



Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 09:23 AM EST

PDB ID : 7UG6
EMDB ID : EMD-26485
Title : Cryo-EM structure of pre-60S ribosomal subunit, unmethylated G2922
Authors : Yelland, J.N.; Bravo, J.P.K.; Black, J.J.B.; Taylor, D.W.; Johnson, A.W.
Deposited on : 2022-03-24
Resolution : 2.90 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:

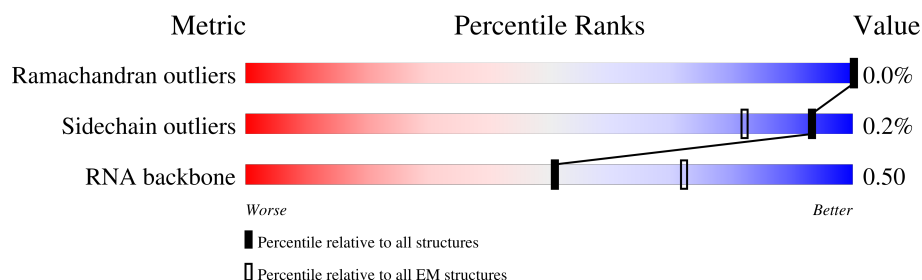
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	3396	
2	2	158	
3	3	121	
4	7	105	
5	A	254	
6	B	387	
7	C	362	
8	D	297	

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Mol	Chain	Length	Quality of chain
9	E	176	
10	F	244	
11	G	256	
12	H	191	
13	I	166	
14	J	174	
15	L	199	
16	M	138	
17	N	204	
18	O	199	
19	P	184	
20	Q	186	
21	R	189	
22	S	172	
23	T	160	
24	U	121	
25	V	137	
26	W	236	
27	X	142	
28	Y	127	
29	Z	136	
30	a	149	
31	b	647	
32	c	175	
33	d	113	

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Mol	Chain	Length	Quality of chain
34	e	130	
35	f	107	
36	g	121	
37	h	120	
38	i	100	
39	j	88	
40	k	78	
41	l	51	
42	m	519	
43	p	92	
44	q	165	
45	r	261	
46	s	520	
47	u	199	
48	v	344	
49	w	203	
50	x	514	
51	y	245	
52	z	106	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 140950 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 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	3058	Total	C	N	O	P	0	0
			65424	29223	11807	21337	3057		

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	158	Total	C	N	O	P	0	0
			3350	1500	586	1107	157		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	121	Total	C	N	O	P	0	0
			2576	1152	461	843	120		

- Molecule 4 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 5 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	213	Total	C	N	O	S	0	0
			1634	1023	326	284	1		

- Molecule 6 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	386	Total	C	N	O	S	0	0
			3082	1956	584	534	8		

- Molecule 7 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	361	Total	C	N	O	S	0	0
			2750	1730	522	495	3		

- Molecule 8 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	257	Total	C	N	O	S	0	0
			2073	1313	362	396	2		

- Molecule 9 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	156	Total	C	N	O	S	0	0
			1240	800	222	217	1		

- Molecule 10 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	222	Total	C	N	O	S	0	0
			1785	1151	324	309	1		

- Molecule 11 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	233	Total	C	N	O	S	0	0
			1818	1159	326	330	3		

- Molecule 12 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	191	Total	C	N	O	S	0	0
			1519	963	274	278	4		

- Molecule 13 is a protein called Bud site selection protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	111	Total	C	N	O	S	0	0
			905	567	170	164	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	112	LEU	VAL	conflict	UNP Q08004

- Molecule 14 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	169	Total	C	N	O	S	0	0
			1354	847	253	250	4		

- Molecule 15 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	187	Total	C	N	O		0	0
			1499	934	307	258			

- Molecule 16 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	137	Total	C	N	O	S	0	0
			1060	678	200	180	2		

- Molecule 17 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	203	Total	C	N	O	S	0	0
			1721	1077	361	282	1		

- Molecule 18 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	197	Total	C	N	O	S	0	0
			1556	1003	289	263	1		

- Molecule 19 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	183	Total	C	N	O		0	0
			1443	896	287	260			

- Molecule 20 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	134	Total	C	N	O	S	0	0
			1035	659	196	179	1		

- Molecule 21 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	156	Total	C	N	O	S	0	0
			1258	781	265	212			

- Molecule 22 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	171	Total	C	N	O	S	0	0
			1438	925	266	244	3		

- Molecule 23 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	119	Total	C	N	O	S	0	0
			943	595	180	165	3		

- Molecule 24 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	106	Total	C	N	O	S	0	0
			844	545	138	161			

- Molecule 25 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	136	Total	C	N	O	S	0	0
			1004	628	189	180	7		

- Molecule 26 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	234	Total	C	N	O	S	0	0
			1885	1194	323	362	6		

- Molecule 27 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	141	Total	C	N	O	S	0	0
			1101	705	196	198	2		

- Molecule 28 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	126	Total	C	N	O		0	0
			994	625	192	177			

- Molecule 29 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	135	Total	C	N	O		0	0
			1093	710	202	181			

- Molecule 30 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	93	Total	C	N	O	S	0	0
			736	479	130	126	1		

- Molecule 31 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	514	Total	C	N	O	S	0	0
			4169	2630	745	773	21		

- Molecule 32 is a protein called Ribosome biogenesis protein ALB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	92	Total	C	N	O		0	0
			743	460	152	131			

- Molecule 33 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	107	Total	C	N	O	S	0	0
			873	553	165	154	1		

- Molecule 34 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 35 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	106	Total	C	N	O	S	0	0
			851	540	165	145	1		

- Molecule 36 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	112	Total	C	N	O	S	0	0
			881	546	179	152	4		

- Molecule 37 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	119	Total	C	N	O	S	0	0
			970	615	186	168	1		

- Molecule 38 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	99	Total	C	N	O	S	0	0
			772	481	156	133	2		

- Molecule 39 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	87	Total	C	N	O	S	0	0
			682	414	148	115	5		

- Molecule 40 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	k	77	Total	C	N	O	0	0
			613	391	115	107		

- Molecule 41 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	50	Total	C	N	O	S	0	0
			437	272	97	66	2		

- Molecule 42 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	469	Total	C	N	O	S	0	0
			3774	2381	685	699	9		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	487	GLY	-	expression tag	UNP P53742
m	488	SER	-	expression tag	UNP P53742
m	489	ASP	-	expression tag	UNP P53742
m	490	TYR	-	expression tag	UNP P53742
m	491	LYS	-	expression tag	UNP P53742
m	492	ASP	-	expression tag	UNP P53742
m	493	ASP	-	expression tag	UNP P53742
m	494	ASP	-	expression tag	UNP P53742
m	495	ASP	-	expression tag	UNP P53742
m	496	LYS	-	expression tag	UNP P53742
m	497	ASP	-	expression tag	UNP P53742
m	498	TYR	-	expression tag	UNP P53742
m	499	LYS	-	expression tag	UNP P53742
m	500	ASP	-	expression tag	UNP P53742
m	501	ASP	-	expression tag	UNP P53742
m	502	ASP	-	expression tag	UNP P53742
m	503	ASP	-	expression tag	UNP P53742
m	504	LYS	-	expression tag	UNP P53742
m	505	ASP	-	expression tag	UNP P53742
m	506	TYR	-	expression tag	UNP P53742
m	507	LYS	-	expression tag	UNP P53742
m	508	ASP	-	expression tag	UNP P53742
m	509	ASP	-	expression tag	UNP P53742
m	510	ASP	-	expression tag	UNP P53742
m	511	ASP	-	expression tag	UNP P53742
m	512	LYS	-	expression tag	UNP P53742
m	513	GLY	-	expression tag	UNP P53742
m	514	HIS	-	expression tag	UNP P53742
m	515	HIS	-	expression tag	UNP P53742
m	516	HIS	-	expression tag	UNP P53742
m	517	HIS	-	expression tag	UNP P53742

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Chain	Residue	Modelled	Actual	Comment	Reference
m	518	HIS	-	expression tag	UNP P53742
m	519	HIS	-	expression tag	UNP P53742

- Molecule 43 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	p	91	Total	C	N	O	S	0	0
			695	429	138	122	6		

- Molecule 44 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	126	Total	C	N	O	S	0	0
			961	606	171	182	2		

- Molecule 45 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	230	Total	C	N	O	S	0	0
			1861	1177	352	325	7		

- Molecule 46 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	69	Total	C	N	O	S	0	0
			573	359	113	98	3		

- Molecule 47 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	u	150	Total	C	N	O	S	0	0
			1265	793	253	210	9		

- Molecule 48 is a protein called Ribosome biogenesis protein RPF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	v	287	Total	C	N	O	S	0	0
			2318	1482	408	412	16		

- Molecule 49 is a protein called Regulator of ribosome biosynthesis.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	w	179	Total	C	N	O	S	0	0
			1425	896	258	266	5		

- Molecule 50 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	x	488	Total	C	N	O	S	0	0
			3808	2398	677	712	21		

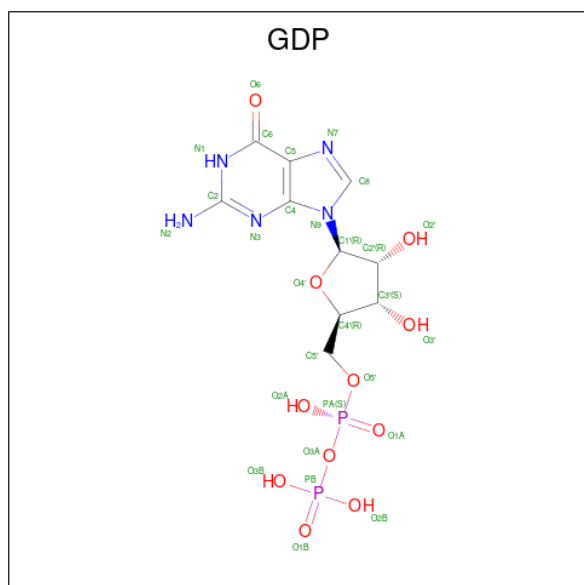
- Molecule 51 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	y	228	Total	C	N	O	S	0	0
			1723	1068	299	349	7		

- Molecule 52 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	z	77	Total	C	N	O	S	0	0
			644	403	130	110	1		

- Molecule 53 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



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

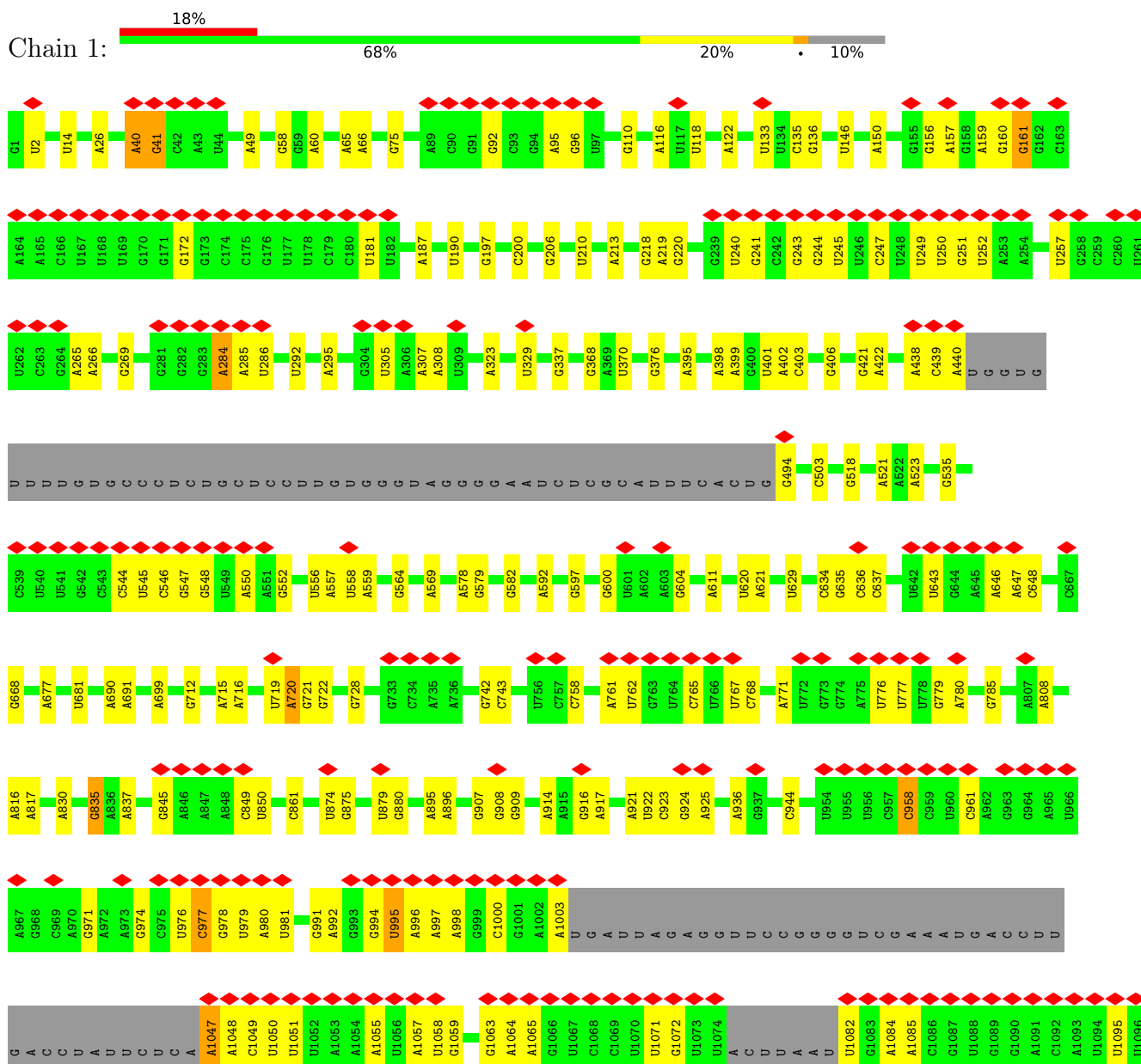
- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
54	m	1	Total 1	Mg 1	0

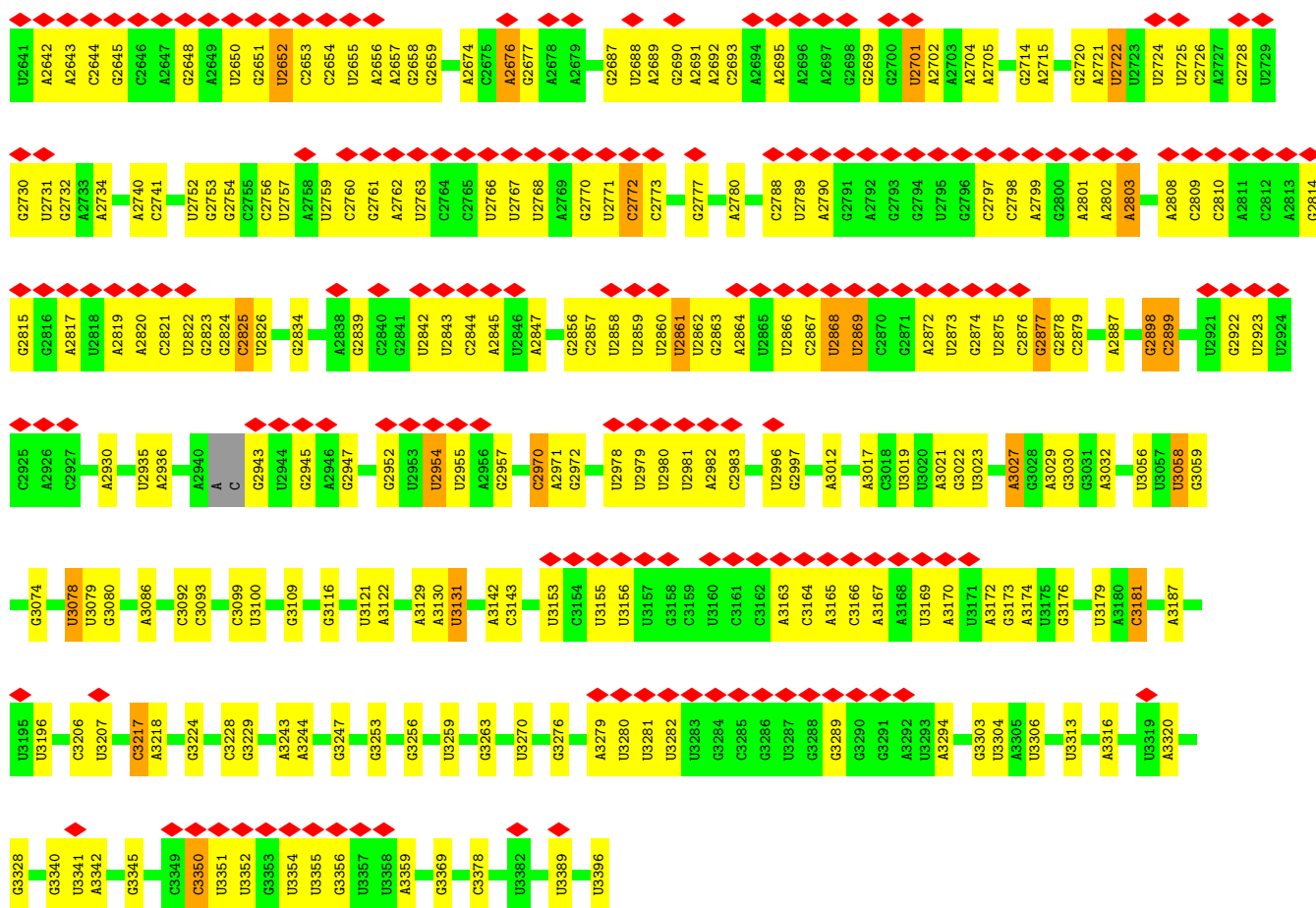
3 Residue-property plots

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

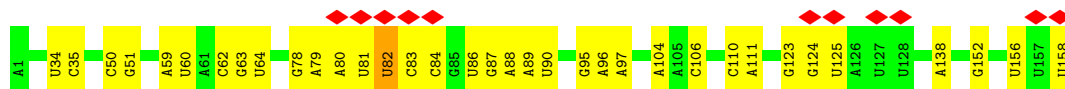
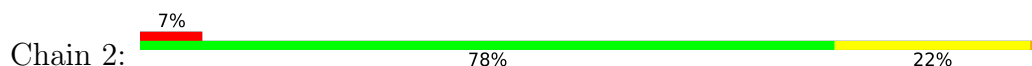
• Molecule 1: 25S rRNA



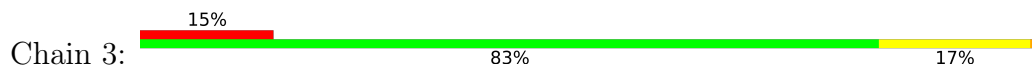




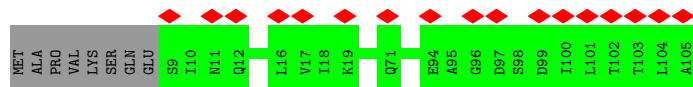
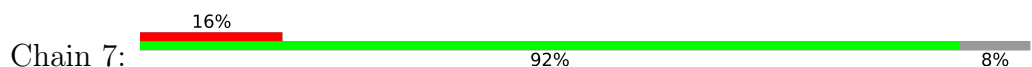
- Molecule 2: 5.8S rRNA



