	-2.95	106.32	109.40
7	7	7	OMU	O4-C4-C5	-2.95	119.97	125.16
1	1	48	OMU	C2'-C1'-N1	-2.93	108.53	114.22
1	1	845	OMU	O4-C4-C5	-2.92	120.03	125.16
1	1	955	A2M	C4-C5-N7	-2.91	106.37	109.40
2	2	667	OMU	O4-C4-C5	-2.90	120.06	125.16
7	7	7	OMU	O2-C2-N1	-2.86	118.99	122.79
2	2	1153	OMU	O2-C2-N1	-2.83	119.03	122.79
1	1	845	OMU	O2-C2-N1	-2.80	119.06	122.79
2	2	572	A2M	C4-C5-N7	-2.79	106.49	109.40
1	1	681	A2M	C4-C5-N7	-2.77	106.51	109.40
1	1	1529	OMC	C2'-C1'-N1	-2.76	108.87	114.22
2	2	1186	A2M	C4-C5-N7	-2.72	106.57	109.40
2	2	1078	OMU	O4-C4-C5	-2.62	120.55	125.16
1	1	1541	A2M	C4-C5-N7	-2.56	106.73	109.40
1	1	927	A2M	C4-C5-N7	-2.55	106.75	109.40
2	2	1404	H2U	O4'-C1'-N1	2.52	112.72	109.30
1	1	959	OMG	C5-C6-N1	2.50	118.36	113.95
2	2	527	A2M	C4-C5-N7	-2.48	106.81	109.40
1	1	1628	OMG	C5-C6-N1	2.48	118.34	113.95
2	2	382	A2M	C4-C5-N7	-2.48	106.81	109.40
1	1	847	OMU	C2'-C1'-N1	-2.48	109.41	114.22
2	2	554	OMC	C2'-C1'-N1	-2.45	109.46	114.22
1	1	48	OMU	O2-C2-N1	-2.44	119.54	122.79
2	2	591	A2M	C4-C5-N7	-2.44	106.86	109.40
1	1	1542	OMG	C5-C6-N1	2.44	118.26	113.95
1	1	847	OMU	O2-C2-N1	-2.44	119.55	122.79
2	2	534	OMG	C8-N7-C5	2.43	107.61	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1526	OMG	C8-N7-C5	2.41	107.58	102.99
2	2	655	OMG	C5-C6-N1	2.40	118.19	113.95
2	2	1254	OMG	C5-C6-N1	2.40	118.19	113.95
2	2	655	OMG	C8-N7-C5	2.38	107.52	102.99
2	2	1230	OMG	C5-C6-N1	2.37	118.14	113.95
1	1	856	OMG	C5-C6-N1	2.36	118.13	113.95
2	2	1078	OMU	C2'-C1'-N1	-2.36	109.64	114.22
2	2	1079	OMG	C8-N7-C5	2.36	107.49	102.99
2	2	1230	OMG	C8-N7-C5	2.34	107.44	102.99
2	2	628	A2M	C4-C5-N7	-2.34	106.96	109.40
2	2	1079	OMG	C5-C6-N1	2.31	118.04	113.95
1	1	36	OMU	O2-C2-N1	-2.31	119.72	122.79
2	2	571	OMG	C5-C6-N1	2.31	118.03	113.95
1	1	1628	OMG	C8-N7-C5	2.31	107.39	102.99
1	1	856	OMG	C8-N7-C5	2.30	107.37	102.99
2	2	71	OMG	C5-C6-N1	2.29	118.00	113.95
2	2	641	OMG	C5-C6-N1	2.28	117.97	113.95
2	2	1254	OMG	C8-N7-C5	2.27	107.32	102.99
1	1	1542	OMG	C8-N7-C5	2.26	107.29	102.99
2	2	571	OMG	C8-N7-C5	2.25	107.28	102.99
1	1	1526	OMG	C5-C6-N1	2.24	117.91	113.95
2	2	667	OMU	O2-C2-N1	-2.21	119.85	122.79
2	2	71	OMG	C8-N7-C5	2.15	107.08	102.99
2	2	534	OMG	C5-C6-N1	2.14	117.73	113.95
2	2	641	OMG	C8-N7-C5	2.13	107.04	102.99
2	2	1078	OMU	O2-C2-N1	-2.11	119.98	122.79
1	1	695	OMC	C5'-C4'-C3'	-2.11	107.28	115.18
2	2	1318	OMC	C2'-C1'-N1	-2.08	110.18	114.22
1	1	959	OMG	C8-N7-C5	2.04	106.88	102.99
2	2	1318	OMC	C5'-C4'-C3'	-2.03	107.58	115.18
7	7	162	A2M	C4-C5-N7	-2.00	107.31	109.40

