wwPDB EM Validation Summary Report

Nov 21, 2022 – 12:50 PM EST

PDB ID	:	7UCJ
EMDB ID	:	EMD-26444
Title	:	Mammalian 80S translation initiation complex with mRNA and Harringtonine
Authors	:	Yang, R.; Arango, D.; Sturgill, D.; Oberdoerffer, S.
Deposited on	:	2022-03-16
Resolution	:	3.10 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (1)) were used in the production of this report:

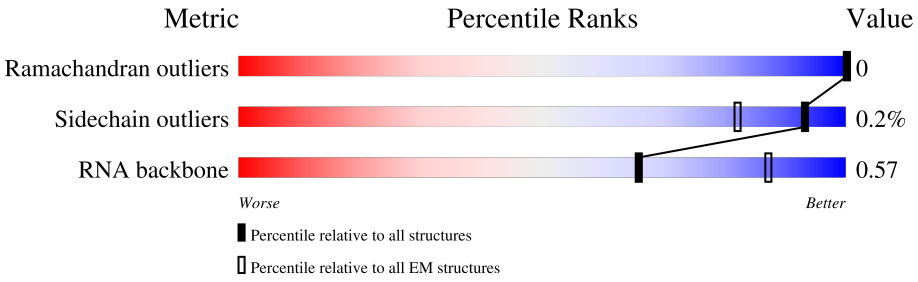
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.10 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	2	76	53% 78% 14% · 5%
2	1	6	17% 67% 33%
3	5	3499	12% 79% 21% ·
4	7	120	· 92% 8%
5	8	156	8% 79% 17% ·
6	9	1698	15% 79% 21% ·
7	A	248	5% 99% ·
8	B	394	9% 100%

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Mol	Chain	Length	Quality of chain
9	C	360	9% 100%
10	D	291	13% 100%
11	E	250	13% 86% 14%
12	F	225	100%
13	G	233	30% 96%
14	H	190	16% 99%
15	I	213	13% 96%
16	J	169	18% 100%
17	L	210	17% 100%
18	M	138	9% 99%
19	N	203	100%
20	O	199	5% 99%
21	P	153	7% 100%
22	Q	187	6% 99%
23	R	180	18% 100%
24	S	176	9% 100%
25	T	159	18% 100%
26	U	98	34% 100%
27	V	130	12% 100%
28	W	95	25% 84% 16%
29	X	118	14% 100%
30	Y	134	11% 100%
31	Z	135	19% 100%
32	a	147	5% 100%
33	b	116	34% 90% 10%

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Mol	Chain	Length	Quality of chain
34	c	95	11% 100%
35	d	107	15% 100%
36	e	128	5% 100%
37	f	109	6% 100%
38	g	114	12% 100%
39	h	122	20% 100%
40	i	102	19% 100%
41	j	86	100%
42	k	69	46% 99%
43	l	50	16% 100%
44	m	51	14% 100%
45	n	25	20% 100%
46	o	103	12% 100%
47	p	91	12% 100%
48	r	124	5% 100%
49	AA	217	18% 100%
50	BB	211	18% 100%
51	CC	221	14% 100%
52	DD	227	52% 100%
53	EE	262	21% 100%
54	FF	191	27% 97%
55	GG	237	53% 100%
56	HH	189	54% 97%
57	II	206	20% 98%
58	JJ	185	21% 100%

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Mol	Chain	Length	Quality of chain
59	KK	96	67% 100%
60	LL	151	12% 95% 5%
61	NN	149	13% 100%
62	OO	136	15% 100%
63	PP	120	55% 99%
64	QQ	142	35% 100%
65	RR	132	55% 100%
66	SS	144	37% 99%
67	TT	141	37% 100%
68	UU	100	61% 99%
69	VV	83	28% 100%
70	WW	129	9% 100%
71	XX	141	13% 100%
72	YY	124	28% 100%
73	ZZ	75	48% 100%
74	Aa	101	17% 100%
75	Bb	83	31% 100%
76	Cc	62	42% 95% 5%
77	Dd	55	22% 100%
78	Ee	55	38% 100%
79	Gg	313	73% 99%

2 Entry composition (i)

There are 82 unique types of molecules in this entry. The entry contains 208732 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 P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	72	1552	694	289	498	71	0	0

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	1	6	130	58	25	41	6	0	0

- Molecule 3 is a RNA chain called 28s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	5	3499	75142	33527	13732	24384	3499	0	0

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	7	120	2558	1141	456	842	119	0	0

- Molecule 5 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	8	150	3192	1424	561	1057	150	0	0

- Molecule 6 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	9	1698	36291	16217	6509	11868	1697	0	0

- Molecule 7 is a protein called 60S ribosomal protein L8.