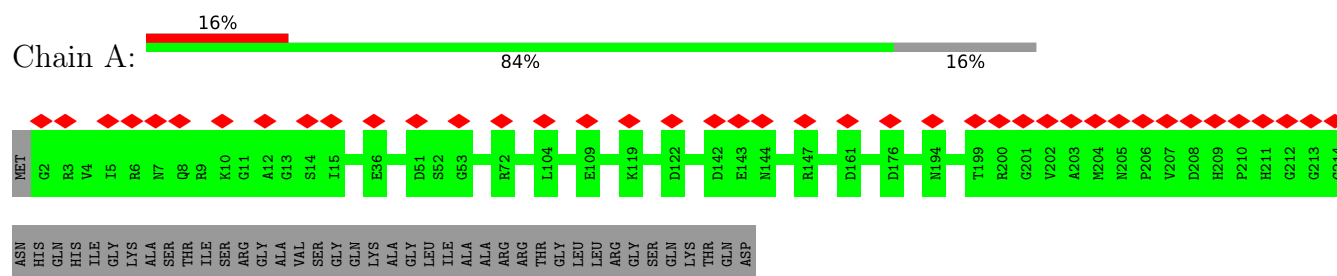
- Molecule 3: 5S rRNA



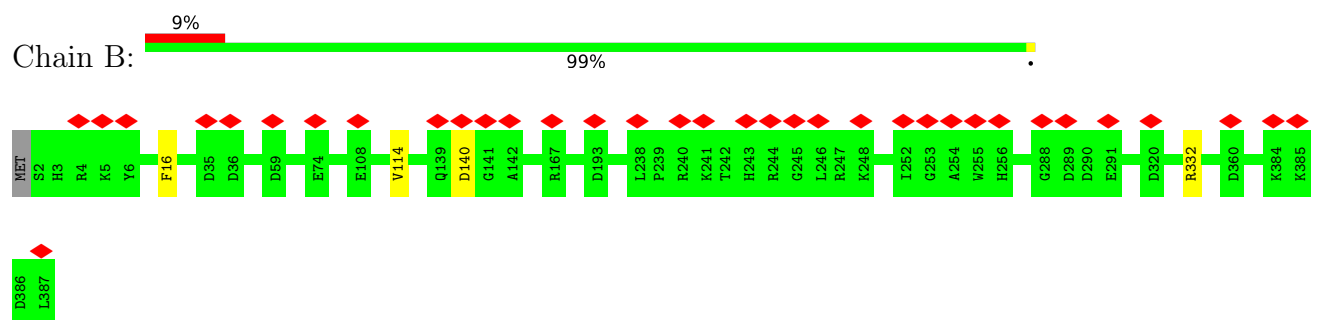
- Molecule 4: 60S ribosomal protein L30



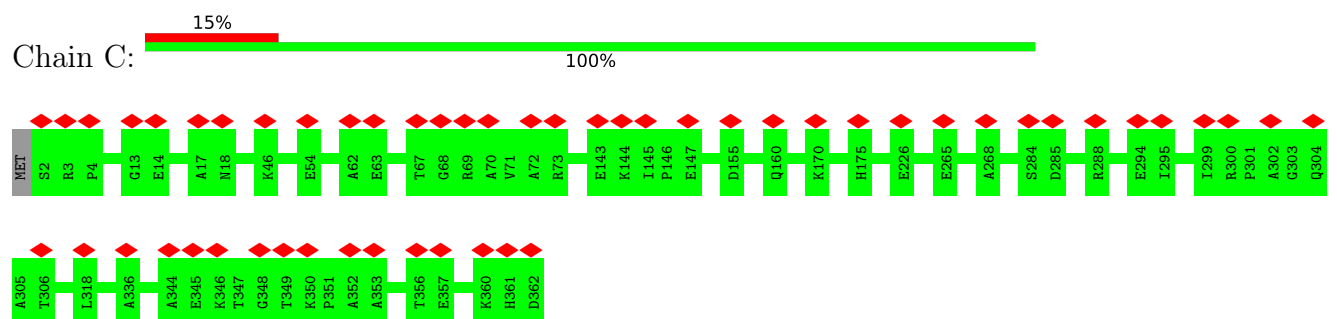
- Molecule 5: 60S ribosomal protein L2-A



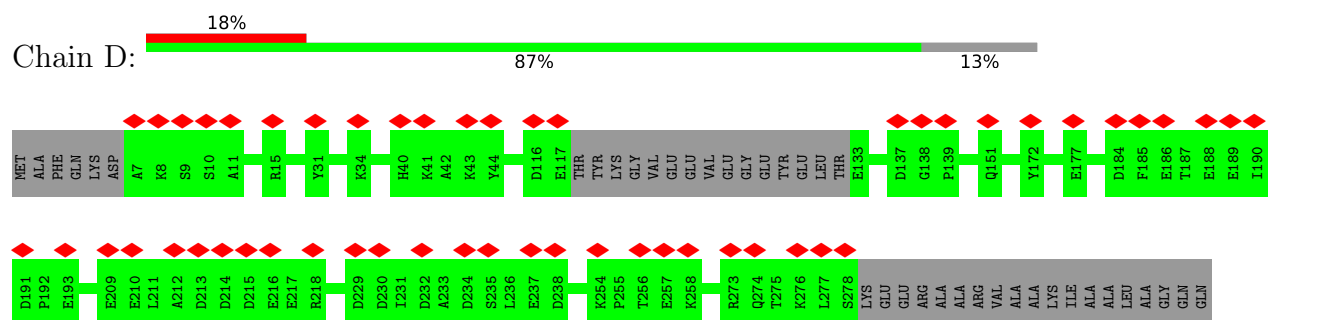
- Molecule 6: 60S ribosomal protein L3



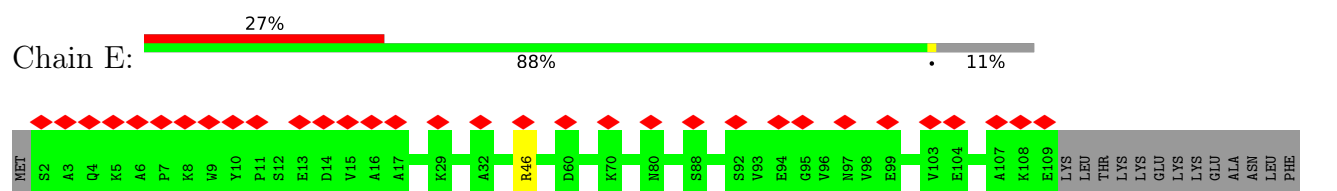
- Molecule 7: 60S ribosomal protein L4-A

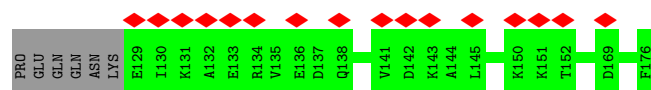


- Molecule 8: 60S ribosomal protein L5

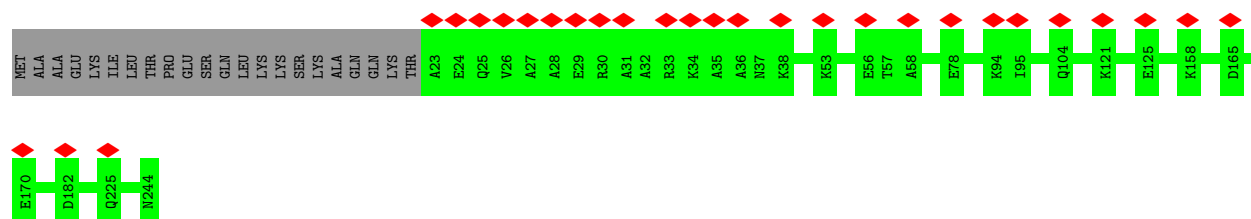


- Molecule 9: 60S ribosomal protein L6-A

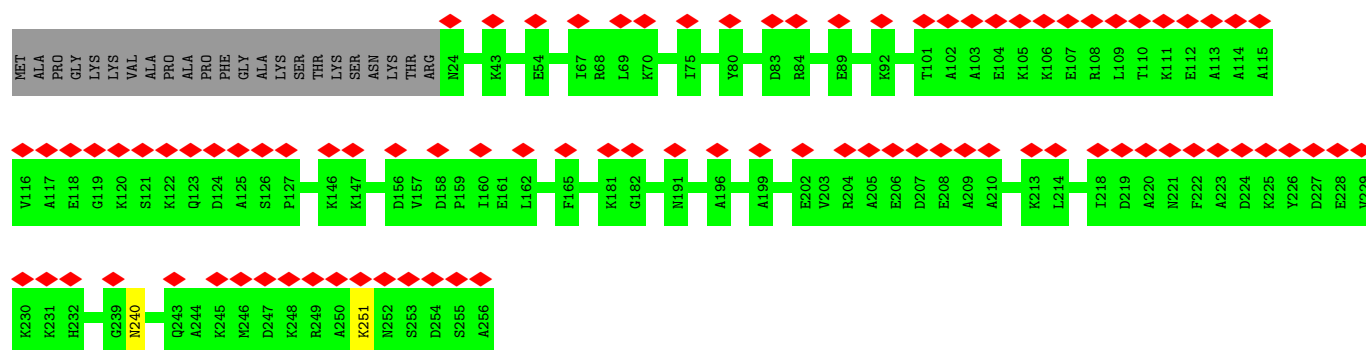
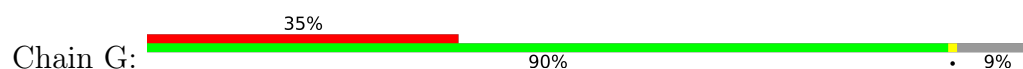




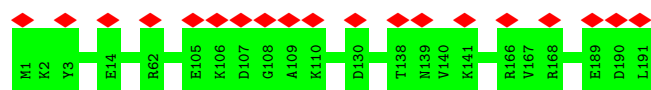
- Molecule 10: 60S ribosomal protein L7-A



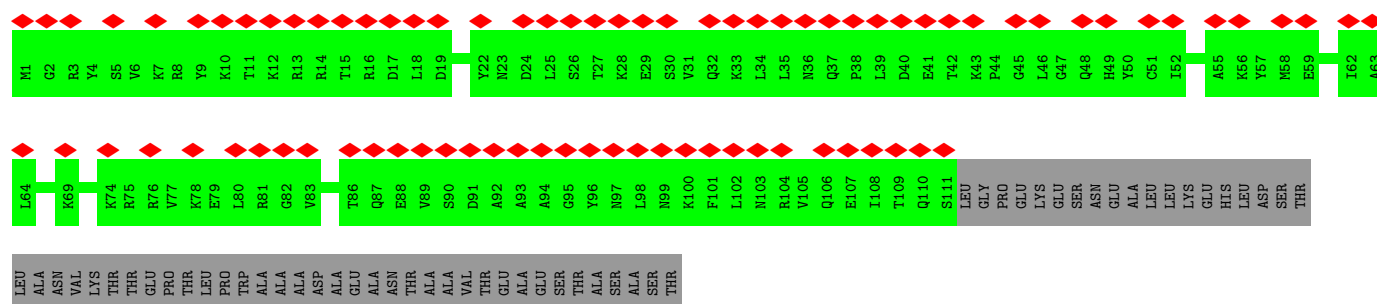
- Molecule 11: 60S ribosomal protein L8-A



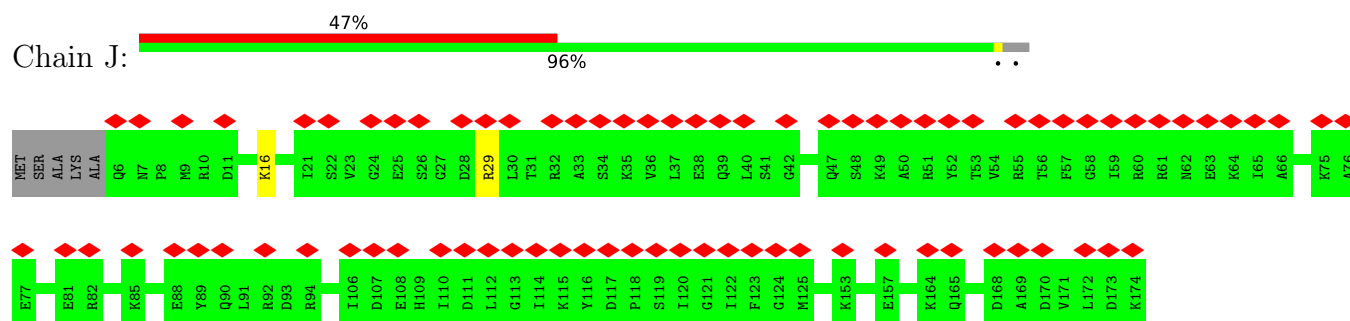
- Molecule 12: 60S ribosomal protein L9-A



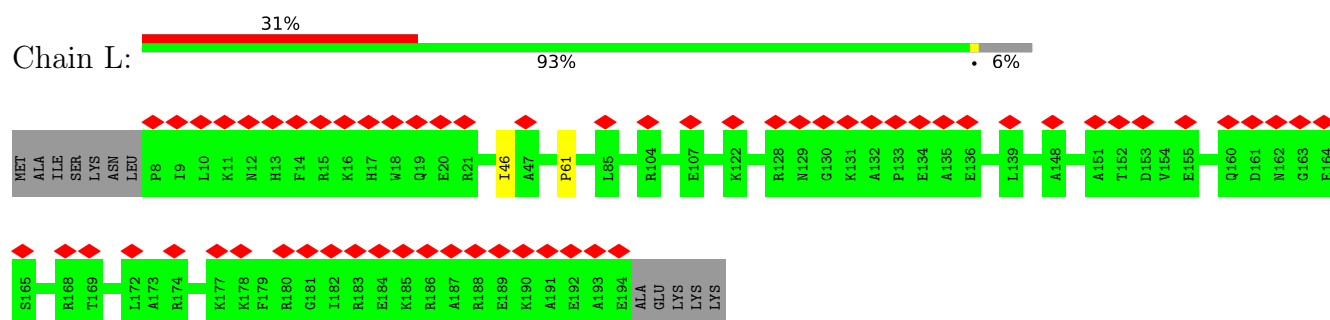
- Molecule 13: Bud site selection protein 20



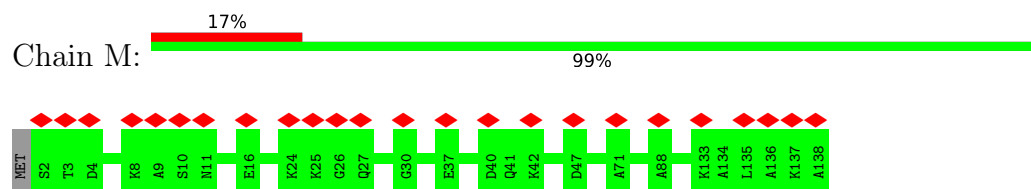
- Molecule 14: 60S ribosomal protein L11-A



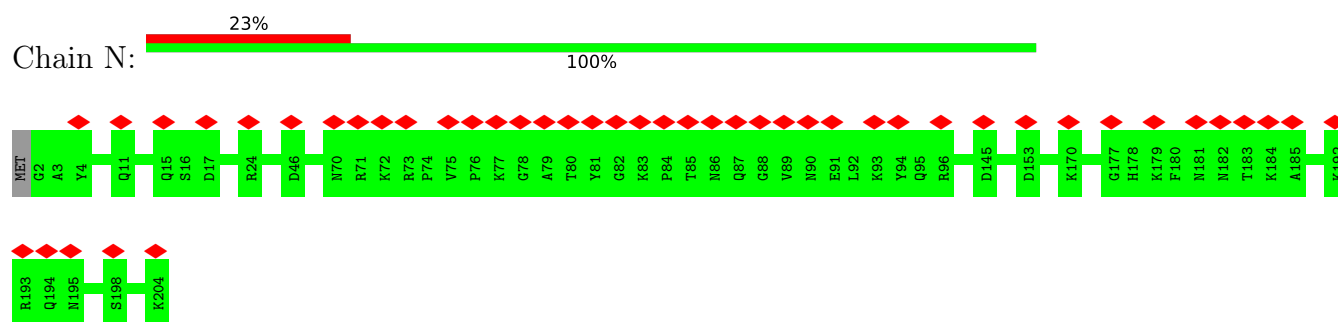
- Molecule 15: 60S ribosomal protein L13-A



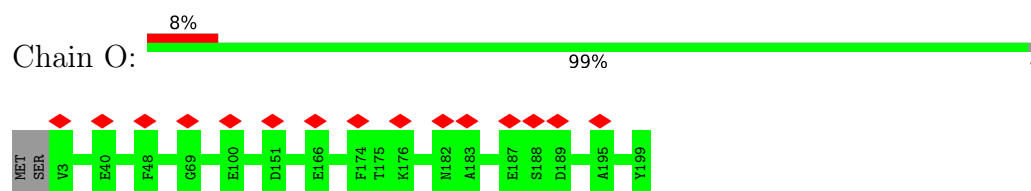
- Molecule 16: 60S ribosomal protein L14-A



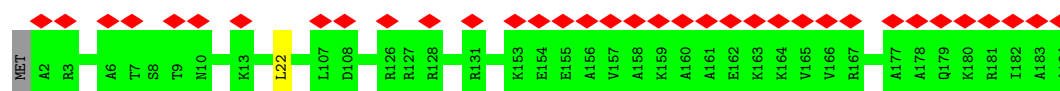
- Molecule 17: 60S ribosomal protein L15-A



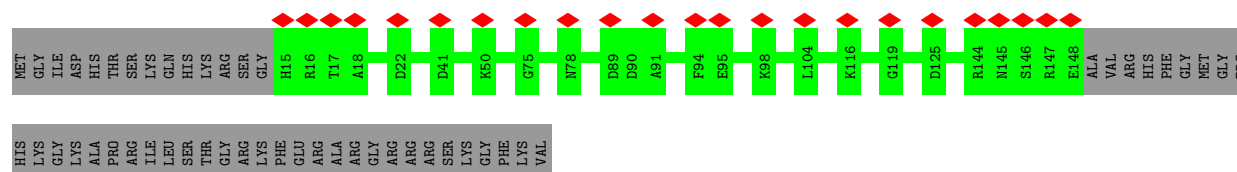
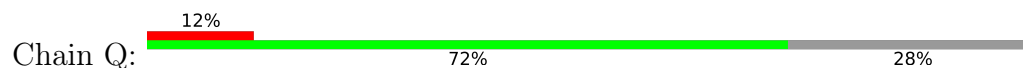
- Molecule 18: 60S ribosomal protein L16-A



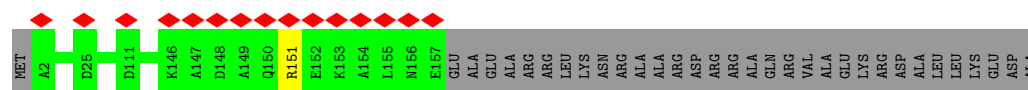
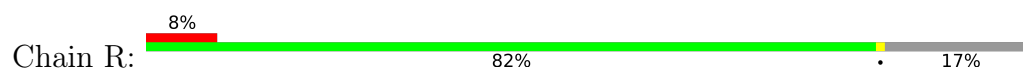
- Molecule 19: 60S ribosomal protein L17-A



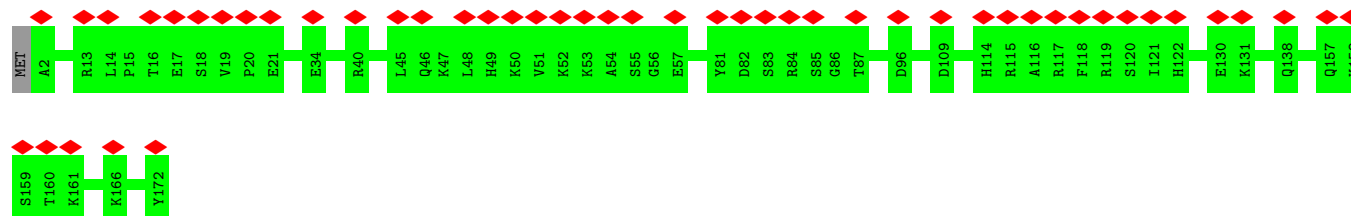
- Molecule 20: 60S ribosomal protein L18-A



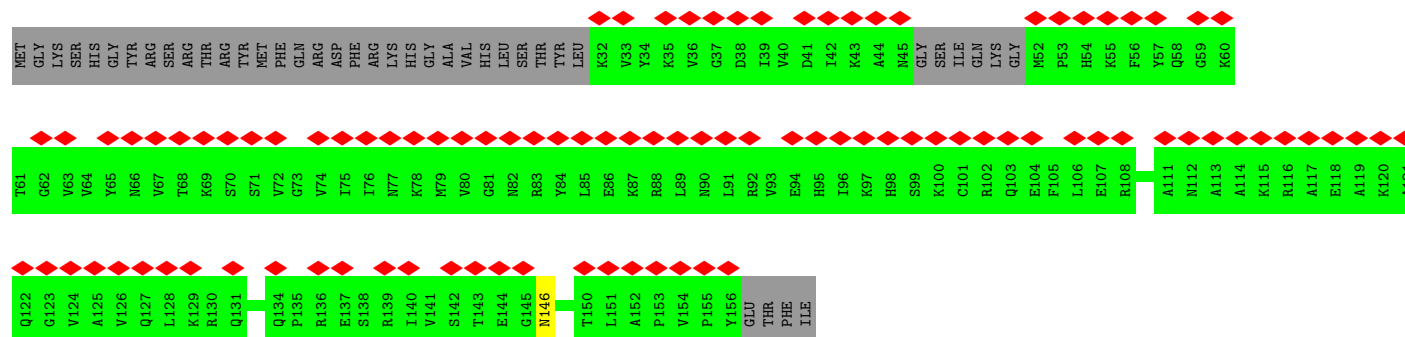
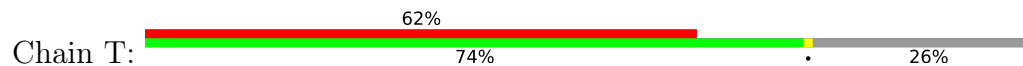
- Molecule 21: 60S ribosomal protein L19-A