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	48	OMU	C3'-C4'-C5'-O5'
1	1	48	OMU	O4'-C4'-C5'-O5'
1	1	681	A2M	O4'-C4'-C5'-O5'
1	1	681	A2M	C3'-C4'-C5'-O5'
1	1	1529	OMC	C3'-C4'-C5'-O5'
1	1	1541	A2M	C1'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
2	2	382	A2M	C1'-C2'-O2'-CM'
2	2	443	OMC	C2'-C1'-N1-C2
2	2	443	OMC	C2'-C1'-N1-C6
2	2	443	OMC	O4'-C4'-C5'-O5'
2	2	527	A2M	O4'-C4'-C5'-O5'
2	2	554	OMC	C3'-C4'-C5'-O5'
2	2	571	OMG	O4'-C4'-C5'-O5'
2	2	571	OMG	C3'-C4'-C5'-O5'
2	2	583	OMC	C3'-C4'-C5'-O5'
2	2	583	OMC	O4'-C4'-C5'-O5'
2	2	667	OMU	C1'-C2'-O2'-CM2
2	2	1186	A2M	C3'-C4'-C5'-O5'
2	2	1230	OMG	C3'-C4'-C5'-O5'
2	2	1230	OMG	C1'-C2'-O2'-CM2
2	2	1254	OMG	O4'-C4'-C5'-O5'
2	2	1254	OMG	C1'-C2'-O2'-CM2
2	2	1318	OMC	C3'-C4'-C5'-O5'
2	2	1404	H2U	O4'-C1'-N1-C2
2	2	1404	H2U	O4'-C1'-N1-C6
7	7	7	OMU	C3'-C2'-O2'-CM2
7	7	7	OMU	C3'-C4'-C5'-O5'
7	7	7	OMU	O4'-C4'-C5'-O5'
1	1	955	A2M	C3'-C4'-C5'-O5'
2	2	554	OMC	O4'-C4'-C5'-O5'
2	2	641	OMG	C3'-C4'-C5'-O5'
2	2	656	OMU	C3'-C4'-C5'-O5'
2	2	667	OMU	C3'-C4'-C5'-O5'
2	2	1079	OMG	O4'-C4'-C5'-O5'
2	2	1254	OMG	C3'-C4'-C5'-O5'
1	1	955	A2M	O4'-C4'-C5'-O5'
1	1	1529	OMC	O4'-C4'-C5'-O5'
2	2	572	A2M	O4'-C4'-C5'-O5'
2	2	572	A2M	C3'-C4'-C5'-O5'
2	2	656	OMU	O4'-C4'-C5'-O5'
2	2	667	OMU	O4'-C4'-C5'-O5'
2	2	1153	OMU	C3'-C4'-C5'-O5'
2	2	1186	A2M	O4'-C4'-C5'-O5'
2	2	1318	OMC	O4'-C4'-C5'-O5'
2	2	1254	OMG	C3'-C2'-O2'-CM2
2	2	1186	A2M	C4'-C5'-O5'-P
1	1	36	OMU	C3'-C4'-C5'-O5'
2	2	591	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	2	1079	OMG	C3'-C4'-C5'-O5'
1	1	36	OMU	O4'-C4'-C5'-O5'
1	1	678	A2M	O4'-C4'-C5'-O5'
1	1	847	OMU	C3'-C4'-C5'-O5'
1	1	847	OMU	O4'-C4'-C5'-O5'
1	1	1541	A2M	O4'-C4'-C5'-O5'
2	2	71	OMG	O4'-C4'-C5'-O5'
2	2	641	OMG	O4'-C4'-C5'-O5'
2	2	1153	OMU	O4'-C4'-C5'-O5'
2	2	1230	OMG	O4'-C4'-C5'-O5'
1	1	1542	OMG	C3'-C4'-C5'-O5'
2	2	71	OMG	C3'-C4'-C5'-O5'
2	2	591	A2M	O4'-C4'-C5'-O5'
1	1	847	OMU	C1'-C2'-O2'-CM2
1	1	1526	OMG	C1'-C2'-O2'-CM2
2	2	656	OMU	C1'-C2'-O2'-CM2
7	7	162	A2M	C1'-C2'-O2'-CM'
2	2	1249	OMC	C4'-C5'-O5'-P
1	1	678	A2M	C3'-C2'-O2'-CM'
2	2	591	A2M	C3'-C2'-O2'-CM'
2	2	443	OMC	O4'-C1'-N1-C6
2	2	656	OMU	C4'-C5'-O5'-P
1	1	681	A2M	C4'-C5'-O5'-P
2	2	443	OMC	O4'-C1'-N1-C2
7	7	7	OMU	C4'-C5'-O5'-P
1	1	1541	A2M	C3'-C4'-C5'-O5'
1	1	678	A2M	C1'-C2'-O2'-CM'
1	1	955	A2M	C1'-C2'-O2'-CM'
1	1	48	OMU	C2'-C1'-N1-C2
1	1	1542	OMG	O4'-C4'-C5'-O5'
2	2	1249	OMC	C3'-C4'-C5'-O5'
2	2	1249	OMC	C2'-C1'-N1-C2
1	1	678	A2M	C3'-C4'-C5'-O5'
1	1	927	A2M	C4'-C5'-O5'-P
2	2	1404	H2U	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 109 ligands modelled in this entry, 109 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