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

- Molecule 8 is a protein called 60S ribosomal protein L3.

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

- Molecule 9 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	360	Total	C	N	O	S	0	0
			2870	1806	575	475	14		

- Molecule 10 is a protein called Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	291	Total	C	N	O	S	0	0
			2381	1506	436	425	14		

- Molecule 11 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	215	Total	C	N	O	S	0	0
			1720	1109	327	281	3		

- Molecule 12 is a protein called 60S ribosomal protein L7.

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

- Molecule 13 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	226	Total	C	N	O	S	0	0
			1830	1167	353	306	4		

- Molecule 14 is a protein called 60S ribosomal protein L9.

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

- Molecule 15 is a protein called Ribosomal protein L10.

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

- Molecule 16 is a protein called 60S ribosomal protein L11.

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

- Molecule 17 is a protein called 60S ribosomal protein L13.

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

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	46	ILE	-	insertion	UNP G1TPV0
L	47	ALA	-	insertion	UNP G1TPV0
L	48	PRO	-	insertion	UNP G1TPV0
L	49	ARG	-	insertion	UNP G1TPV0
L	50	PRO	-	insertion	UNP G1TPV0
L	51	ALA	-	insertion	UNP G1TPV0
L	52	ALA	-	insertion	UNP G1TPV0
L	53	GLY	-	insertion	UNP G1TPV0
L	54	PRO	-	insertion	UNP G1TPV0

- Molecule 18 is a protein called 60S ribosomal protein L14.

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

- Molecule 19 is a protein called 60S ribosomal protein L15.

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

- Molecule 20 is a protein called 60S ribosomal protein L13a.

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

- Molecule 21 is a protein called 60S ribosomal protein L17.

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

- Molecule 22 is a protein called 60S ribosomal protein L18.

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

- Molecule 23 is a protein called 60S ribosomal protein L19.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	38	ARG	HIS	conflict	UNP G1TYL6
R	151	ARG	HIS	conflict	UNP G1TYL6

- Molecule 24 is a protein called 60S ribosomal protein L18a.

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

- Molecule 25 is a protein called 60S ribosomal protein L21.

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

- Molecule 26 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	98	Total	C	N	O	S	0	0
			800	514	139	145	2		

- Molecule 27 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	130	Total	C	N	O	S	0	0
			973	615	183	170	5		

- Molecule 28 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	80	Total	C	N	O	S	0	0
			654	412	130	109	3		

- Molecule 29 is a protein called 60S ribosomal protein L23a.

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

- Molecule 30 is a protein called 60S ribosomal protein L26.

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

- Molecule 31 is a protein called 60S ribosomal protein L27.

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

- Molecule 32 is a protein called 60S ribosomal protein L27a.

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

- Molecule 33 is a protein called 60S ribosomal protein L29.

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

- Molecule 34 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	95	Total	C	N	O	S	0	0
			738	467	131	134	6		

- Molecule 35 is a protein called 60S ribosomal protein L31.

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

- Molecule 36 is a protein called 60S ribosomal protein L32.

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

- Molecule 37 is a protein called 60S ribosomal protein L35a.

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

- Molecule 38 is a protein called 60S ribosomal protein L34.

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

- Molecule 39 is a protein called 60S ribosomal protein L35.

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

- Molecule 40 is a protein called 60S ribosomal protein L36.

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

- Molecule 41 is a protein called 60S ribosomal protein L37.

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

- Molecule 42 is a protein called 60S ribosomal protein L38.

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

- Molecule 43 is a protein called 60S ribosomal protein L39.

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

- Molecule 44 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	51	Total	C	N	O	S	0	0
			420	261	88	65	6		

- Molecule 45 is a protein called eL41.

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

- Molecule 46 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	103	Total	C	N	O	S	0	0
			842	528	172	136	6		

- Molecule 47 is a protein called 60S ribosomal protein L37a.

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

- Molecule 48 is a protein called 60S ribosomal protein L28.

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

- Molecule 49 is a protein called 40S_SA_C domain-containing protein.

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

- Molecule 50 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BB	211	Total	C	N	O	S	0	0
			1715	1088	307	306	14		

- Molecule 51 is a protein called 40S ribosomal protein S2.