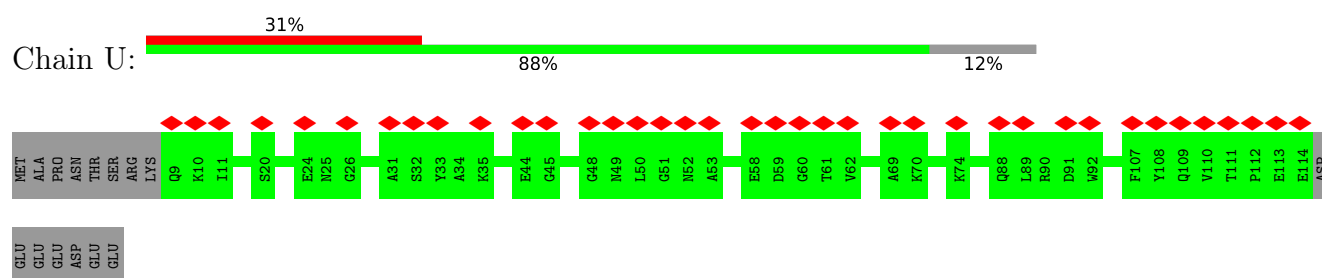
- Molecule 22: 60S ribosomal protein L20-A



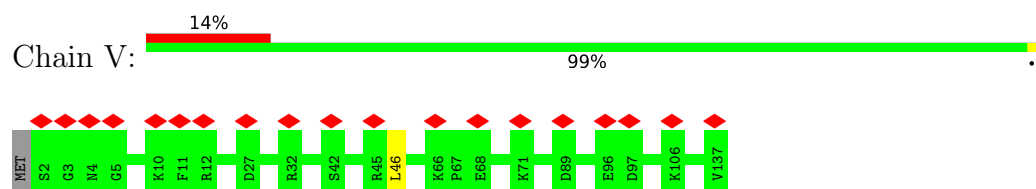
- Molecule 23: 60S ribosomal protein L21-A



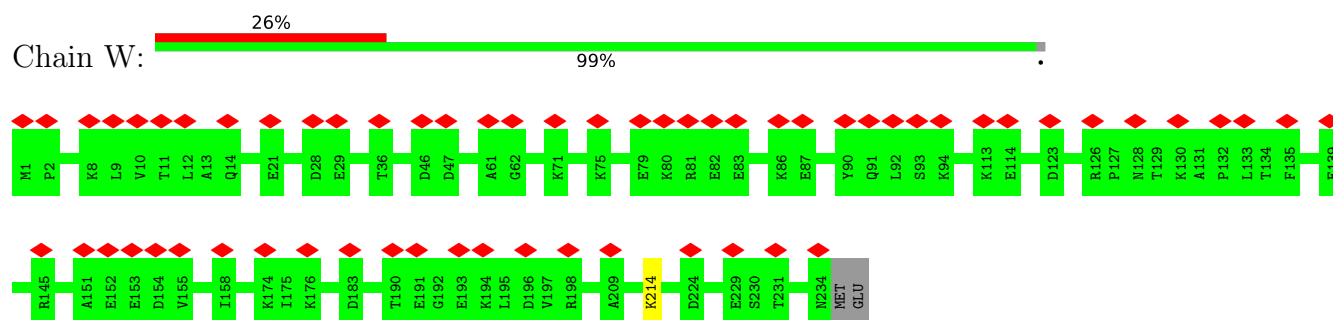
- Molecule 24: 60S ribosomal protein L22-A



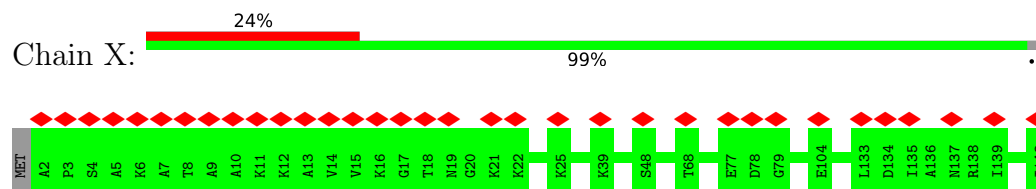
- Molecule 25: 60S ribosomal protein L23-A



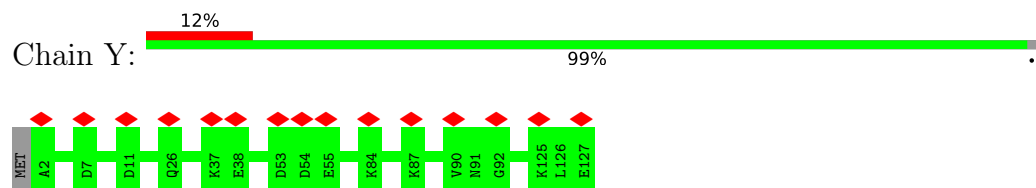
- Molecule 26: Ribosome assembly factor MRT4



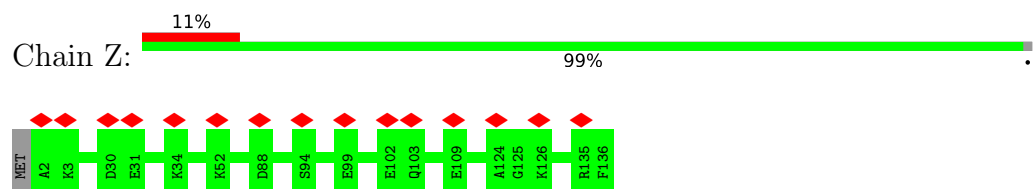
- Molecule 27: 60S ribosomal protein L25



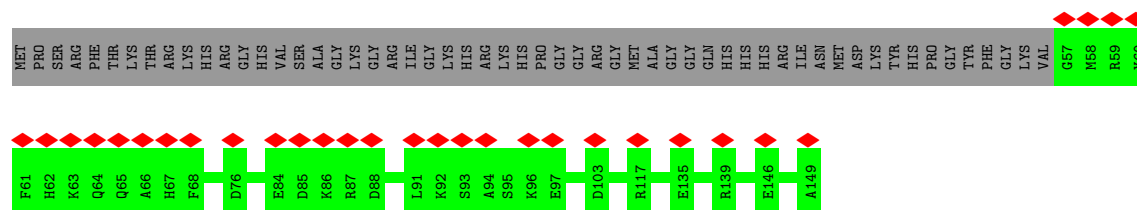
- Molecule 28: 60S ribosomal protein L26-A



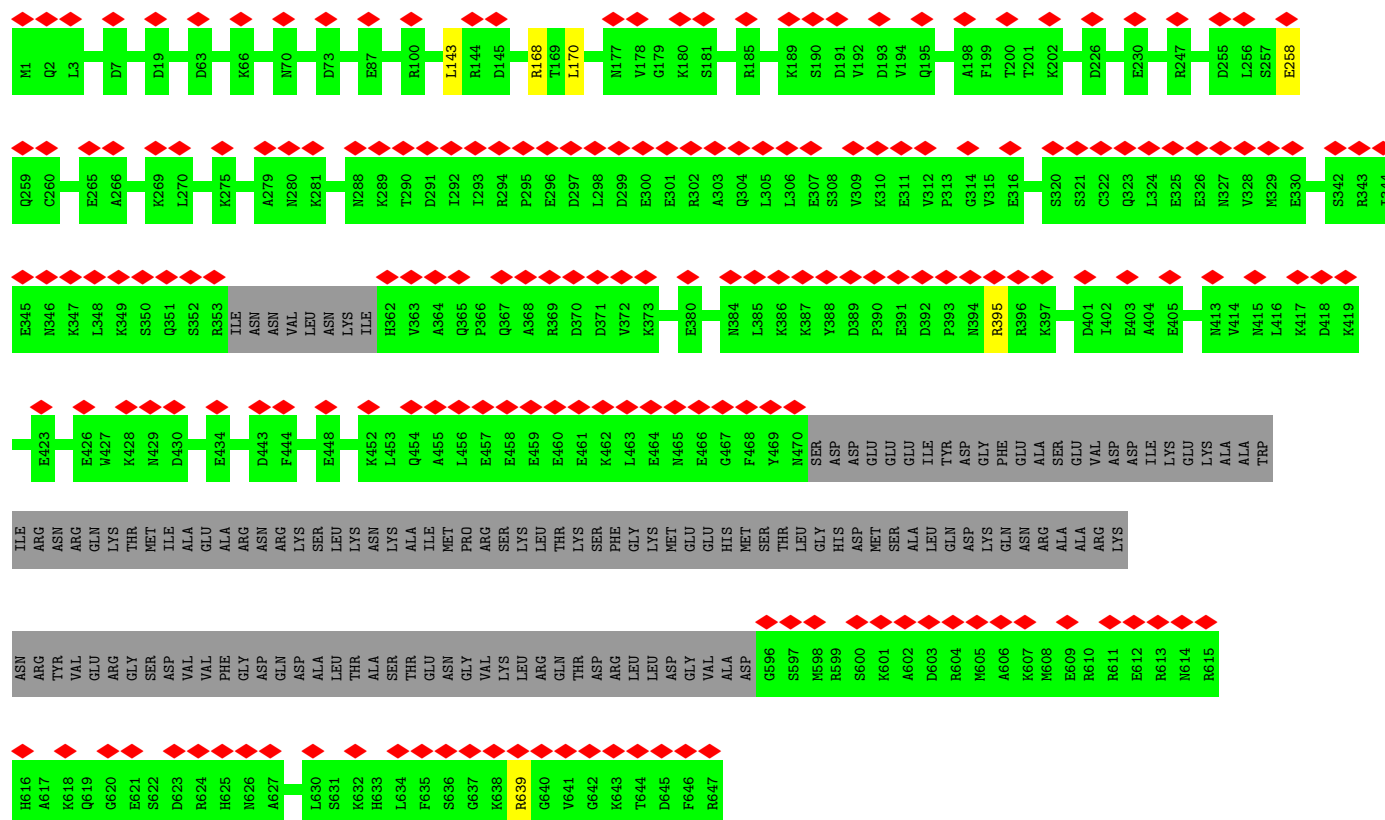
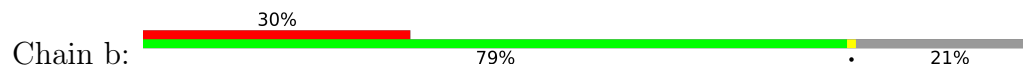
- Molecule 29: 60S ribosomal protein L27-A



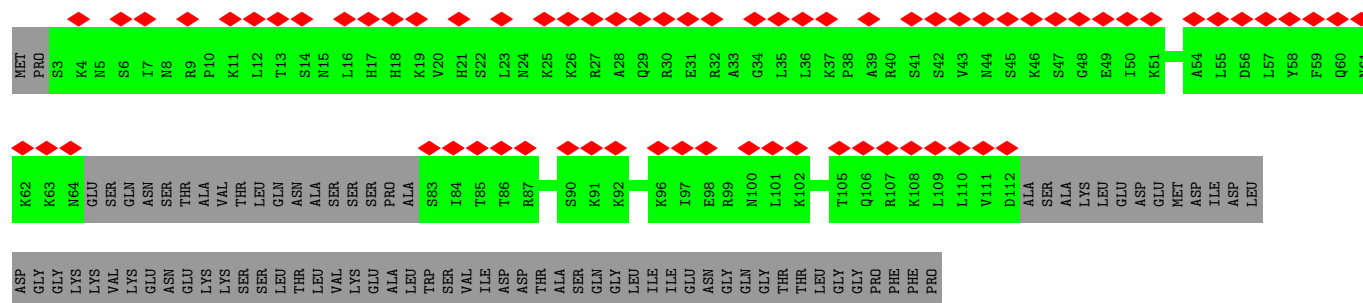
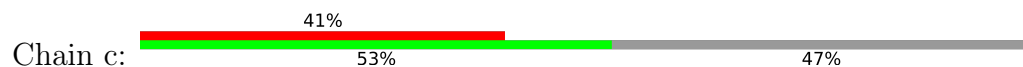
- Molecule 30: 60S ribosomal protein L28



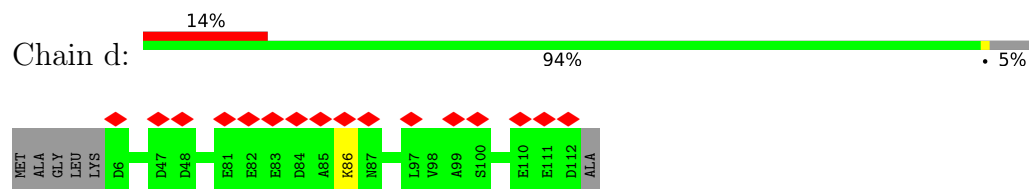
• Molecule 31: Nucleolar GTP-binding protein 1



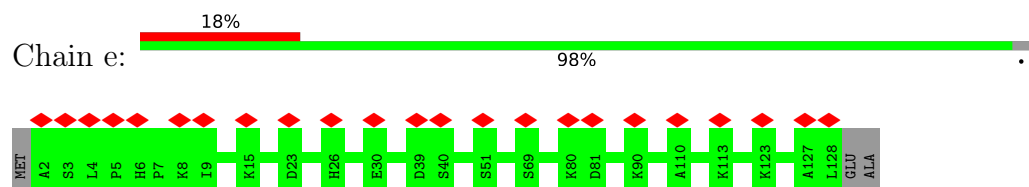
• Molecule 32: Ribosome biogenesis protein ALB1



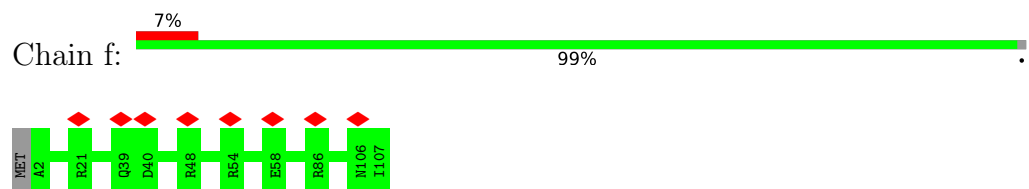
- Molecule 33: 60S ribosomal protein L31-A



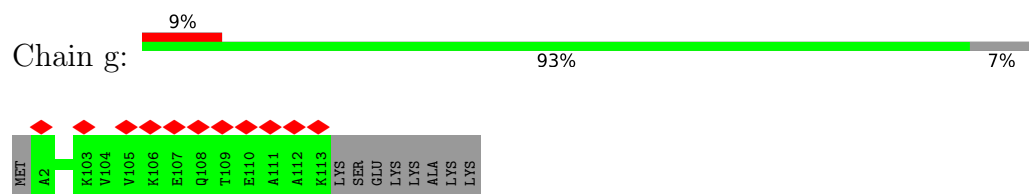
- Molecule 34: 60S ribosomal protein L32



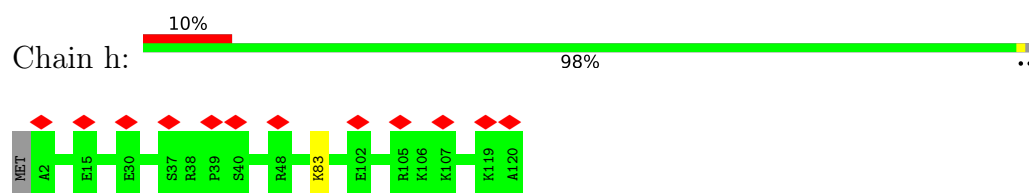
- Molecule 35: 60S ribosomal protein L33-A



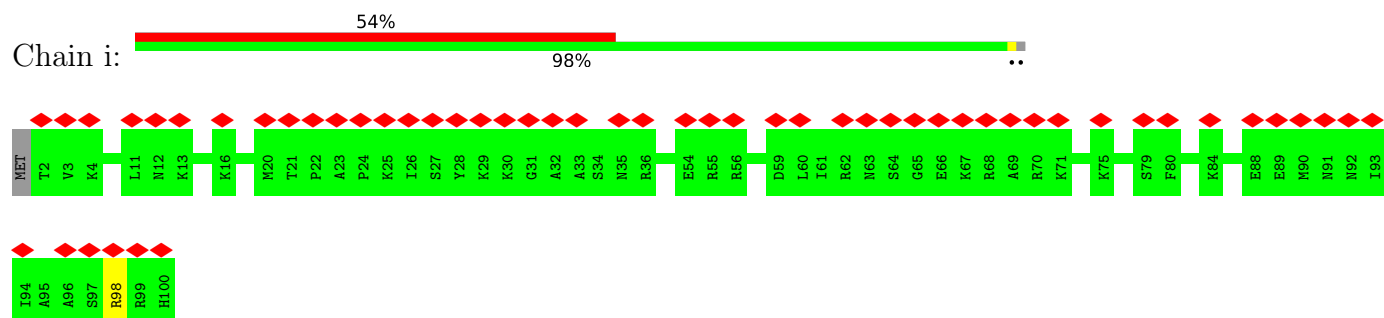
- Molecule 36: 60S ribosomal protein L34-A



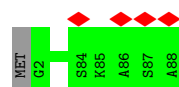
- Molecule 37: 60S ribosomal protein L35-A



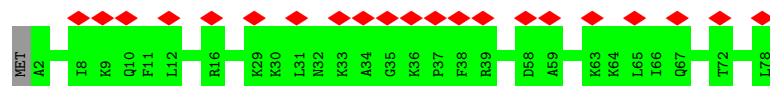
- Molecule 38: 60S ribosomal protein L36-A



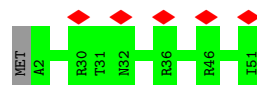
- Molecule 39: 60S ribosomal protein L37-A



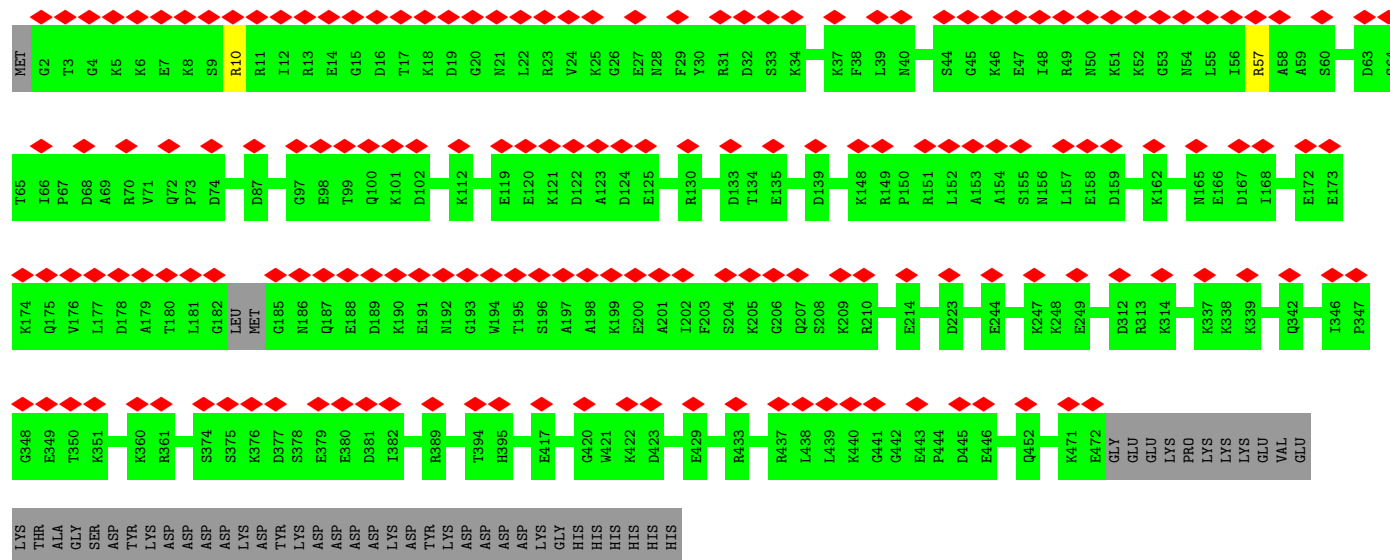
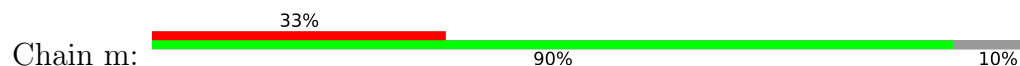
- Molecule 40: 60S ribosomal protein L38



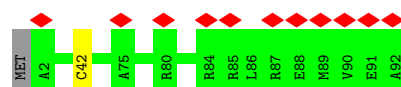
- Molecule 41: 60S ribosomal protein L39