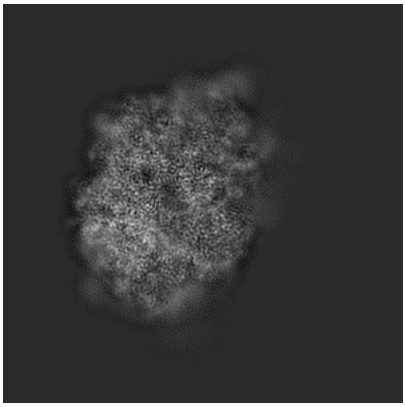
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6583. These allow visual inspection of the internal detail of the map and identification of artifacts.

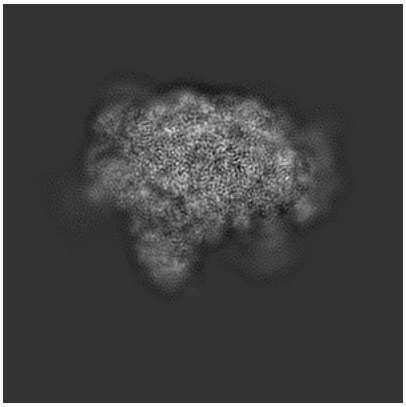
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

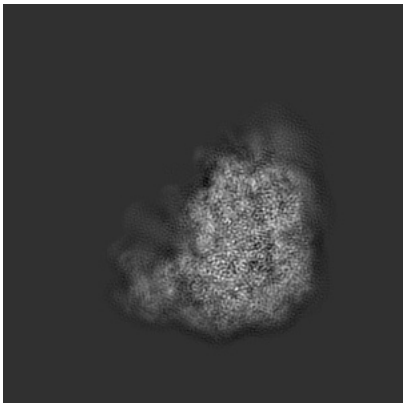
6.1.1 Primary map



X



Y

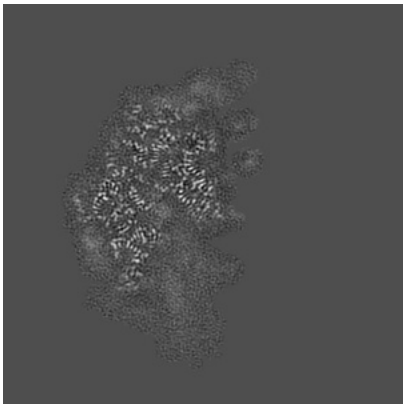


Z

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

6.2 Central slices

6.2.1 Primary map



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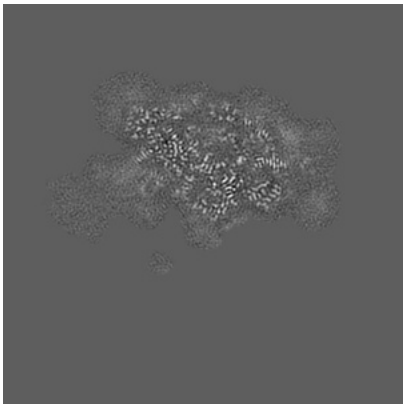
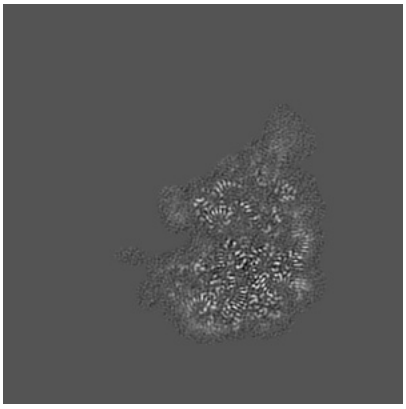