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	73	MET	VAL	conflict	UNP G1TUT9
CC	101	SER	ALA	conflict	UNP G1TUT9
CC	119	GLY	ALA	conflict	UNP G1TUT9
CC	194	ARG	HIS	conflict	UNP G1TUT9
CC	215	MET	LEU	conflict	UNP G1TUT9
CC	227	ARG	TRP	conflict	UNP G1TUT9

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

- Molecule 52 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	DD	227	Total	C	N	O	S	0	0
			1760	1121	317	315	7		

- Molecule 53 is a protein called 40S ribosomal protein S4.

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

- Molecule 54 is a protein called Ribosomal protein S5.

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

- Molecule 55 is a protein called 40S ribosomal protein S6.

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

- Molecule 56 is a protein called 40S ribosomal protein S7.

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

- Molecule 57 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	II	203	Total	C	N	O	S	0	0
			1668	1047	328	288	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
II	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 58 is a protein called 40S ribosomal protein S9.

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

- Molecule 59 is a protein called 40S ribosomal protein S10.

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

- Molecule 60 is a protein called 40S ribosomal protein S11.

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

- Molecule 61 is a protein called 40S ribosomal protein S13.

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

- Molecule 62 is a protein called 40S ribosomal protein S14.

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

- Molecule 63 is a protein called 40S ribosomal protein S15.

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

- Molecule 64 is a protein called 40S ribosomal protein S16.

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

- Molecule 65 is a protein called 40S ribosomal protein S17.

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

- Molecule 66 is a protein called 40S ribosomal protein S18.

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

- Molecule 67 is a protein called 40S ribosomal protein S19.

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

- Molecule 68 is a protein called 40S ribosomal protein S20.

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

- Molecule 69 is a protein called eS21.

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
VV	3	ASN	SER	conflict	UNP G1TM82
VV	4	ASP	ASN	conflict	UNP G1TM82
VV	33	GLN	PRO	conflict	UNP G1TM82
VV	50	PHE	SER	conflict	UNP G1TM82
VV	75	ALA	SER	conflict	UNP G1TM82
VV	76	ASP	HIS	conflict	UNP G1TM82

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Chain	Residue	Modelled	Actual	Comment	Reference
VV	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 70 is a protein called 40S ribosomal protein S15a.

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

- Molecule 71 is a protein called 40S ribosomal protein S23.

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

- Molecule 72 is a protein called 40S ribosomal protein S24.

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

- Molecule 73 is a protein called 40S ribosomal protein S25.

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

- Molecule 74 is a protein called eS26.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	28	ARG	CYS	conflict	UNP G1TFE8
Aa	56	ALA	VAL	conflict	UNP G1TFE8

- Molecule 75 is a protein called 40S ribosomal protein S27.

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

- Molecule 76 is a protein called 40S ribosomal protein S28.

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

- Molecule 77 is a protein called 40S ribosomal protein S29.

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

- Molecule 78 is a protein called 40S ribosomal protein S30.

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

- Molecule 79 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 80 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
80	5	196	Total	Mg	0
			196	196	
80	7	7	Total	Mg	0
			7	7	
80	8	7	Total	Mg	0
			7	7	
80	9	77	Total	Mg	0
			77	77	
80	A	1	Total	Mg	0
			1	1	
80	I	1	Total	Mg	0
			1	1	

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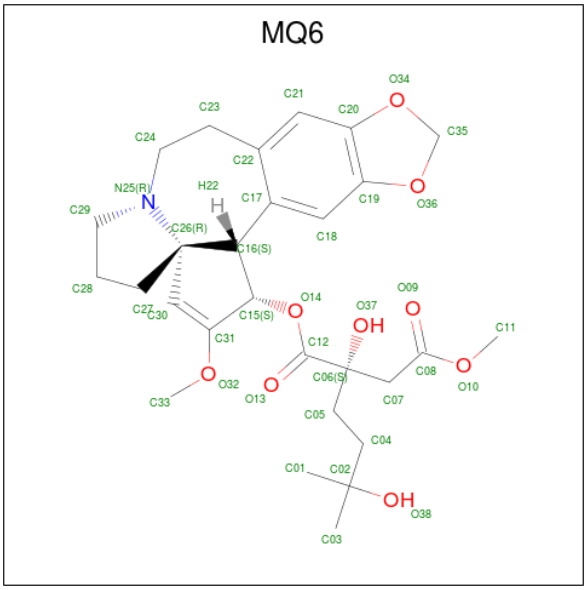
Mol	Chain	Residues	Atoms	AltConf
80	N	1	Total Mg 1 1	0
80	P	1	Total Mg 1 1	0
80	V	1	Total Mg 1 1	0
80	a	1	Total Mg 1 1	0
80	g	1	Total Mg 1 1	0
80	FF	1	Total Mg 1 1	0
80	TT	1	Total Mg 1 1	0