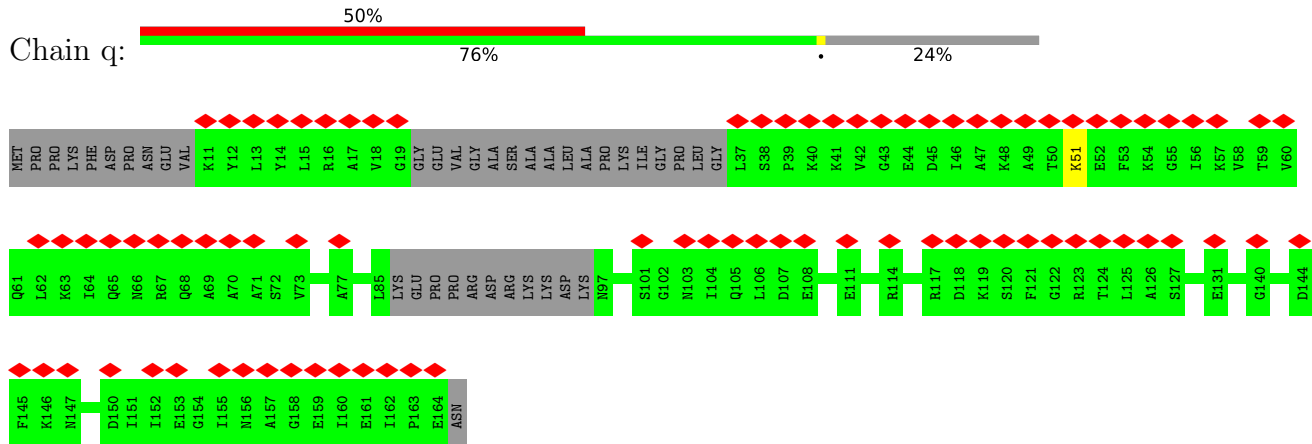
- Molecule 42: Nucleolar GTP-binding protein 2



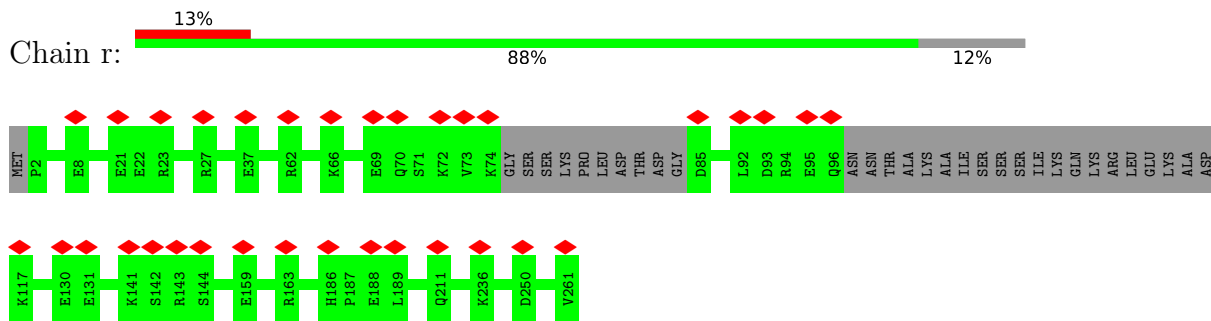
- Molecule 43: 60S ribosomal protein L43-A



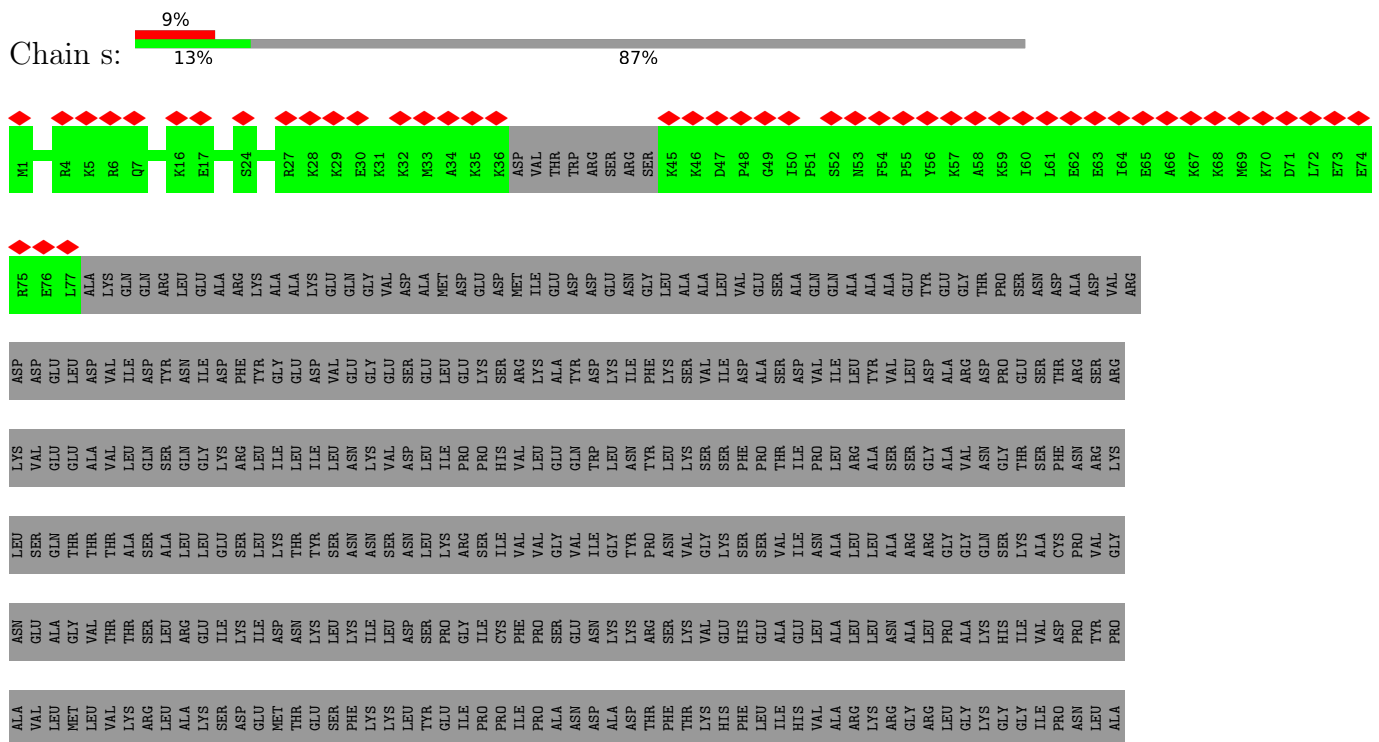
- Molecule 44: 60S ribosomal protein L12-A

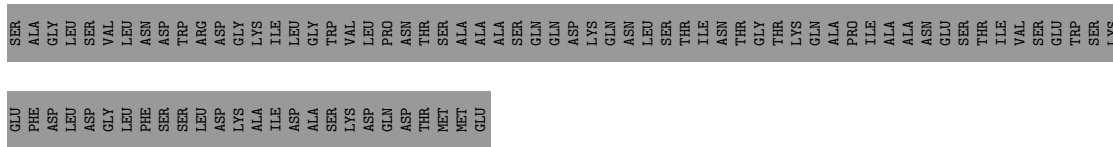


- Molecule 45: Ribosome biogenesis protein NSA2

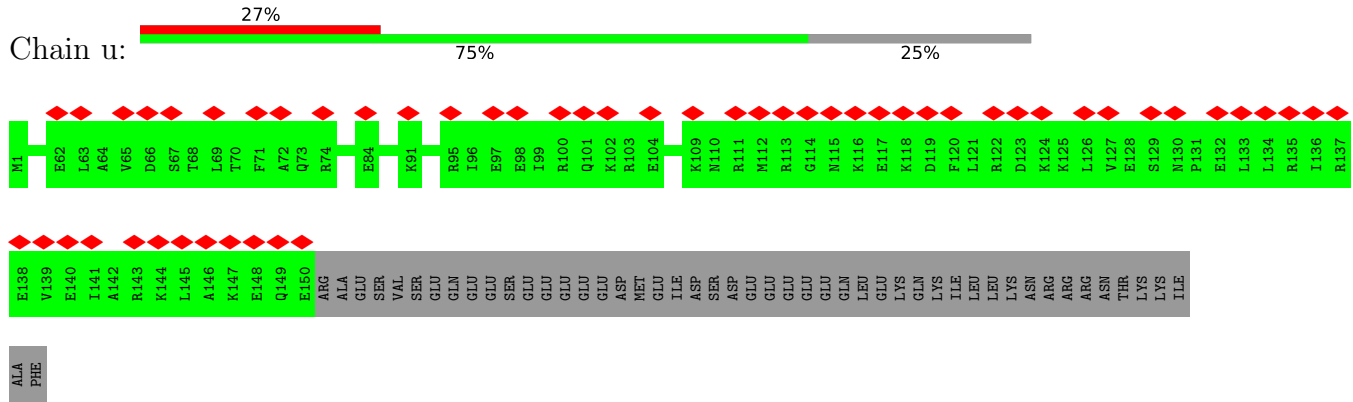


- Molecule 46: Nuclear GTP-binding protein NUG1

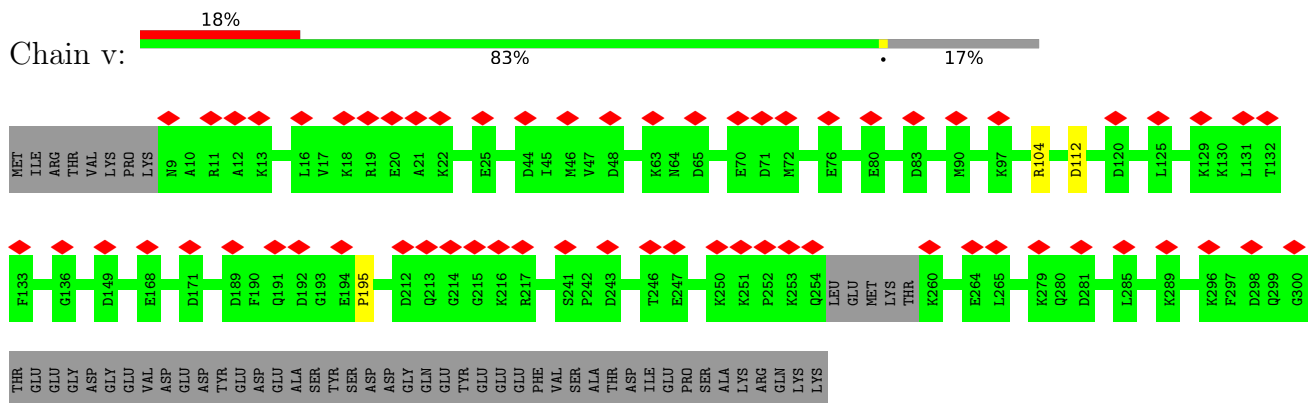




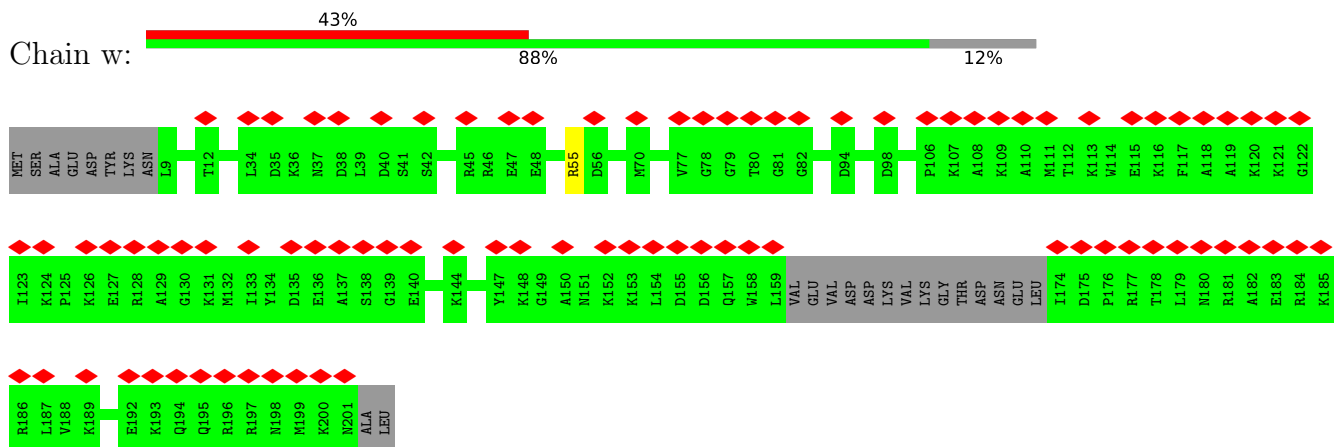
- Molecule 47: Ribosome biogenesis protein RLP24



- Molecule 48: Ribosome biogenesis protein RPF2

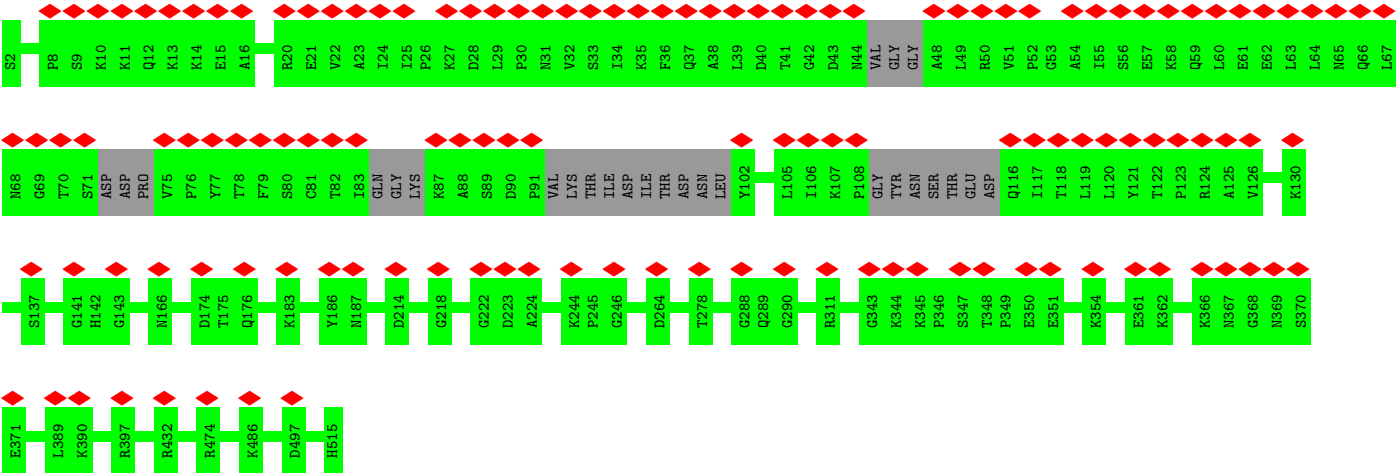


- Molecule 49: Regulator of ribosome biosynthesis

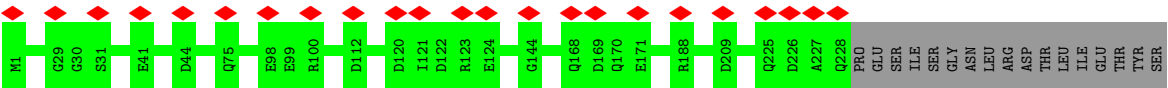
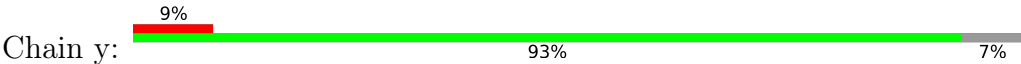


- Molecule 50: Ribosome assembly protein 4





• Molecule 51: Eukaryotic translation initiation factor 6



• Molecule 52: UPF0642 protein YBL028C



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15954	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.756	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.18	Depositor
Map size (\AA)	414.72, 414.72, 414.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.81, 0.81, 0.81	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.03	2/73231 (0.0%)	0.98	190/114163 (0.2%)
2	2	1.16	0/3743	0.91	5/5828 (0.1%)
3	3	0.91	0/2880	0.96	6/4487 (0.1%)
4	7	0.55	0/751	0.51	0/1008
5	A	0.59	0/1666	0.57	0/2241
6	B	0.59	2/3153 (0.1%)	0.58	1/4239 (0.0%)
7	C	0.50	0/2802	0.51	0/3792
8	D	0.50	0/2119	0.57	0/2859
9	E	0.47	0/1261	0.56	0/1694
10	F	0.54	0/1822	0.52	0/2451
11	G	0.44	0/1850	0.55	0/2495
12	H	0.56	0/1540	0.58	0/2073
13	I	0.38	0/919	0.48	0/1232
14	J	0.42	0/1375	0.59	0/1842
15	L	0.48	0/1524	0.53	0/2046
16	M	0.49	0/1075	0.50	0/1446
17	N	0.53	0/1758	0.53	0/2354
18	O	0.57	0/1586	0.54	0/2128
19	P	0.52	0/1466	0.53	1/1968 (0.1%)
20	Q	0.46	0/1050	0.52	0/1419
21	R	0.54	0/1275	0.49	0/1702
22	S	0.53	0/1474	0.57	0/1980
23	T	0.37	0/957	0.58	0/1285
24	U	0.47	0/861	0.60	0/1167
25	V	0.55	0/1019	0.59	1/1369 (0.1%)
26	W	0.43	0/1918	0.54	0/2586
27	X	0.55	0/1117	0.55	0/1503
28	Y	0.50	0/1005	0.57	0/1341
29	Z	0.58	0/1119	0.52	0/1497
30	a	0.42	0/752	0.58	0/1013
31	b	0.48	0/4243	0.55	2/5704 (0.0%)
32	c	0.34	0/749	0.46	0/994

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.53	0/887	0.51	0/1191
34	e	0.49	0/1041	0.51	0/1394
35	f	0.60	0/869	0.55	0/1168
36	g	0.57	0/891	0.58	0/1191
37	h	0.52	0/979	0.53	0/1301
38	i	0.35	0/779	0.52	0/1034
39	j	0.61	0/697	0.54	0/923
40	k	0.49	0/619	0.60	0/826
41	l	0.58	0/444	0.62	0/588
42	m	0.47	0/3848	0.53	0/5181
43	p	0.63	1/702 (0.1%)	0.54	0/934
44	q	0.39	0/969	0.60	0/1301
45	r	0.53	0/1893	0.53	0/2528
46	s	0.35	0/577	0.49	0/752
47	u	0.50	0/1287	0.49	0/1711
48	v	0.50	0/2361	0.64	1/3153 (0.0%)
49	w	0.41	0/1448	0.57	0/1948
50	x	0.50	0/3898	0.60	0/5282
51	y	0.50	0/1744	0.58	0/2373
52	z	0.36	0/651	0.51	0/854
All	All	0.82	5/150644 (0.0%)	0.82	207/219539 (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
15	L	0	1
31	b	0	1
37	h	0	1
44	q	0	1
48	v	0	2
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	114	VAL	CB-CG1	-6.30	1.39	1.52
6	B	16	PHE	C-N	-5.94	1.20	1.34
1	1	2898	G	C5-C6	-5.66	1.36	1.42
1	1	2898	G	N9-C4	-5.46	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	p	42	CYS	CB-SG	-5.04	1.73	1.81