Y Index: 192

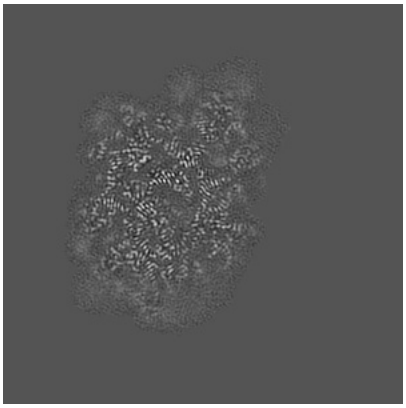


Z Index: 192

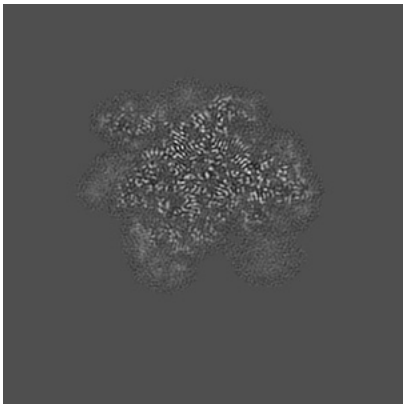
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

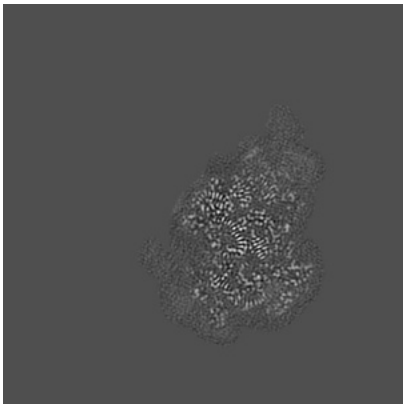
6.3.1 Primary map



X Index: 228



Y Index: 123



Z Index: 213

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

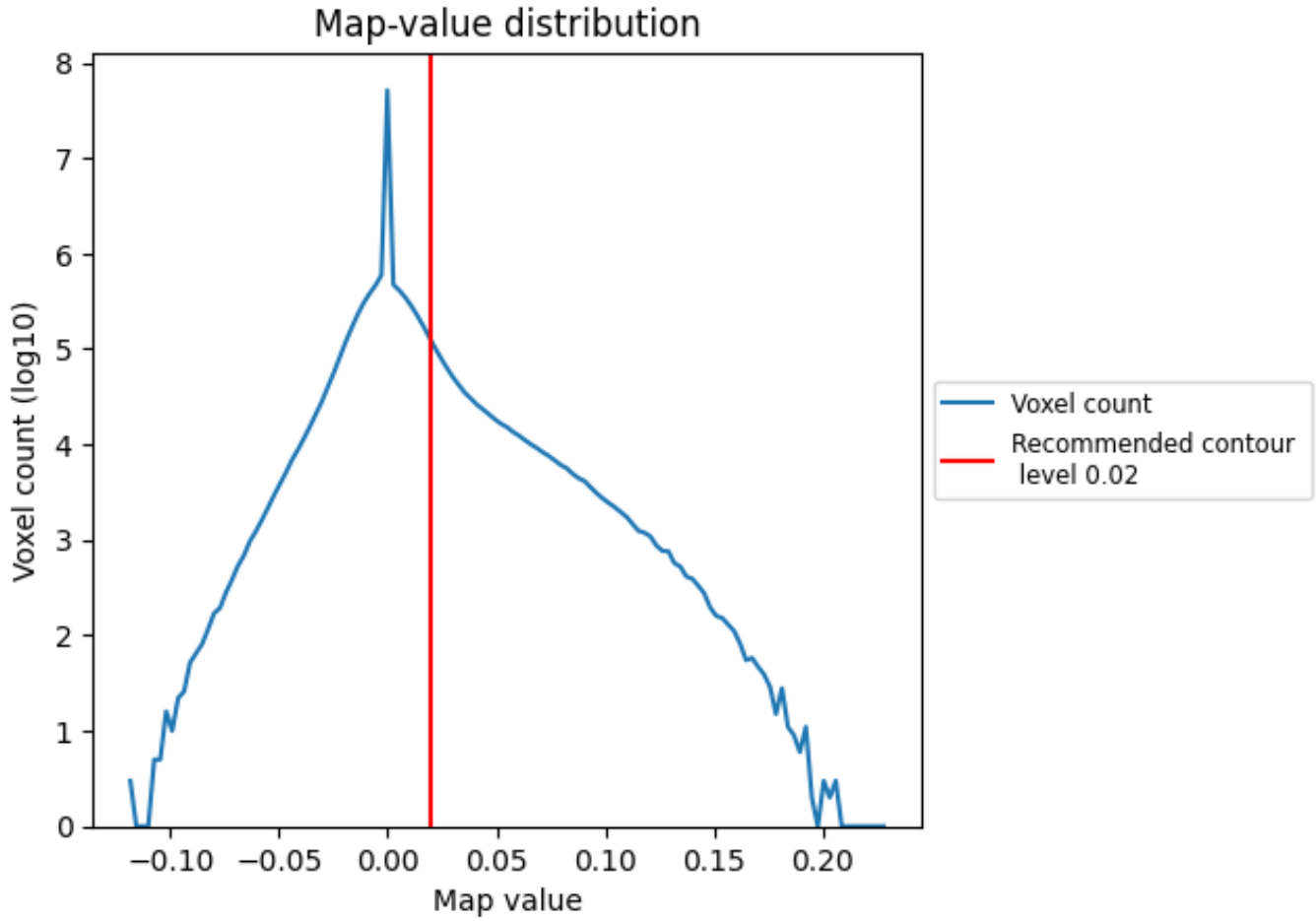
6.5 Mask visualisation (i)