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1279	C	C5-C6-N1	11.43	126.72	121.00
3	3	98	C	N1-C2-O2	10.70	125.32	118.90
1	1	1279	C	C6-N1-C2	-10.50	116.10	120.30
1	1	2376	G	O4'-C1'-N9	10.30	116.44	108.20
3	3	98	C	C2-N1-C1'	10.28	130.11	118.80
1	1	3217	C	N1-C2-O2	10.22	125.03	118.90
1	1	3217	C	C2-N1-C1'	8.89	128.58	118.80
1	1	2979	U	C2-N1-C1'	8.84	128.30	117.70
3	3	98	C	N3-C2-O2	-8.69	115.82	121.90
1	1	3217	C	N3-C2-O2	-8.69	115.82	121.90
1	1	2898	G	C4-C5-N7	8.66	114.26	110.80
1	1	3153	U	C2-N1-C1'	8.48	127.88	117.70
3	3	98	C	C6-N1-C2	-8.48	116.91	120.30
1	1	1567	U	C2-N1-C1'	8.47	127.86	117.70
1	1	3027	A	N1-C2-N3	8.37	133.48	129.30
1	1	2898	G	C5-C6-O6	-8.33	123.60	128.60
1	1	3153	U	N1-C2-O2	8.31	128.62	122.80
1	1	2979	U	N1-C2-O2	8.17	128.52	122.80
1	1	2257	C	N1-C2-O2	8.11	123.77	118.90
1	1	2759	U	C2-N1-C1'	8.09	127.40	117.70
1	1	1567	U	N1-C2-O2	8.04	128.43	122.80
1	1	2943	G	OP1-P-OP2	-7.86	107.81	119.60
1	1	1227	C	C2-N1-C1'	7.85	127.43	118.80
1	1	2652	U	C2-N1-C1'	7.78	127.03	117.70
1	1	2970	C	C5-C6-N1	7.77	124.88	121.00
1	1	977	C	N1-C2-O2	7.75	123.55	118.90
1	1	2257	C	C2-N1-C1'	7.66	127.23	118.80
1	1	1496	C	C2-N1-C1'	7.57	127.12	118.80
1	1	1567	U	N3-C2-O2	-7.51	116.94	122.20
1	1	2652	U	N1-C2-O2	7.48	128.03	122.80
1	1	2898	G	N1-C6-O6	7.47	124.38	119.90
1	1	2376	G	N9-C1'-C2'	7.46	123.70	114.00
3	3	98	C	C5-C6-N1	7.43	124.72	121.00
1	1	2898	G	C2-N3-C4	-7.32	108.24	111.90
1	1	1187	C	C2-N1-C1'	7.26	126.79	118.80
1	1	2248	C	N1-C2-O2	7.21	123.23	118.90
1	1	2724	U	N1-C2-O2	7.19	127.83	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2094	C	N3-C2-O2	-7.18	116.87	121.90
1	1	3027	A	C2-N3-C4	-7.18	107.01	110.60
1	1	1227	C	C5-C6-N1	7.16	124.58	121.00
1	1	2652	U	N3-C2-O2	-7.15	117.20	122.20
1	1	2376	G	OP1-P-OP2	-7.12	108.93	119.60
1	1	3023	U	N3-C2-O2	-7.10	117.23	122.20
1	1	2979	U	N3-C2-O2	-7.07	117.25	122.20
1	1	977	C	N3-C2-O2	-7.00	117.00	121.90
1	1	2501	U	OP1-P-OP2	-6.95	109.18	119.60
1	1	3306	U	N3-C2-O2	-6.95	117.34	122.20
1	1	494	G	OP1-P-OP2	-6.94	109.19	119.60
1	1	3058	U	C2-N1-C1'	6.93	126.01	117.70
1	1	922	U	C2-N1-C1'	6.88	125.95	117.70
1	1	2724	U	N3-C2-O2	-6.87	117.39	122.20
1	1	3131	U	C2-N1-C1'	6.87	125.94	117.70
1	1	2861	U	C2-N1-C1'	6.87	125.94	117.70
1	1	2877	G	O4'-C1'-N9	6.84	113.68	108.20
1	1	2257	C	N3-C2-O2	-6.81	117.13	121.90
6	B	140	ASP	CB-CG-OD1	6.76	124.39	118.30
1	1	2898	G	C5-N7-C8	-6.75	100.93	104.30
1	1	2093	A	OP1-P-OP2	-6.74	109.49	119.60
1	1	2760	C	C2-N1-C1'	6.73	126.21	118.80
1	1	3019	U	N3-C2-O2	-6.73	117.49	122.20
1	1	292	U	C2-N1-C1'	6.69	125.73	117.70
1	1	1187	C	N3-C2-O2	-6.65	117.25	121.90
1	1	2313	A	OP1-P-OP2	-6.59	109.71	119.60
1	1	977	C	C2-N1-C1'	6.56	126.02	118.80
1	1	2112	U	N3-C2-O2	-6.55	117.61	122.20
1	1	1255	C	C2-N1-C1'	6.55	126.00	118.80
1	1	1082	U	OP1-P-OP2	-6.53	109.80	119.60
3	3	98	C	C6-N1-C1'	-6.53	112.96	120.80
1	1	2970	C	C6-N1-C2	-6.53	117.69	120.30
1	1	3217	C	C6-N1-C1'	-6.46	113.05	120.80
1	1	1047	A	OP1-P-OP2	-6.43	109.96	119.60
1	1	2825	C	C2-N1-C1'	6.38	125.81	118.80
1	1	406	G	O4'-C1'-N9	6.37	113.30	108.20
1	1	3023	U	C2-N1-C1'	6.28	125.24	117.70
2	2	82	U	N1-C2-O2	6.26	127.18	122.80
1	1	1604	G	C4-N9-C1'	6.25	134.63	126.50
1	1	2235	C	N1-C2-O2	6.22	122.63	118.90
1	1	2869	U	N1-C2-O2	6.20	127.14	122.80
1	1	2541	U	P-O3'-C3'	6.17	127.11	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	835	G	O4'-C1'-N9	6.17	113.13	108.20
1	1	2550	U	N1-C2-O2	6.16	127.11	122.80
1	1	2898	G	C6-C5-N7	-6.15	126.71	130.40
1	1	3153	U	C6-N1-C1'	-6.12	112.63	121.20
1	1	2676	A	O4'-C1'-N9	6.12	113.09	108.20
1	1	3058	U	N1-C2-O2	6.10	127.07	122.80
2	2	82	U	N3-C2-O2	-6.08	117.94	122.20
1	1	1561	G	O4'-C1'-N9	6.07	113.06	108.20
1	1	1117	G	O4'-C1'-N9	6.03	113.03	108.20
1	1	961	C	C2-N1-C1'	6.03	125.43	118.80
1	1	1283	C	N3-C2-O2	-6.02	117.68	121.90
1	1	1299	U	C2-N1-C1'	6.00	124.89	117.70
1	1	1187	C	N1-C2-O2	5.91	122.44	118.90
1	1	292	U	N3-C2-O2	-5.90	118.07	122.20
1	1	3181	C	N1-C2-O2	5.89	122.43	118.90
1	1	1400	G	N3-C4-N9	-5.88	122.47	126.00
1	1	2979	U	C6-N1-C1'	-5.86	112.99	121.20
1	1	2825	C	C2-N3-C4	5.84	122.82	119.90
1	1	2759	U	N1-C2-O2	5.83	126.88	122.80
1	1	2112	U	C2-N1-C1'	5.80	124.66	117.70
1	1	1103	A	P-O3'-C3'	5.79	126.65	119.70
48	v	104	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	1	3058	U	N3-C2-O2	-5.78	118.16	122.20
1	1	2550	U	N3-C2-O2	-5.77	118.16	122.20
1	1	648	C	N1-C2-O2	5.75	122.35	118.90
1	1	2869	U	N3-C2-O2	-5.74	118.18	122.20
1	1	2549	G	C4-N9-C1'	5.74	133.97	126.50
1	1	3019	U	C2-N1-C1'	5.74	124.59	117.70
1	1	958	C	C2-N1-C1'	5.73	125.11	118.80
31	b	143	LEU	CA-CB-CG	5.73	128.47	115.30
1	1	2235	C	N3-C2-O2	-5.72	117.90	121.90
1	1	3306	U	C2-N1-C1'	5.71	124.55	117.70
1	1	1604	G	C8-N9-C1'	-5.70	119.59	127.00
25	V	46	LEU	C-N-CA	-5.70	107.46	121.70
1	1	244	G	N3-C4-N9	5.69	129.41	126.00
1	1	3181	C	C2-N1-C1'	5.68	125.04	118.80
1	1	2899	C	C2-N1-C1'	5.67	125.04	118.80
2	2	64	U	N3-C2-O2	-5.66	118.24	122.20
1	1	1278	A	C8-N9-C4	-5.64	103.55	105.80
1	1	922	U	N1-C2-O2	5.64	126.75	122.80
1	1	1496	C	C6-N1-C1'	-5.63	114.04	120.80
1	1	2629	U	N3-C2-O2	-5.62	118.26	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1227	C	C6-N1-C2	-5.60	118.06	120.30
1	1	2825	C	C5-C6-N1	5.60	123.80	121.00
1	1	2979	U	C5-C6-N1	5.60	125.50	122.70
1	1	2428	U	C2-N1-C1'	5.60	124.42	117.70
1	1	3153	U	C5-C6-N1	5.59	125.50	122.70
1	1	2759	U	C6-N1-C1'	-5.58	113.39	121.20
1	1	1724	U	O4'-C1'-N1	5.57	112.66	108.20
1	1	2248	C	C2-N1-C1'	5.55	124.91	118.80
1	1	2550	U	C2-N1-C1'	5.52	124.33	117.70
1	1	2629	U	N1-C2-O2	5.52	126.66	122.80
2	2	156	U	C2-N1-C1'	5.51	124.31	117.70
1	1	3153	U	N3-C2-O2	-5.51	118.34	122.20
1	1	2624	G	N3-C4-N9	-5.50	122.70	126.00
1	1	2868	U	OP1-P-O3'	5.50	117.31	105.20
1	1	2722	U	C2-N1-C1'	5.50	124.30	117.70
19	P	22	LEU	CB-CG-CD1	-5.49	101.66	111.00
1	1	284	A	P-O3'-C3'	5.48	126.28	119.70
1	1	1567	U	C6-N1-C1'	-5.48	113.53	121.20
1	1	2094	C	N1-C2-O2	5.48	122.19	118.90
1	1	2760	C	N1-C2-O2	5.46	122.18	118.90
1	1	3306	U	N1-C2-O2	5.46	126.62	122.80
1	1	1227	C	N1-C2-O2	5.45	122.17	118.90
1	1	995	U	N1-C2-O2	5.45	126.61	122.80
1	1	3181	C	N3-C2-O2	-5.44	118.09	121.90
1	1	2248	C	N3-C2-O2	-5.43	118.10	121.90
1	1	2772	C	C2-N1-C1'	5.43	124.78	118.80
1	1	40	A	P-O3'-C3'	5.39	126.17	119.70
1	1	995	U	C2-N1-C1'	5.36	124.14	117.70
1	1	1199	C	C2-N1-C1'	5.36	124.69	118.80
1	1	3078	U	P-O3'-C3'	5.35	126.12	119.70
1	1	1124	U	N3-C2-O2	-5.34	118.46	122.20
1	1	1878	G	C4-N9-C1'	5.34	133.44	126.50
1	1	545	U	N1-C2-O2	5.34	126.54	122.80
1	1	1568	U	P-O3'-C3'	5.33	126.09	119.70
1	1	2862	U	N3-C2-O2	-5.31	118.48	122.20
31	b	170	LEU	CA-CB-CG	5.31	127.51	115.30
1	1	648	C	C2-N1-C1'	5.30	124.63	118.80
1	1	1400	G	N3-C4-C5	5.29	131.25	128.60
1	1	1770	G	C4-N9-C1'	5.29	133.37	126.50
1	1	2257	C	C6-N1-C2	-5.28	118.19	120.30
1	1	977	C	C6-N1-C2	-5.28	118.19	120.30
1	1	2701	U	C5-C6-N1	5.27	125.34	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1235	U	C5-C4-O4	-5.27	122.74	125.90
1	1	1227	C	C6-N1-C1'	-5.26	114.48	120.80
1	1	244	G	C4-N9-C1'	5.26	133.34	126.50
1	1	1604	G	N3-C4-N9	5.26	129.15	126.00
1	1	1255	C	C6-N1-C1'	-5.25	114.49	120.80
1	1	1355	A	P-O3'-C3'	5.24	125.99	119.70
1	1	1283	C	N1-C2-O2	5.24	122.04	118.90
1	1	2406	C	C2-N1-C1'	5.24	124.56	118.80
1	1	2112	U	N1-C2-O2	5.23	126.46	122.80
1	1	1187	C	C6-N1-C1'	-5.22	114.53	120.80
1	1	2629	U	C2-N1-C1'	5.22	123.96	117.70
1	1	2861	U	N1-C2-O2	5.22	126.45	122.80
1	1	244	G	C6-C5-N7	-5.19	127.28	130.40
1	1	2257	C	C6-N1-C1'	-5.19	114.57	120.80
1	1	1495	U	N1-C2-N3	5.18	118.01	114.90
1	1	1278	A	O4'-C1'-N9	5.18	112.35	108.20
1	1	1255	C	N3-C2-O2	-5.18	118.28	121.90
1	1	2759	U	N3-C2-O2	-5.17	118.58	122.20
1	1	2954	U	OP2-P-O3'	5.17	116.58	105.20
1	1	2619	G	OP1-P-OP2	-5.17	111.85	119.60
1	1	161	G	N7-C8-N9	5.14	115.67	113.10
1	1	2528	G	O4'-C1'-N9	5.12	112.30	108.20
1	1	3116	G	N1-C6-O6	-5.12	116.83	119.90
1	1	1201	C	C2-N1-C1'	5.11	124.43	118.80
1	1	2513	U	P-O3'-C3'	5.11	125.83	119.70
1	1	720	A	P-O3'-C3'	5.10	125.82	119.70
1	1	2760	C	N3-C2-O2	-5.10	118.33	121.90
1	1	922	U	N3-C2-O2	-5.09	118.64	122.20
1	1	40	A	OP1-P-O3'	5.09	116.39	105.20
1	1	2278	C	C2-N1-C1'	5.09	124.40	118.80
1	1	3155	U	C2-N1-C1'	5.08	123.80	117.70
2	2	156	U	N3-C2-O2	-5.08	118.64	122.20
1	1	1123	U	C2-N1-C1'	5.06	123.78	117.70
1	1	3217	C	C6-N1-C2	-5.05	118.28	120.30
1	1	2537	U	P-O3'-C3'	5.04	125.75	119.70
1	1	3350	C	C2-N1-C1'	5.04	124.35	118.80
1	1	2803	A	N1-C6-N6	-5.04	115.58	118.60
1	1	1269	U	C2-N1-C1'	5.03	123.73	117.70
1	1	3027	A	O4'-C1'-N9	5.03	112.22	108.20
1	1	2699	G	N9-C4-C5	-5.02	103.39	105.40
1	1	1763	U	N3-C2-O2	-5.01	118.69	122.20
1	1	1302	A	OP1-P-O3'	5.01	116.22	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	41	G	C4-N9-C1'	5.01	133.01	126.50
1	1	2542	U	O4'-C1'-N1	5.01	112.20	108.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	L	46	ILE	Peptide
31	b	258	GLU	Peptide
37	h	83	LYS	Peptide
44	q	51	LYS	Peptide
48	v	112	ASP	Peptide
48	v	195	PRO	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	7	95/105 (90%)	93 (98%)	2 (2%)	0	100	100
5	A	211/254 (83%)	198 (94%)	13 (6%)	0	100	100
6	B	384/387 (99%)	368 (96%)	16 (4%)	0	100	100
7	C	359/362 (99%)	348 (97%)	11 (3%)	0	100	100
8	D	253/297 (85%)	241 (95%)	12 (5%)	0	100	100
9	E	152/176 (86%)	145 (95%)	7 (5%)	0	100	100
10	F	220/244 (90%)	216 (98%)	4 (2%)	0	100	100
11	G	231/256 (90%)	217 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	H	189/191 (99%)	180 (95%)	9 (5%)	0	100	100
13	I	109/166 (66%)	103 (94%)	6 (6%)	0	100	100
14	J	167/174 (96%)	153 (92%)	14 (8%)	0	100	100
15	L	185/199 (93%)	175 (95%)	9 (5%)	1 (0%)	29	61
16	M	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
17	N	201/204 (98%)	190 (94%)	11 (6%)	0	100	100
18	O	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
19	P	181/184 (98%)	173 (96%)	8 (4%)	0	100	100
20	Q	132/186 (71%)	128 (97%)	4 (3%)	0	100	100
21	R	154/189 (82%)	154 (100%)	0	0	100	100
22	S	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
23	T	115/160 (72%)	106 (92%)	9 (8%)	0	100	100
24	U	104/121 (86%)	95 (91%)	9 (9%)	0	100	100
25	V	134/137 (98%)	130 (97%)	4 (3%)	0	100	100
26	W	232/236 (98%)	217 (94%)	15 (6%)	0	100	100
27	X	139/142 (98%)	130 (94%)	9 (6%)	0	100	100
28	Y	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
29	Z	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
30	a	91/149 (61%)	84 (92%)	7 (8%)	0	100	100
31	b	508/647 (78%)	490 (96%)	18 (4%)	0	100	100
32	c	88/175 (50%)	87 (99%)	1 (1%)	0	100	100
33	d	105/113 (93%)	101 (96%)	4 (4%)	0	100	100
34	e	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
35	f	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
36	g	110/121 (91%)	107 (97%)	3 (3%)	0	100	100
37	h	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
38	i	97/100 (97%)	91 (94%)	6 (6%)	0	100	100
39	j	85/88 (97%)	81 (95%)	4 (5%)	0	100	100
40	k	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
41	l	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
42	m	465/519 (90%)	442 (95%)	23 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	p	89/92 (97%)	82 (92%)	7 (8%)	0	100	100
44	q	120/165 (73%)	109 (91%)	11 (9%)	0	100	100
45	r	224/261 (86%)	217 (97%)	7 (3%)	0	100	100
46	s	65/520 (12%)	63 (97%)	2 (3%)	0	100	100
47	u	148/199 (74%)	144 (97%)	4 (3%)	0	100	100
48	v	283/344 (82%)	271 (96%)	12 (4%)	0	100	100
49	w	175/203 (86%)	166 (95%)	9 (5%)	0	100	100
50	x	476/514 (93%)	439 (92%)	37 (8%)	0	100	100
51	y	226/245 (92%)	210 (93%)	16 (7%)	0	100	100
52	z	73/106 (69%)	71 (97%)	2 (3%)	0	100	100
All	All	8600/10189 (84%)	8202 (95%)	397 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	L	61	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	7	81/88 (92%)	81 (100%)	0	100	100
5	A	166/196 (85%)	166 (100%)	0	100	100
6	B	322/323 (100%)	321 (100%)	1 (0%)	92	98
7	C	288/289 (100%)	288 (100%)	0	100	100
8	D	216/245 (88%)	216 (100%)	0	100	100
9	E	134/153 (88%)	133 (99%)	1 (1%)	84	95
10	F	186/205 (91%)	186 (100%)	0	100	100
11	G	191/208 (92%)	189 (99%)	2 (1%)	76	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	H	171/171 (100%)	171 (100%)	0	100	100
13	I	99/141 (70%)	99 (100%)	0	100	100
14	J	147/150 (98%)	145 (99%)	2 (1%)	67	89
15	L	149/159 (94%)	149 (100%)	0	100	100
16	M	108/109 (99%)	108 (100%)	0	100	100
17	N	175/176 (99%)	175 (100%)	0	100	100
18	O	160/162 (99%)	160 (100%)	0	100	100
19	P	145/146 (99%)	145 (100%)	0	100	100
20	Q	110/151 (73%)	110 (100%)	0	100	100
21	R	129/154 (84%)	128 (99%)	1 (1%)	81	94
22	S	155/156 (99%)	155 (100%)	0	100	100
23	T	102/137 (74%)	101 (99%)	1 (1%)	76	92
24	U	93/107 (87%)	93 (100%)	0	100	100
25	V	104/105 (99%)	104 (100%)	0	100	100
26	W	211/213 (99%)	210 (100%)	1 (0%)	88	96
27	X	117/118 (99%)	117 (100%)	0	100	100
28	Y	109/110 (99%)	109 (100%)	0	100	100
29	Z	115/116 (99%)	115 (100%)	0	100	100
30	a	76/119 (64%)	76 (100%)	0	100	100
31	b	459/573 (80%)	456 (99%)	3 (1%)	84	95
32	c	84/153 (55%)	84 (100%)	0	100	100
33	d	94/97 (97%)	93 (99%)	1 (1%)	73	92
34	e	109/111 (98%)	109 (100%)	0	100	100
35	f	90/91 (99%)	90 (100%)	0	100	100
36	g	95/103 (92%)	95 (100%)	0	100	100
37	h	104/105 (99%)	104 (100%)	0	100	100
38	i	81/82 (99%)	80 (99%)	1 (1%)	71	91
39	j	70/71 (99%)	70 (100%)	0	100	100
40	k	68/69 (99%)	68 (100%)	0	100	100
41	l	45/46 (98%)	45 (100%)	0	100	100
42	m	413/459 (90%)	411 (100%)	2 (0%)	88	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	p	71/72 (99%)	71 (100%)	0	100	100
44	q	105/136 (77%)	105 (100%)	0	100	100
45	r	203/229 (89%)	203 (100%)	0	100	100
46	s	62/445 (14%)	62 (100%)	0	100	100
47	u	133/180 (74%)	133 (100%)	0	100	100
48	v	258/309 (84%)	258 (100%)	0	100	100
49	w	158/179 (88%)	157 (99%)	1 (1%)	86	96
50	x	428/450 (95%)	428 (100%)	0	100	100
51	y	195/211 (92%)	195 (100%)	0	100	100
52	z	69/95 (73%)	69 (100%)	0	100	100
All	All	7453/8673 (86%)	7436 (100%)	17 (0%)	93	98

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	332	ARG
9	E	46	ARG
11	G	240	ASN
11	G	251	LYS
14	J	16	LYS
14	J	29	ARG
21	R	151	ARG
23	T	146	ASN
26	W	214	LYS
31	b	168	ARG
31	b	395	ARG
31	b	639	ARG
33	d	86	LYS
38	i	98	ARG
42	m	10	ARG
42	m	57	ARG
49	w	55	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	79	ASN

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Mol	Chain	Res	Type
6	B	231	HIS
12	H	59	ASN
12	H	102	ASN
14	J	109	HIS
21	R	134	HIS
22	S	88	HIS
32	c	24	ASN
40	k	10	GLN
44	q	65	GLN
45	r	256	ASN
48	v	99	ASN
48	v	187	GLN
49	w	180	ASN
49	w	198	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3050/3396 (89%)	698 (22%)	50 (1%)
2	2	157/158 (99%)	33 (21%)	1 (0%)
3	3	120/121 (99%)	21 (17%)	1 (0%)
All	All	3327/3675 (90%)	752 (22%)	52 (1%)

All (752) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	U
1	1	14	U
1	1	26	A
1	1	40	A
1	1	41	G
1	1	49	A
1	1	58	G
1	1	60	A
1	1	65	A
1	1	66	A
1	1	75	G
1	1	92	G
1	1	95	A
1	1	96	G
1	1	110	G

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Mol	Chain	Res	Type
1	1	116	A
1	1	118	U
1	1	122	A
1	1	133	U
1	1	135	C
1	1	136	G
1	1	146	U
1	1	150	A
1	1	156	G
1	1	157	A
1	1	159	A
1	1	161	G
1	1	172	G
1	1	181	U
1	1	187	A
1	1	190	U
1	1	197	G
1	1	200	C
1	1	206	G
1	1	210	U
1	1	213	A
1	1	218	G
1	1	219	A
1	1	220	G
1	1	240	U
1	1	241	G
1	1	243	G
1	1	245	U
1	1	247	C
1	1	249	U
1	1	250	U
1	1	251	G
1	1	252	U
1	1	257	U
1	1	265	A
1	1	266	A
1	1	269	G
1	1	284	A
1	1	285	A
1	1	286	U
1	1	295	A
1	1	305	U

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Mol	Chain	Res	Type
1	1	307	A
1	1	308	A
1	1	323	A
1	1	329	U
1	1	337	G
1	1	368	G
1	1	370	U
1	1	376	G
1	1	395	A
1	1	398	A
1	1	399	A
1	1	401	U
1	1	402	A
1	1	403	C
1	1	421	G
1	1	422	A
1	1	438	A
1	1	439	C
1	1	440	A
1	1	503	C
1	1	518	G
1	1	521	A
1	1	523	A
1	1	535	G
1	1	544	C
1	1	546	C
1	1	547	G
1	1	548	G
1	1	550	A
1	1	552	G
1	1	556	U
1	1	557	A
1	1	558	U
1	1	559	A
1	1	564	G
1	1	569	A
1	1	578	A
1	1	579	G
1	1	582	G
1	1	592	A
1	1	597	G
1	1	600	G

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Mol	Chain	Res	Type
1	1	604	G
1	1	611	A
1	1	620	U
1	1	621	A
1	1	629	U
1	1	634	C
1	1	635	G
1	1	636	C
1	1	637	C
1	1	643	U
1	1	646	A
1	1	647	A
1	1	668	G
1	1	677	A
1	1	681	U
1	1	690	A
1	1	691	A
1	1	699	A
1	1	712	G
1	1	715	A
1	1	716	A
1	1	719	U
1	1	720	A
1	1	721	G
1	1	722	G
1	1	728	G
1	1	742	G
1	1	743	C
1	1	758	C
1	1	762	U
1	1	765	C
1	1	767	U
1	1	768	C
1	1	771	A
1	1	776	U
1	1	777	U
1	1	779	G
1	1	780	A
1	1	785	G
1	1	808	A
1	1	816	A
1	1	817	A

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Mol	Chain	Res	Type
1	1	830	A
1	1	835	G
1	1	837	A
1	1	845	G
1	1	849	C
1	1	850	U
1	1	861	C
1	1	874	U
1	1	875	G
1	1	879	U
1	1	880	G
1	1	895	A
1	1	896	A
1	1	907	G
1	1	908	G
1	1	909	G
1	1	914	A
1	1	916	G
1	1	917	A
1	1	921	A
1	1	923	C
1	1	924	G
1	1	925	A
1	1	936	A
1	1	944	C
1	1	958	C
1	1	971	G
1	1	974	G
1	1	976	U
1	1	977	C
1	1	978	G
1	1	979	U
1	1	980	A
1	1	981	U
1	1	991	G
1	1	992	A
1	1	994	G
1	1	995	U
1	1	996	A
1	1	997	A
1	1	998	A
1	1	1000	C

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Mol	Chain	Res	Type
1	1	1003	A
1	1	1048	A
1	1	1049	C
1	1	1050	U
1	1	1051	U
1	1	1055	A
1	1	1057	A
1	1	1058	U
1	1	1059	G
1	1	1063	G
1	1	1064	A
1	1	1065	A
1	1	1071	U
1	1	1072	G
1	1	1084	A
1	1	1085	A
1	1	1095	U
1	1	1097	G
1	1	1098	A
1	1	1103	A
1	1	1104	G
1	1	1105	A
1	1	1107	C
1	1	1108	U
1	1	1111	U
1	1	1112	A
1	1	1115	G
1	1	1117	G
1	1	1118	C
1	1	1127	G
1	1	1128	U
1	1	1129	A
1	1	1130	A
1	1	1132	C
1	1	1143	A
1	1	1144	U
1	1	1152	G
1	1	1153	A
1	1	1154	A
1	1	1159	A
1	1	1160	C
1	1	1179	A

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Mol	Chain	Res	Type
1	1	1180	A
1	1	1181	U
1	1	1182	A
1	1	1192	C
1	1	1193	A
1	1	1196	C
1	1	1197	A
1	1	1198	C
1	1	1199	C
1	1	1200	A
1	1	1201	C
1	1	1202	A
1	1	1204	A
1	1	1208	U
1	1	1209	G
1	1	1221	A
1	1	1222	G
1	1	1223	A
1	1	1227	C
1	1	1235	U
1	1	1241	U
1	1	1242	G
1	1	1245	A
1	1	1250	G
1	1	1252	A
1	1	1258	U
1	1	1263	A
1	1	1271	A
1	1	1272	C
1	1	1278	A
1	1	1279	C
1	1	1286	A
1	1	1287	A
1	1	1302	A
1	1	1303	A
1	1	1304	A
1	1	1305	U
1	1	1307	G
1	1	1313	G
1	1	1325	U
1	1	1330	A
1	1	1348	U

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Mol	Chain	Res	Type
1	1	1349	G
1	1	1352	A
1	1	1354	G
1	1	1355	A
1	1	1356	U
1	1	1357	G
1	1	1386	A
1	1	1399	A
1	1	1400	G
1	1	1408	G
1	1	1417	G
1	1	1419	A
1	1	1431	G
1	1	1434	G
1	1	1437	C
1	1	1446	A
1	1	1469	C
1	1	1483	G
1	1	1484	U
1	1	1487	G
1	1	1503	A
1	1	1508	C
1	1	1527	C
1	1	1533	U
1	1	1555	U
1	1	1556	C
1	1	1561	G
1	1	1562	C
1	1	1566	A
1	1	1567	U
1	1	1568	U
1	1	1569	U
1	1	1573	G
1	1	1580	A
1	1	1581	C
1	1	1582	C
1	1	1583	A
1	1	1587	A
1	1	1589	A
1	1	1590	G
1	1	1593	A
1	1	1613	A

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Mol	Chain	Res	Type
1	1	1620	U
1	1	1629	U
1	1	1631	C
1	1	1639	C
1	1	1643	A
1	1	1657	C
1	1	1677	G
1	1	1717	U
1	1	1724	U
1	1	1725	C
1	1	1741	A
1	1	1742	U
1	1	1750	A
1	1	1751	G
1	1	1761	C
1	1	1762	C
1	1	1763	U
1	1	1764	U
1	1	1765	U
1	1	1770	G
1	1	1775	G
1	1	1780	G
1	1	1796	G
1	1	1797	A
1	1	1810	A
1	1	1813	A
1	1	1814	A
1	1	1815	U
1	1	1816	A
1	1	1817	G
1	1	1820	U
1	1	1821	U
1	1	1839	A
1	1	1842	A
1	1	1846	C
1	1	1847	A
1	1	1849	C
1	1	1850	A
1	1	1878	G
1	1	1880	U
1	1	1906	G
1	1	1909	A

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Mol	Chain	Res	Type
1	1	1935	G
1	1	1951	C
1	1	1952	G
1	1	1953	G
1	1	2094	C
1	1	2112	U
1	1	2113	A
1	1	2121	G
1	1	2122	G
1	1	2126	A
1	1	2131	A
1	1	2140	U
1	1	2149	A
1	1	2158	A
1	1	2169	G
1	1	2176	U
1	1	2193	U
1	1	2194	G
1	1	2195	C
1	1	2196	C
1	1	2198	A
1	1	2201	G
1	1	2205	U
1	1	2207	A
1	1	2209	U
1	1	2210	G
1	1	2212	C
1	1	2220	A
1	1	2222	A
1	1	2225	U
1	1	2239	G
1	1	2242	A
1	1	2243	A
1	1	2244	A
1	1	2246	G
1	1	2247	G
1	1	2248	C
1	1	2249	G
1	1	2250	G
1	1	2255	A
1	1	2256	A
1	1	2262	A

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Mol	Chain	Res	Type
1	1	2264	U
1	1	2267	C
1	1	2268	U
1	1	2269	U
1	1	2270	A
1	1	2271	A
1	1	2272	G
1	1	2278	C
1	1	2279	A
1	1	2280	A
1	1	2316	G
1	1	2317	A
1	1	2318	U
1	1	2334	U
1	1	2335	G
1	1	2336	U
1	1	2371	G
1	1	2388	U
1	1	2393	G
1	1	2397	A
1	1	2398	A
1	1	2401	A
1	1	2402	A
1	1	2404	A
1	1	2409	G
1	1	2410	U
1	1	2411	U
1	1	2412	G
1	1	2413	A
1	1	2414	G
1	1	2418	G
1	1	2442	G
1	1	2445	A
1	1	2502	A
1	1	2503	G
1	1	2504	U
1	1	2507	C
1	1	2509	U
1	1	2511	A
1	1	2512	C
1	1	2514	U
1	1	2522	G

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Mol	Chain	Res	Type
1	1	2528	G
1	1	2529	A
1	1	2530	G
1	1	2531	C
1	1	2532	U
1	1	2533	G
1	1	2537	U
1	1	2538	U
1	1	2540	A
1	1	2541	U
1	1	2542	U
1	1	2543	U
1	1	2544	U
1	1	2545	C
1	1	2546	C
1	1	2547	A
1	1	2548	C
1	1	2551	U
1	1	2552	C
1	1	2559	U
1	1	2561	A
1	1	2569	A
1	1	2570	U
1	1	2571	U
1	1	2572	C
1	1	2573	G
1	1	2576	G
1	1	2586	G
1	1	2593	A
1	1	2594	C
1	1	2606	G
1	1	2607	G
1	1	2613	U
1	1	2614	G
1	1	2615	G
1	1	2620	G
1	1	2621	G
1	1	2623	G
1	1	2624	G
1	1	2625	C
1	1	2627	C
1	1	2628	A

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Mol	Chain	Res	Type
1	1	2632	G
1	1	2634	U
1	1	2638	C
1	1	2640	A
1	1	2642	A
1	1	2643	A
1	1	2644	C
1	1	2645	G
1	1	2648	G
1	1	2650	U
1	1	2651	G
1	1	2652	U
1	1	2653	C
1	1	2654	C
1	1	2655	U
1	1	2656	A
1	1	2657	A
1	1	2658	G
1	1	2659	G
1	1	2674	A
1	1	2676	A
1	1	2677	G
1	1	2687	G
1	1	2688	U
1	1	2689	A
1	1	2690	G
1	1	2691	A
1	1	2692	A
1	1	2693	C
1	1	2695	A
1	1	2701	U
1	1	2702	A
1	1	2704	A
1	1	2705	A
1	1	2714	G
1	1	2715	A
1	1	2720	G
1	1	2721	A
1	1	2722	U
1	1	2725	U
1	1	2726	C
1	1	2728	G

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Mol	Chain	Res	Type
1	1	2730	G
1	1	2731	U
1	1	2732	G
1	1	2734	A
1	1	2740	A
1	1	2741	C
1	1	2752	U
1	1	2754	G
1	1	2756	C
1	1	2757	U
1	1	2761	G
1	1	2762	A
1	1	2763	U
1	1	2766	U
1	1	2767	U
1	1	2768	U
1	1	2770	G
1	1	2771	U
1	1	2772	C
1	1	2773	C
1	1	2777	G
1	1	2780	A
1	1	2788	C
1	1	2789	U
1	1	2790	A
1	1	2797	C
1	1	2798	C
1	1	2799	A
1	1	2801	A
1	1	2802	A
1	1	2803	A
1	1	2809	C
1	1	2810	C
1	1	2814	G
1	1	2815	G
1	1	2817	A
1	1	2819	A
1	1	2820	A
1	1	2821	C
1	1	2822	U
1	1	2823	G
1	1	2824	G

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Mol	Chain	Res	Type
1	1	2825	C
1	1	2826	U
1	1	2834	G
1	1	2839	G
1	1	2842	U
1	1	2843	U
1	1	2844	C
1	1	2845	A
1	1	2847	A
1	1	2856	G
1	1	2857	C
1	1	2858	U
1	1	2859	U
1	1	2860	U
1	1	2861	U
1	1	2863	G
1	1	2864	A
1	1	2866	U
1	1	2867	C
1	1	2868	U
1	1	2869	U
1	1	2872	A
1	1	2873	U
1	1	2874	G
1	1	2875	U
1	1	2876	C
1	1	2877	G
1	1	2878	G
1	1	2879	C
1	1	2887	A
1	1	2898	G
1	1	2899	C
1	1	2922	G
1	1	2923	U
1	1	2930	A
1	1	2935	U
1	1	2936	A
1	1	2945	G
1	1	2947	G
1	1	2952	G
1	1	2954	U
1	1	2955	U

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Mol	Chain	Res	Type
1	1	2957	G
1	1	2970	C
1	1	2971	A
1	1	2972	G
1	1	2978	U
1	1	2980	U
1	1	2981	U
1	1	2982	A
1	1	2983	C
1	1	2996	U
1	1	2997	G
1	1	3012	A
1	1	3017	A
1	1	3021	A
1	1	3022	G
1	1	3027	A
1	1	3029	A
1	1	3030	G
1	1	3032	A
1	1	3056	U
1	1	3058	U
1	1	3059	G
1	1	3074	G
1	1	3078	U
1	1	3079	U
1	1	3080	G
1	1	3086	A
1	1	3092	C
1	1	3093	C
1	1	3099	C
1	1	3100	U
1	1	3109	G
1	1	3122	A
1	1	3129	A
1	1	3130	A
1	1	3131	U
1	1	3142	A
1	1	3143	C
1	1	3156	U
1	1	3163	A
1	1	3164	C
1	1	3165	A

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Mol	Chain	Res	Type
1	1	3166	C
1	1	3167	A
1	1	3169	U
1	1	3170	A
1	1	3172	A
1	1	3173	G
1	1	3174	A
1	1	3176	G
1	1	3179	U
1	1	3181	C
1	1	3187	A
1	1	3196	U
1	1	3206	C
1	1	3207	U
1	1	3217	C
1	1	3218	A
1	1	3224	G
1	1	3229	G
1	1	3243	A
1	1	3244	A
1	1	3247	G
1	1	3253	G
1	1	3256	G
1	1	3259	U
1	1	3263	G
1	1	3270	U
1	1	3276	G
1	1	3279	A
1	1	3280	U
1	1	3281	U
1	1	3282	U
1	1	3289	G
1	1	3294	A
1	1	3303	G
1	1	3304	U
1	1	3313	U
1	1	3316	A
1	1	3320	A
1	1	3328	G
1	1	3341	U
1	1	3342	A
1	1	3345	G

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Mol	Chain	Res	Type
1	1	3350	C
1	1	3351	U
1	1	3352	U
1	1	3354	U
1	1	3355	U
1	1	3356	G
1	1	3359	A
1	1	3369	G
1	1	3378	C
1	1	3389	U
1	1	3396	U
2	2	34	U
2	2	35	C
2	2	50	C
2	2	51	G
2	2	59	A
2	2	60	U
2	2	62	C
2	2	63	G
2	2	78	G
2	2	79	A
2	2	80	A
2	2	81	U
2	2	82	U
2	2	83	C
2	2	84	C
2	2	86	U
2	2	87	G
2	2	88	A
2	2	89	A
2	2	90	U
2	2	95	G
2	2	96	A
2	2	97	A
2	2	104	A
2	2	106	C
2	2	110	C
2	2	111	A
2	2	123	G
2	2	124	G
2	2	125	U
2	2	138	A

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Mol	Chain	Res	Type
2	2	152	G
2	2	158	U
3	3	7	G
3	3	16	U
3	3	52	G
3	3	53	U
3	3	54	U
3	3	64	A
3	3	65	G
3	3	73	C
3	3	74	C
3	3	76	A
3	3	83	U
3	3	84	A
3	3	86	U
3	3	87	G
3	3	98	C
3	3	99	G
3	3	100	C
3	3	102	A
3	3	103	A
3	3	112	G
3	3	121	U

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	40	A
1	1	160	G
1	1	284	A
1	1	646	A
1	1	720	A
1	1	761	A
1	1	849	C
1	1	916	G
1	1	1047	A
1	1	1064	A
1	1	1097	G
1	1	1102	A
1	1	1103	A
1	1	1128	U
1	1	1129	A

Continued on next page...

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Mol	Chain	Res	Type
1	1	1159	A
1	1	1192	C
1	1	1241	U
1	1	1302	A
1	1	1329	U
1	1	1355	A
1	1	1567	U
1	1	1568	U
1	1	1816	A
1	1	1820	U
1	1	1842	A
1	1	2209	U
1	1	2263	C
1	1	2269	U
1	1	2317	A
1	1	2397	A
1	1	2410	U
1	1	2501	U
1	1	2511	A
1	1	2513	U
1	1	2537	U
1	1	2541	U
1	1	2593	A
1	1	2651	G
1	1	2753	G
1	1	2808	A
1	1	2824	G
1	1	2868	U
1	1	2954	U
1	1	3021	A
1	1	3078	U
1	1	3121	U
1	1	3228	C
1	1	3340	G
1	1	3350	C
2	2	123	G
3	3	52	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
53	GDP	m	601	54	24,30,30	1.06	1 (4%)	30,47,47	1.39	5 (16%)

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
53	GDP	m	601	54	-	3/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	m	601	GDP	C6-N1	-3.20	1.33	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	m	601	GDP	PA-O3A-PB	-3.98	119.16	132.83
53	m	601	GDP	C5-C6-N1	2.75	118.82	113.95
53	m	601	GDP	C8-N7-C5	2.34	107.45	102.99
53	m	601	GDP	C3'-C2'-C1'	2.30	104.45	100.98
53	m	601	GDP	O6-C6-C5	-2.11	120.25	124.37

There are no chirality outliers.

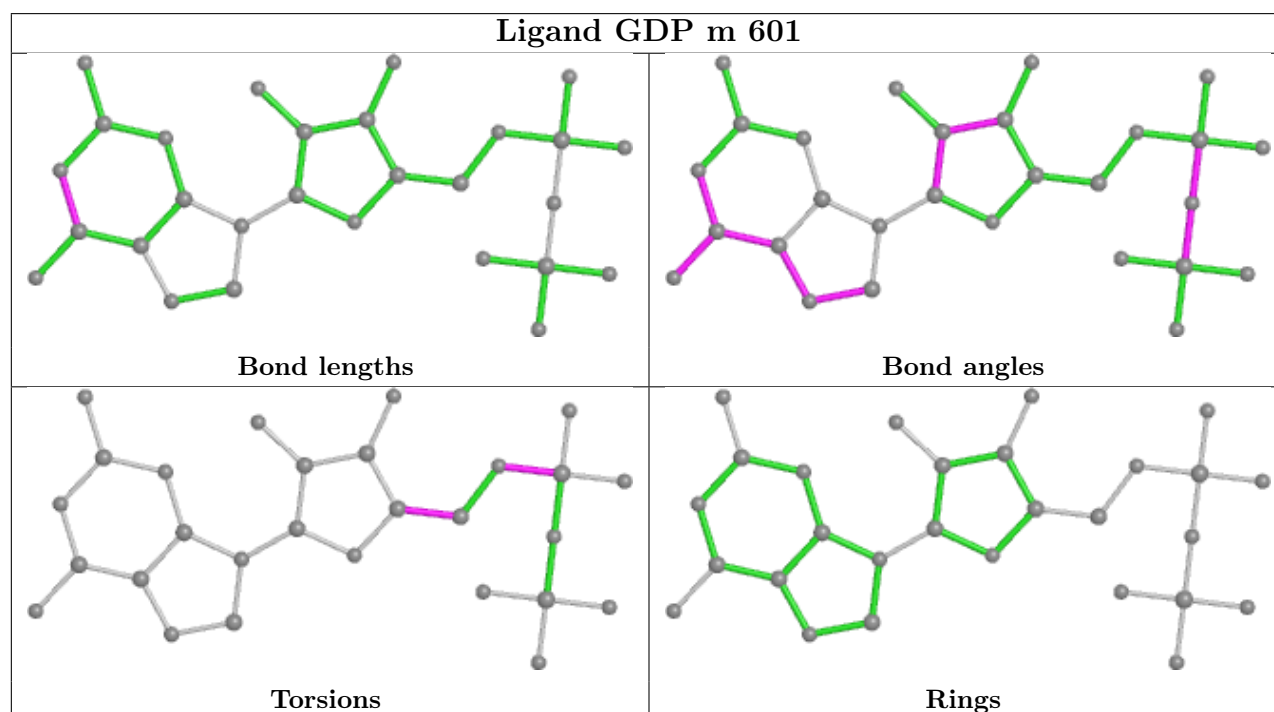
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	m	601	GDP	C3'-C4'-C5'-O5'
53	m	601	GDP	O4'-C4'-C5'-O5'
53	m	601	GDP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	16:PHE	C	17:LEU	N	1.20

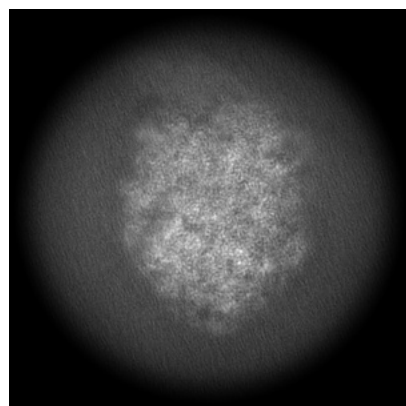
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26485. These allow visual inspection of the internal detail of the map and identification of artifacts.