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

7 Map analysis

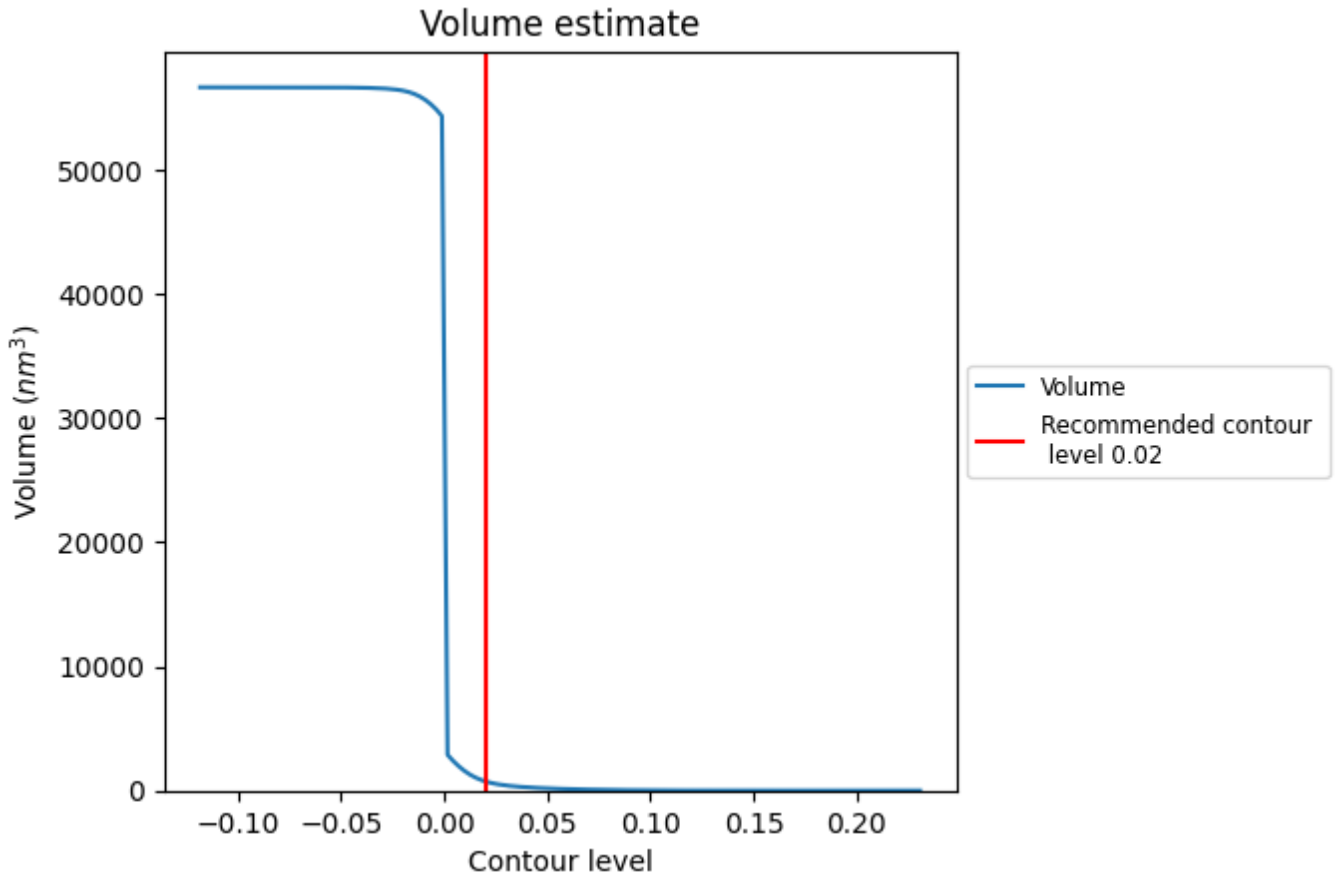
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

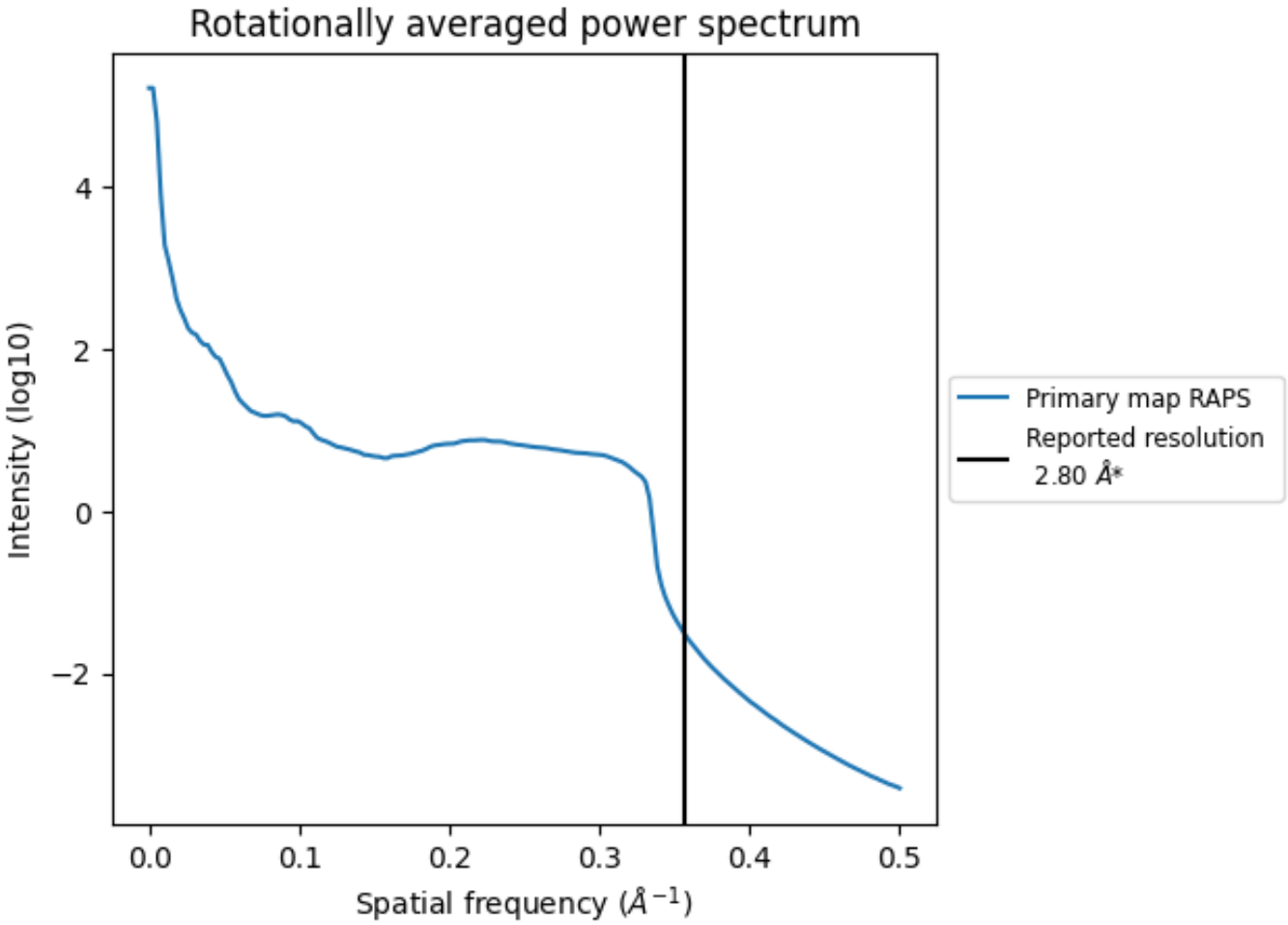
7.2 Volume estimate



The volume at the recommended contour level is 742 nm^3; this corresponds to an approximate mass of 670 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 (i)



*Reported resolution corresponds to spatial frequency of 0.357 $Å^{-1}$

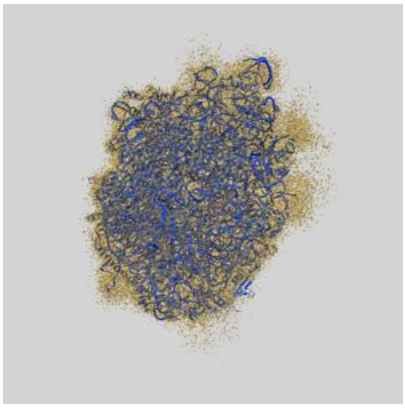
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

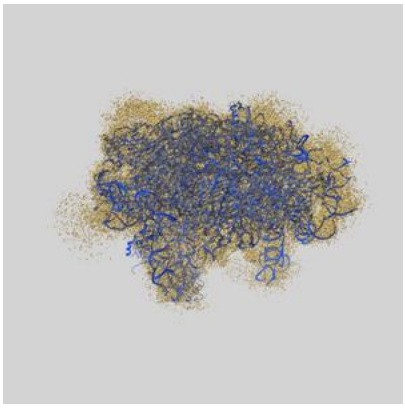
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6583 and PDB model 3JCS. Per-residue inclusion information can be found in section 3 on page 14.