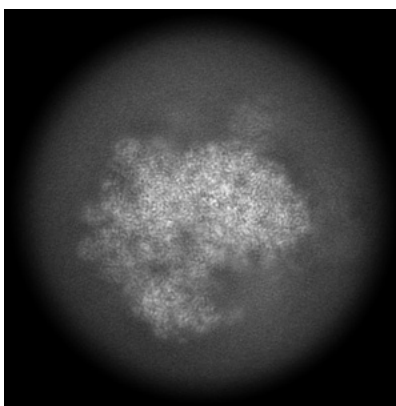
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

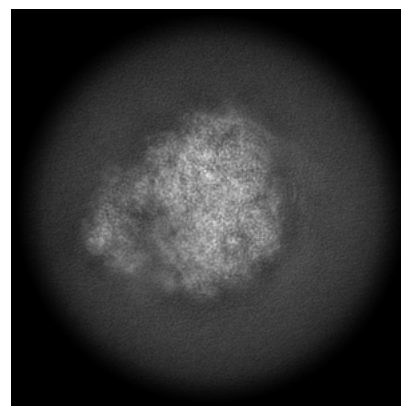
6.1.1 Primary map



X

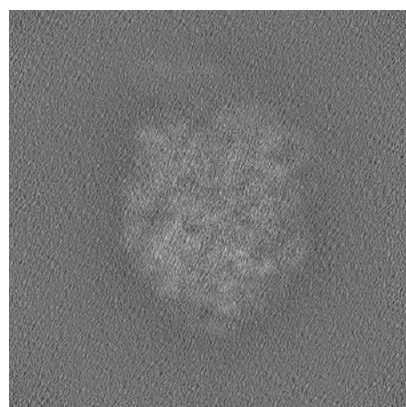


Y

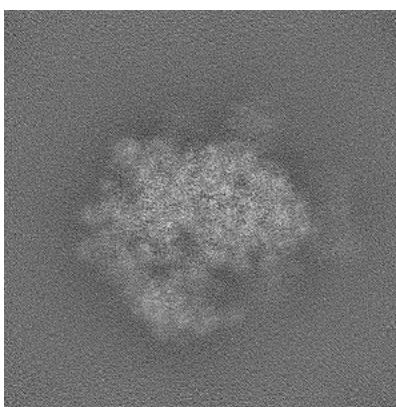


Z

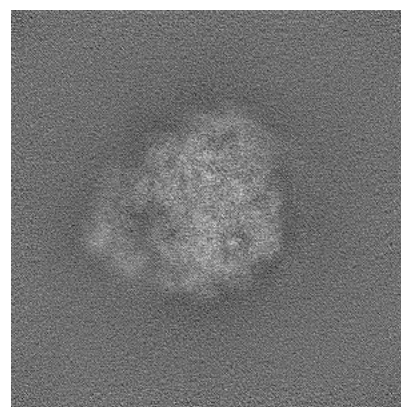
6.1.2 Raw map



X



Y

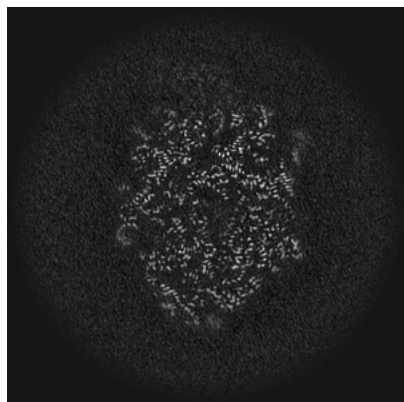


Z

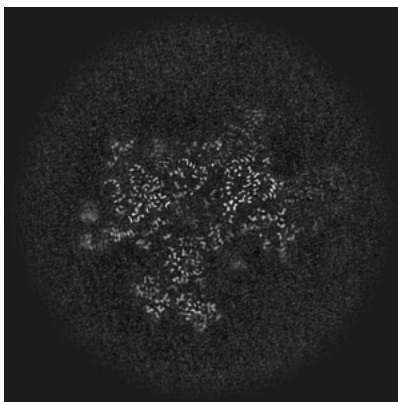
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

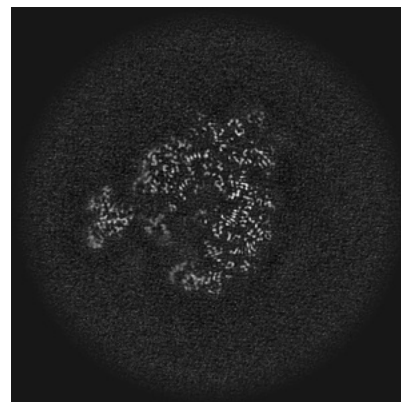
6.2.1 Primary map



X Index: 256

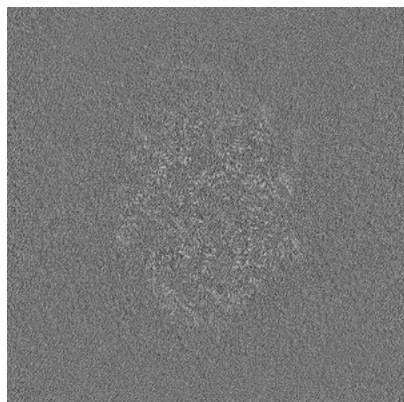


Y Index: 256

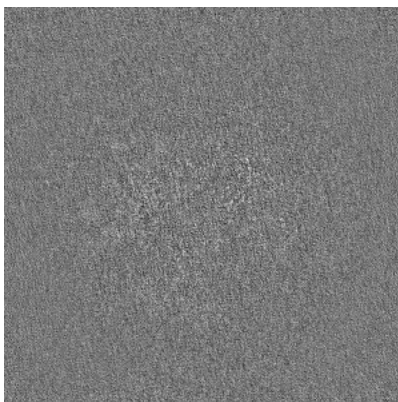


Z Index: 256

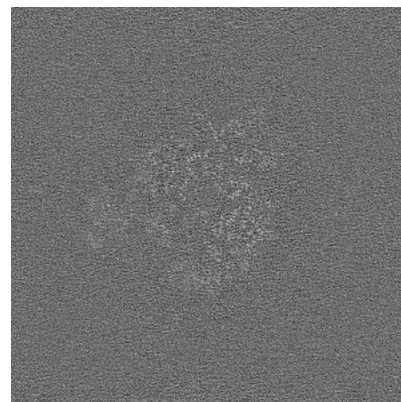
6.2.2 Raw map



X Index: 256



Y Index: 256

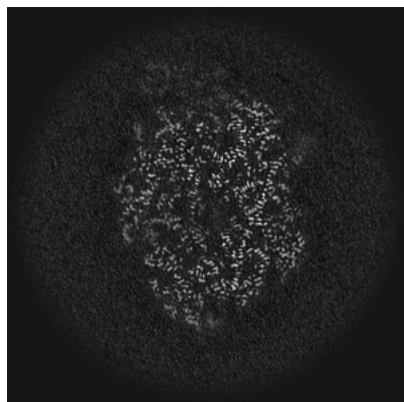


Z Index: 256

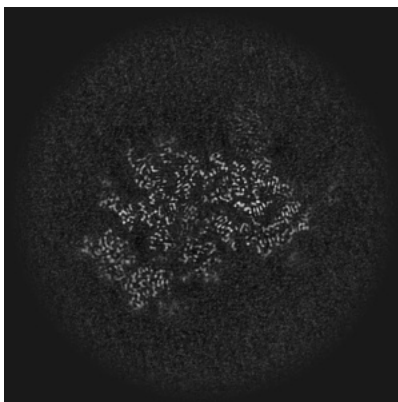
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

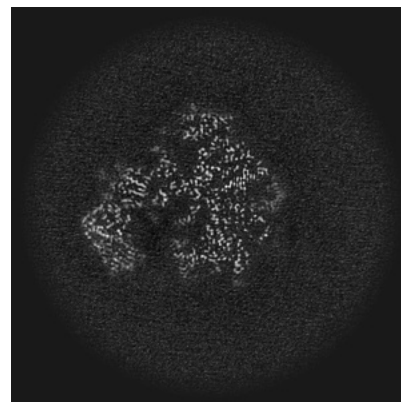
6.3.1 Primary map



X Index: 249

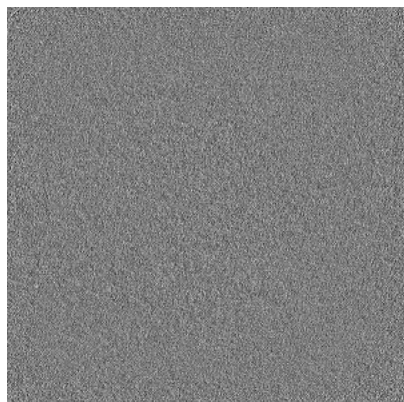


Y Index: 289

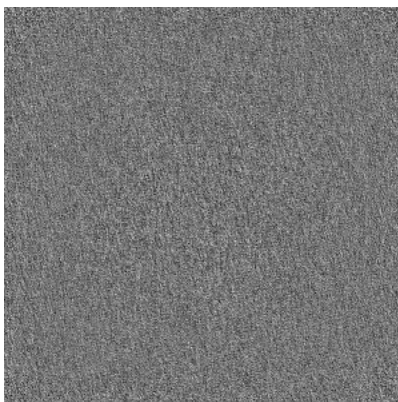


Z Index: 197

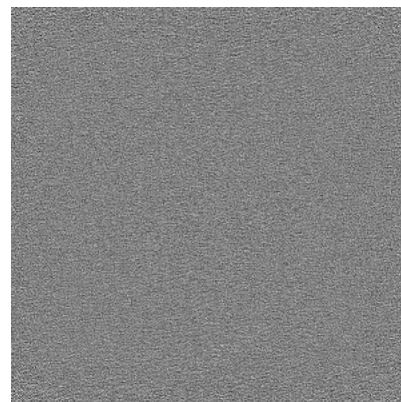
6.3.2 Raw map



X Index: 0



Y Index: 0

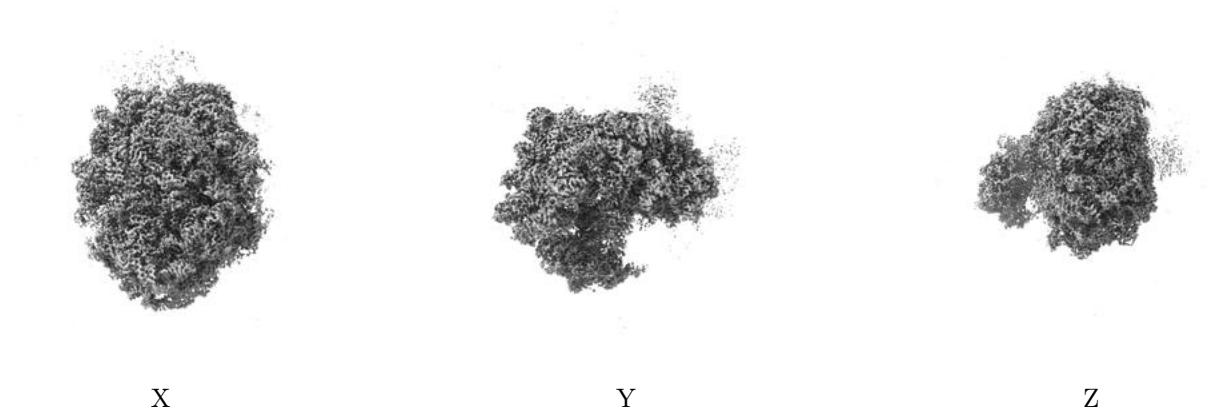


Z Index: 0

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

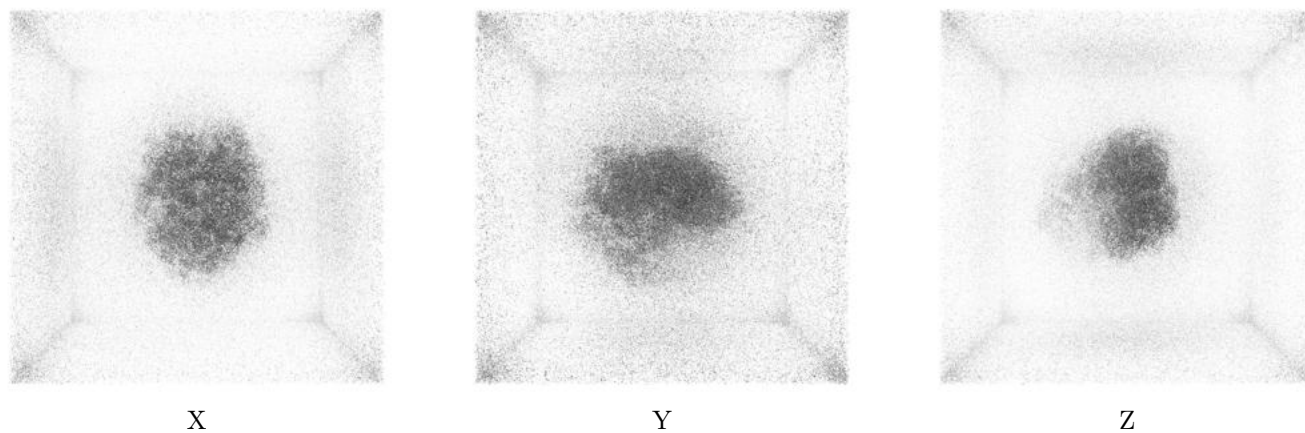
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

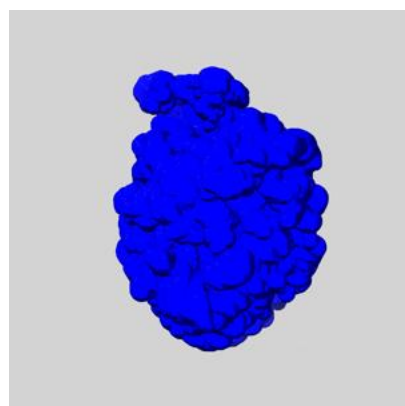
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

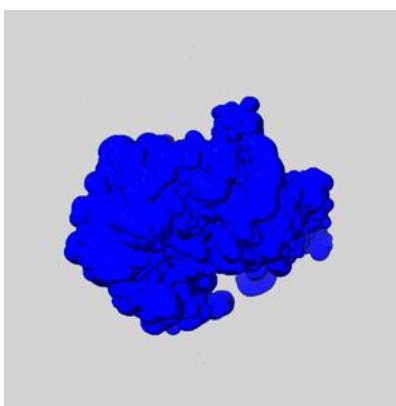
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

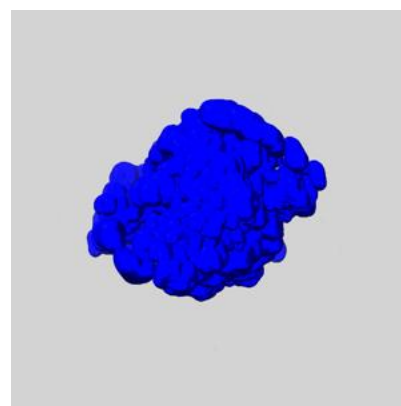
6.5.1 emd_26485_msk_1.map [i](#)



X



Y

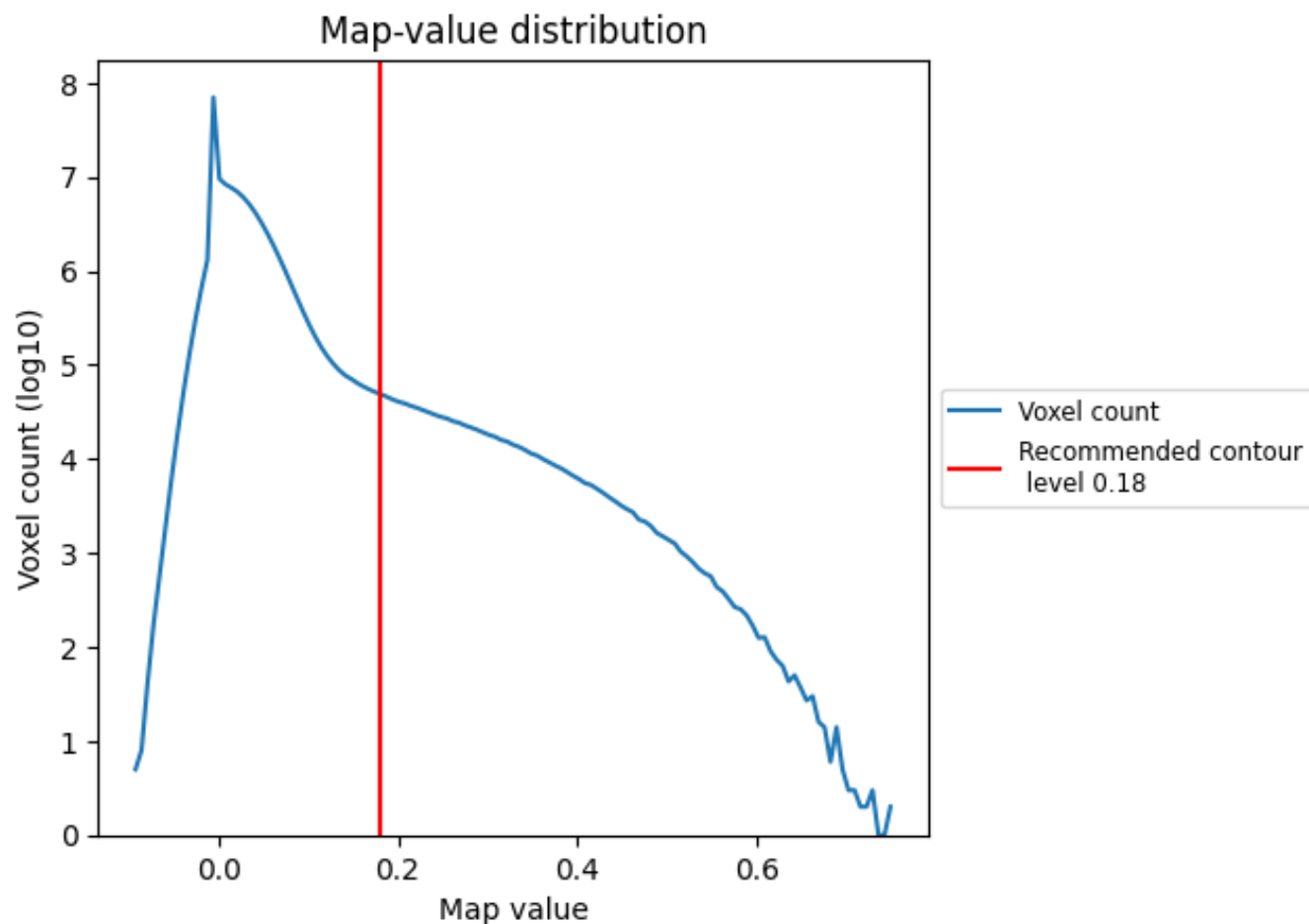


Z

7 Map analysis [i](#)

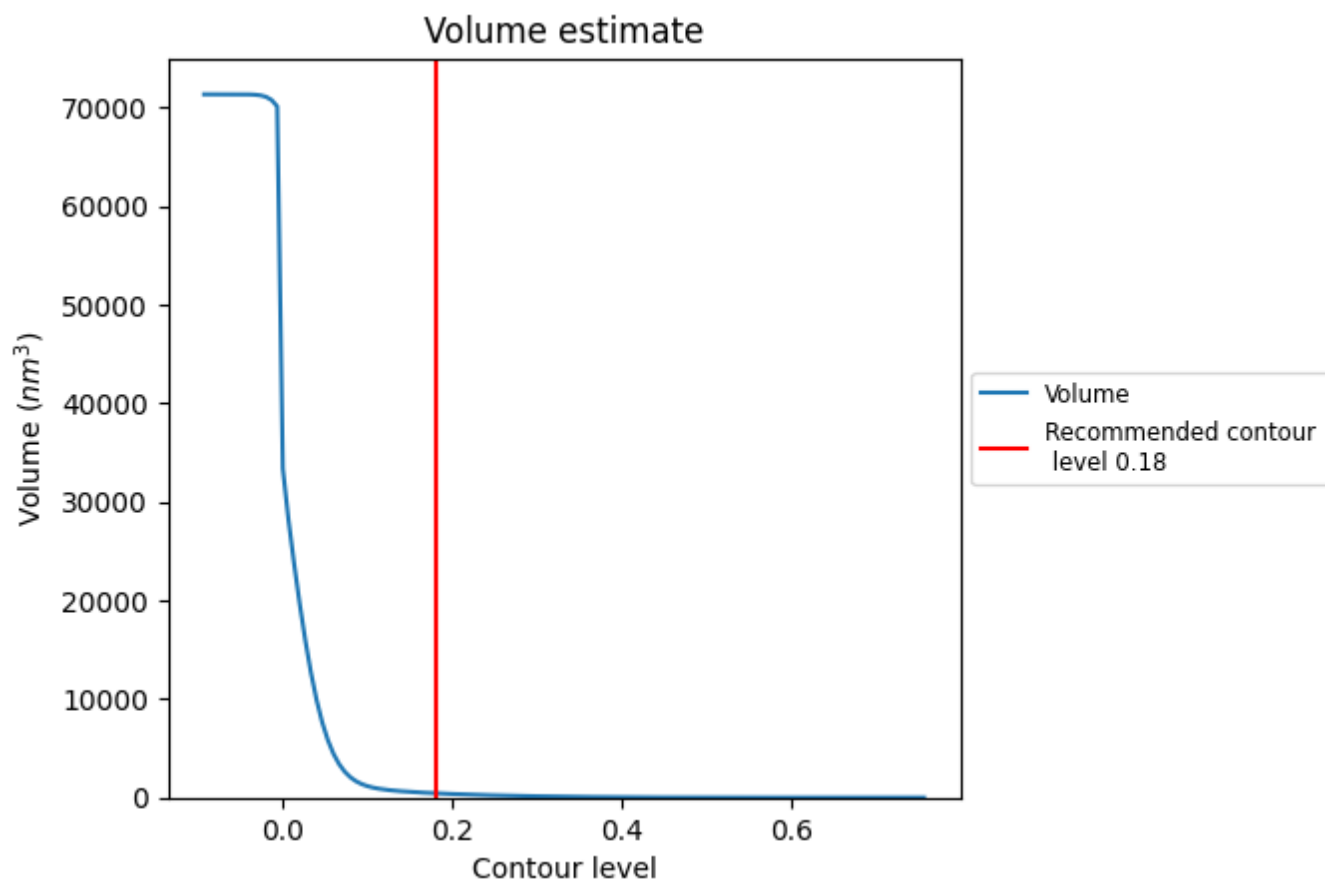
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