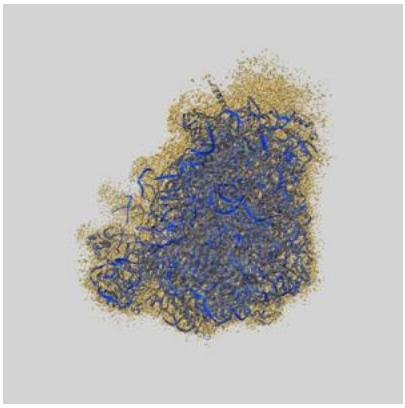
9.1 Map-model overlay



X



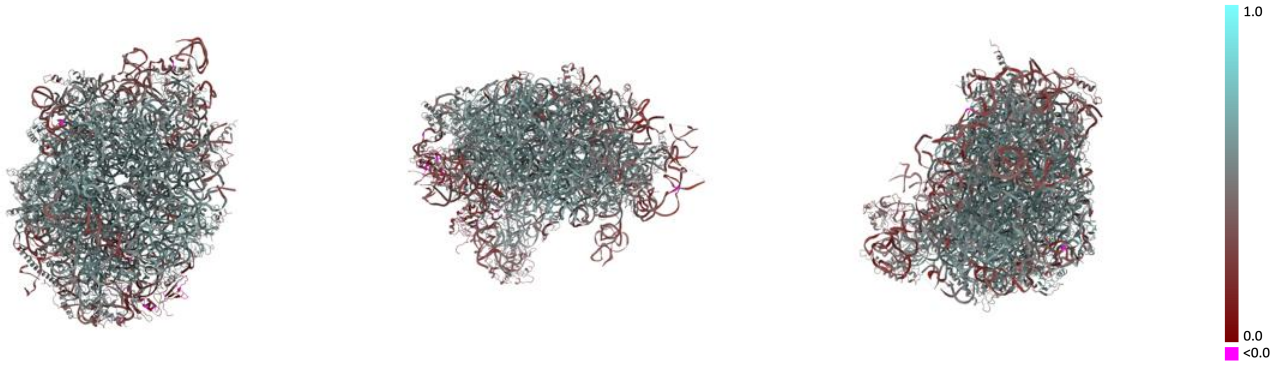
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

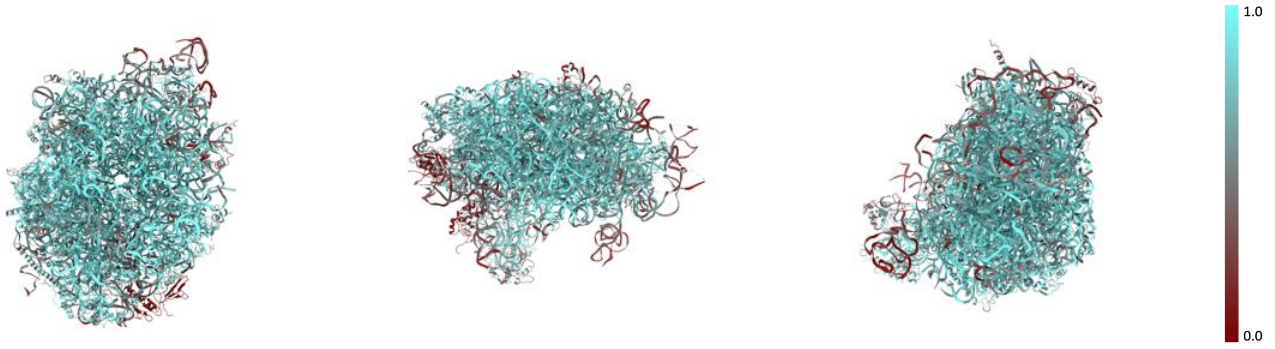
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