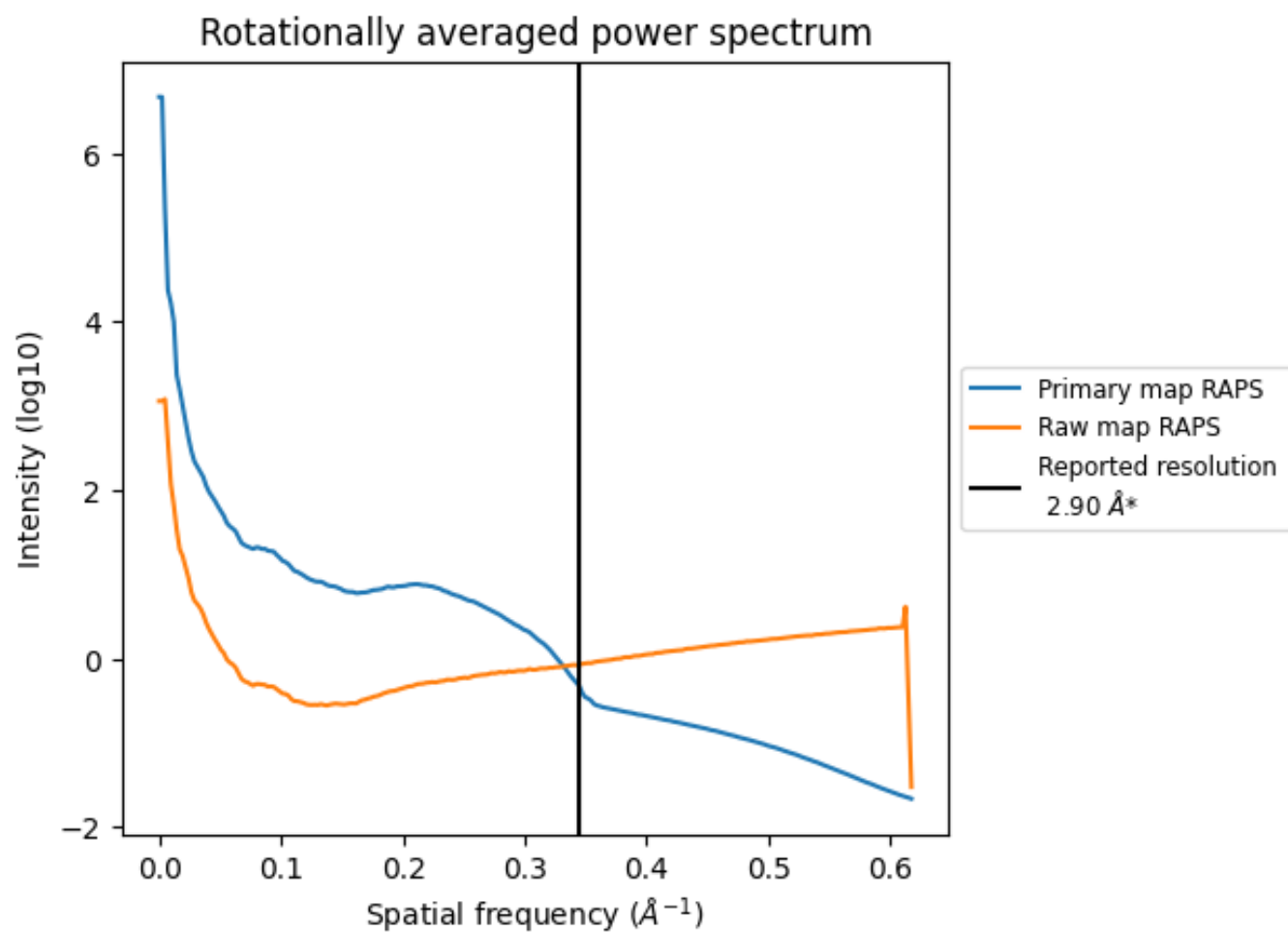
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 436 nm³; this corresponds to an approximate mass of 394 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

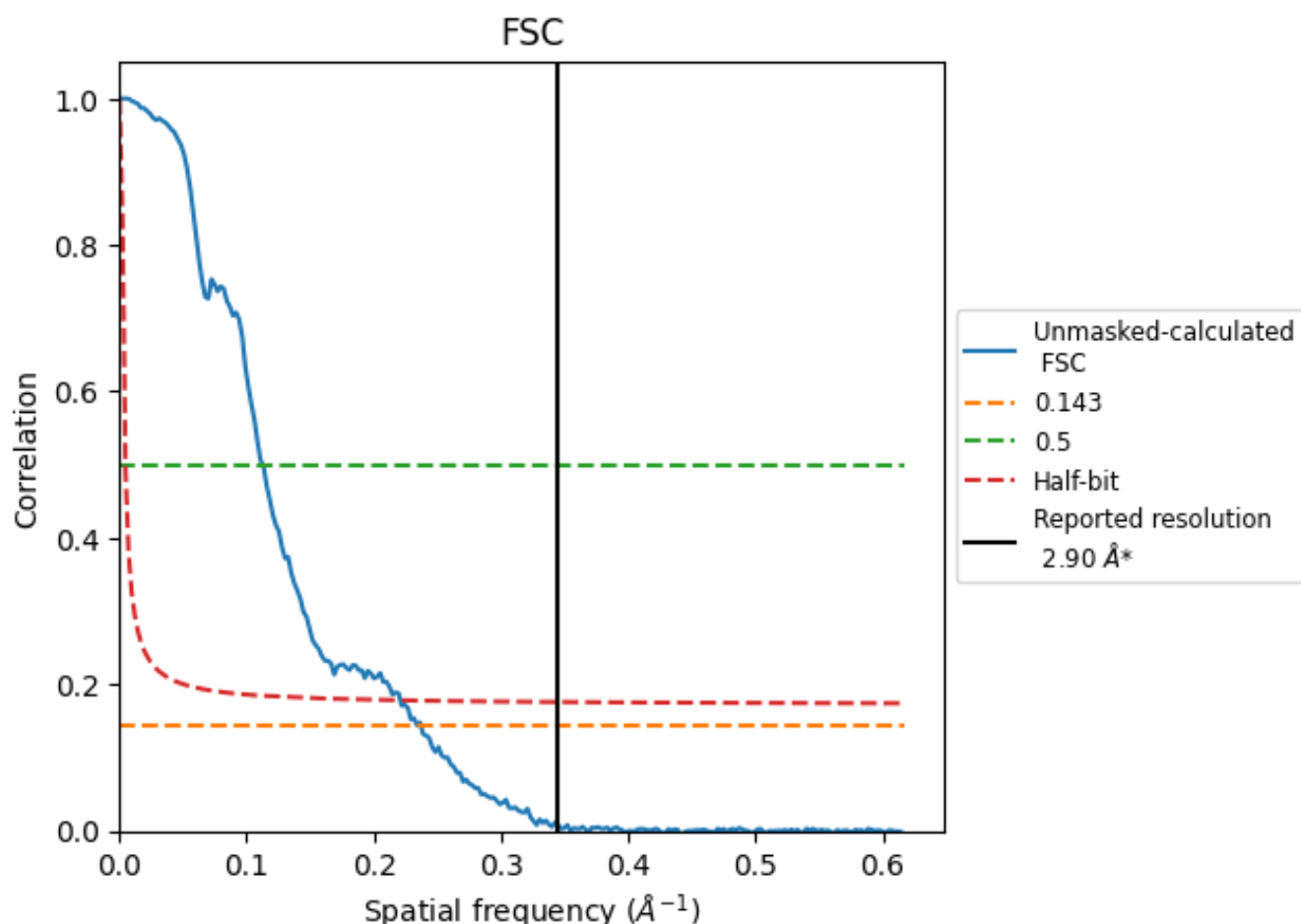


*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

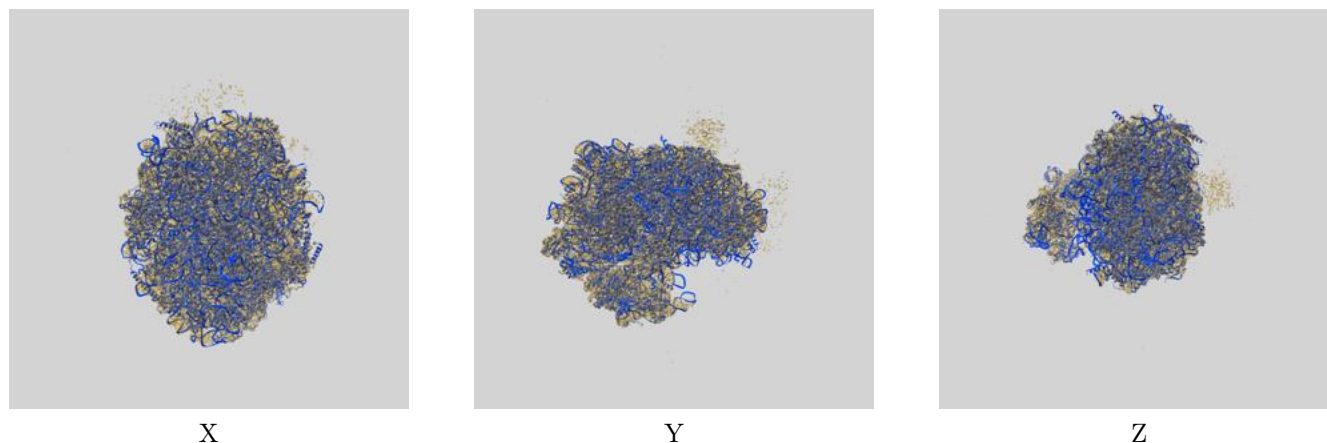
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.22	8.89	4.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.22 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

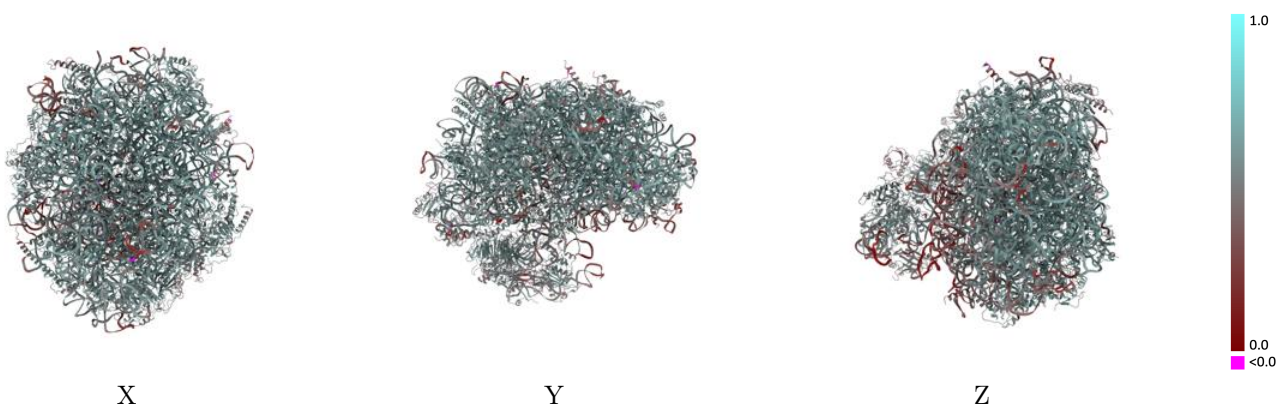
This section contains information regarding the fit between EMDB map EMD-26485 and PDB model 7UG6. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



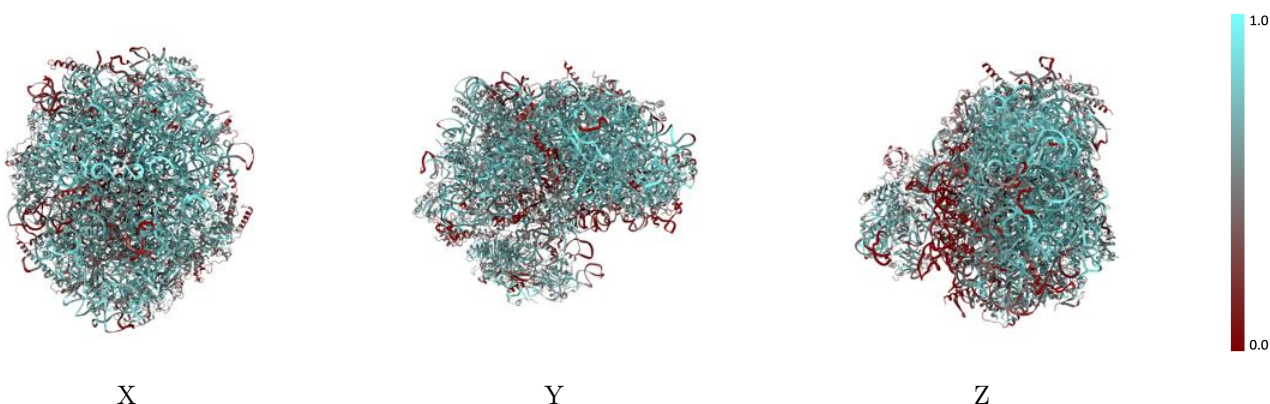
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



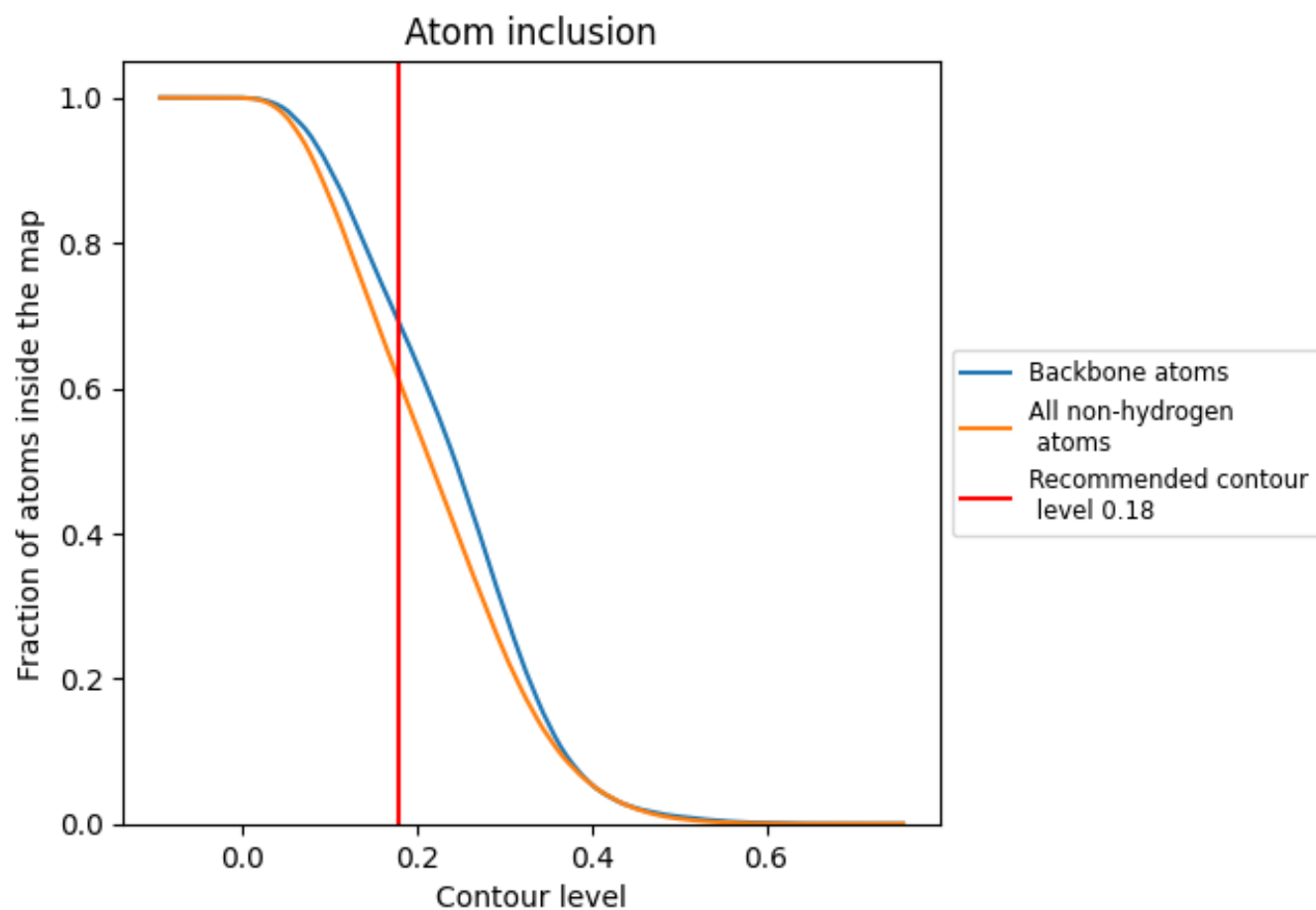
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 61% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6110	 0.5330
1	 0.6627	 0.5230
2	 0.8024	 0.5820
3	 0.6840	 0.4580
7	 0.6129	 0.5520
A	 0.6138	 0.5680
B	 0.6647	 0.5890
C	 0.6187	 0.5810
D	 0.5878	 0.5080
E	 0.5206	 0.5500
F	 0.6196	 0.5690
G	 0.4574	 0.5060
H	 0.6526	 0.5770
I	 0.2864	 0.5280
J	 0.4050	 0.4190
L	 0.4789	 0.5290
M	 0.5905	 0.5670
N	 0.5800	 0.5690
O	 0.6733	 0.5930
P	 0.5884	 0.5650
Q	 0.5581	 0.5530
R	 0.6865	 0.5760
S	 0.5176	 0.5420
T	 0.2283	 0.4550
U	 0.4723	 0.4930
V	 0.6337	 0.5780
W	 0.5239	 0.5130
X	 0.6043	 0.5810
Y	 0.6412	 0.5730
Z	 0.6716	 0.5750
a	 0.4799	 0.4970
b	 0.4725	 0.5200
c	 0.2780	 0.5130
d	 0.6375	 0.5630
e	 0.5744	 0.5850



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Chain	Atom inclusion	Q-score
f	 0.6557	 0.6010
g	 0.6596	 0.5850
h	 0.6441	 0.5750
i	 0.3579	 0.4940
j	 0.7454	 0.6050
k	 0.5283	 0.5550
l	 0.6683	 0.5980
m	 0.4821	 0.5270
p	 0.6582	 0.5760
q	 0.3147	 0.4630
r	 0.6099	 0.5720
s	 0.2509	 0.4440
u	 0.5206	 0.5280
v	 0.5839	 0.5230
w	 0.4226	 0.4910
x	 0.5394	 0.5060
y	 0.6423	 0.5610
z	 0.3435	 0.5190