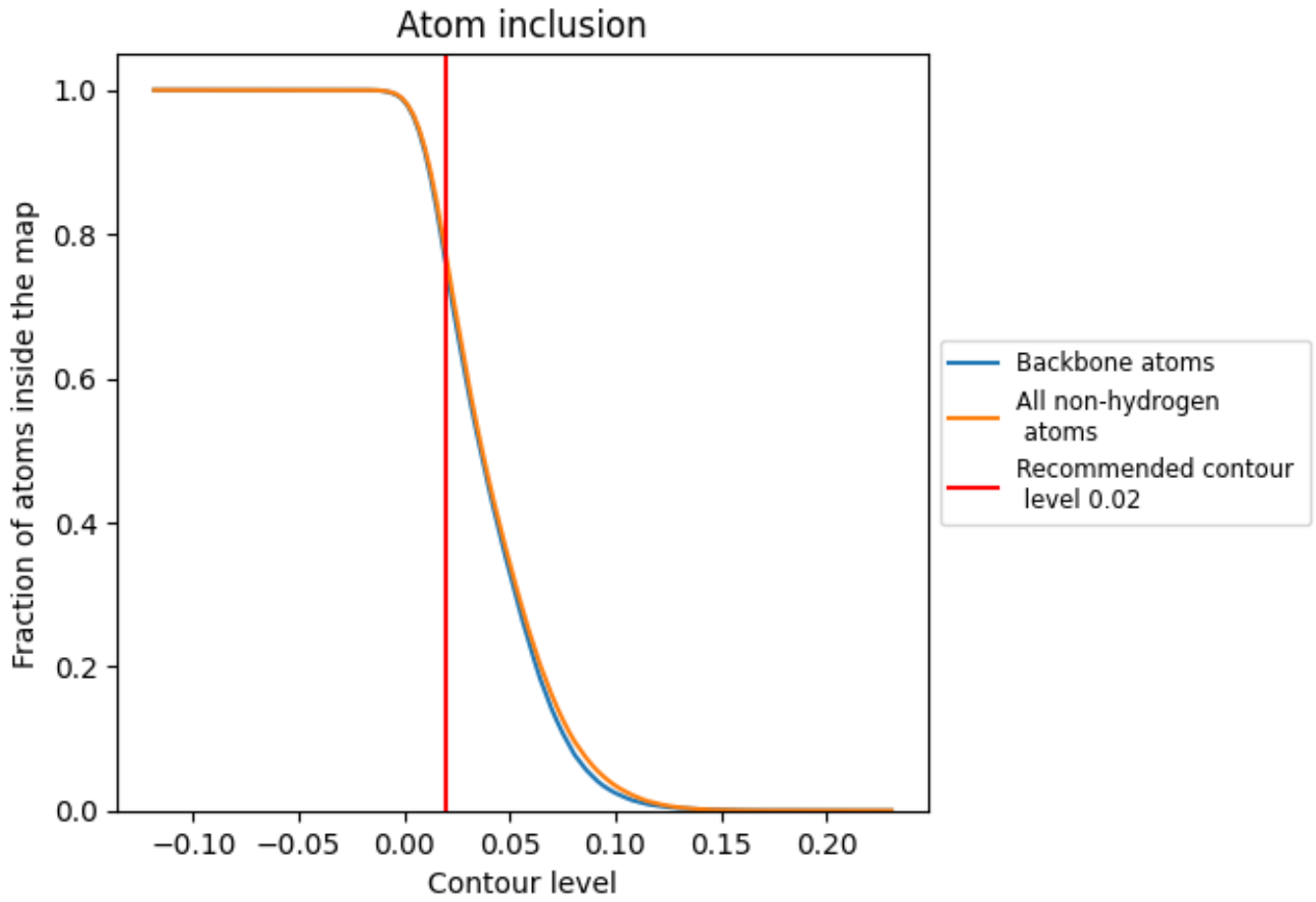
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 77% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7677	0.4990
1	0.8182	0.5060
2	0.7556	0.4850
3	0.6910	0.4460
4	0.7952	0.4970
5	0.8879	0.5440
6	0.6724	0.3910
7	0.8930	0.5550
8	0.8056	0.4420
A	0.8575	0.5770
B	0.8237	0.5530
C	0.8482	0.5580
D	0.4593	0.3530
E	0.1210	0.2290
F	0.8041	0.5200
G	0.7575	0.5140
H	0.7841	0.5300
I	0.8463	0.5620
J	0.8232	0.5510
K	0.7090	0.4450
L	0.8397	0.5570
M	0.8664	0.5820
N	0.0709	0.2100
O	0.7577	0.4740
P	0.8268	0.5570
Q	0.7303	0.5080
R	0.8151	0.5220
S	0.7307	0.5060
T	0.8349	0.5590
U	0.4480	0.3960
V	0.8283	0.5500
W	0.8306	0.5460
X	0.7286	0.5210
Y	0.7685	0.4950
Z	0.6279	0.4930

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Chain	Atom inclusion	Q-score
a	0.8038	0.5310
b	0.8320	0.5530
c	0.8069	0.5410
d	0.6437	0.4540
e	0.7910	0.5220
f	0.8237	0.5580
g	0.8669	0.5780
h	0.7497	0.5290
i	0.7340	0.5140
j	0.8740	0.5930
k	0.5531	0.4250
l	0.8278	0.5680
m	0.7578	0.5320
n	0.6646	0.4980