- Molecule 81 is Harringtonine (three-letter code: MQ6) (formula: $C_{28}H_{37}NO_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
81	5	1	Total C N O 38 28 1 9	0

- Molecule 82 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
82	g	1	Total Zn 1 1	0

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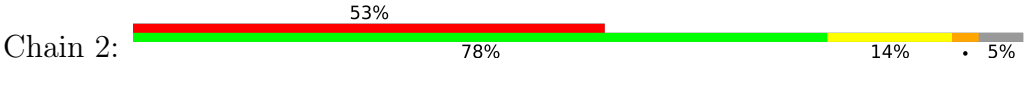
Mol	Chain	Residues	Atoms	AltConf
82	j	1	Total Zn 1 1	0
82	m	1	Total Zn 1 1	0
82	o	1	Total Zn 1 1	0
82	p	1	Total Zn 1 1	0
82	Aa	1	Total Zn 1 1	0
82	Dd	1	Total Zn 1 1	0

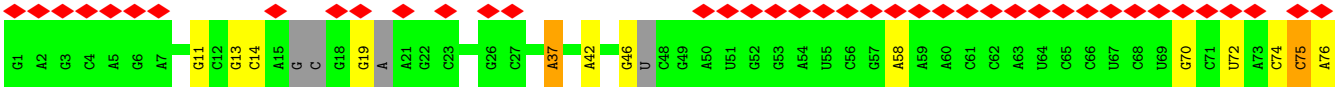
3 Residue-property plots (i)

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: P-site tRNA

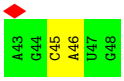
Chain 2:





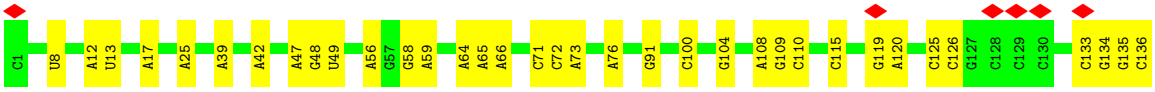
- Molecule 2: mRNA

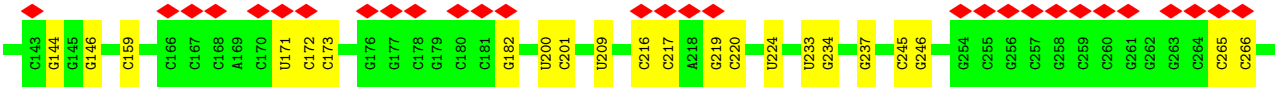
Chain 1:

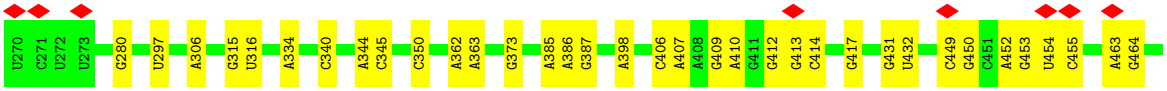


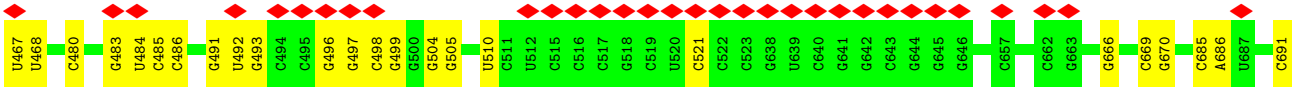
- Molecule 3: 28s rRNA

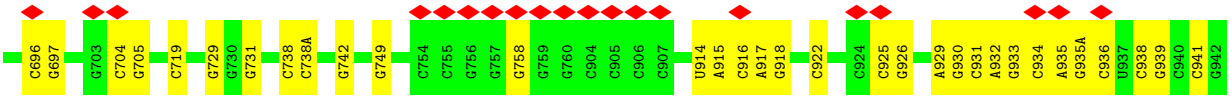
Chain 5:

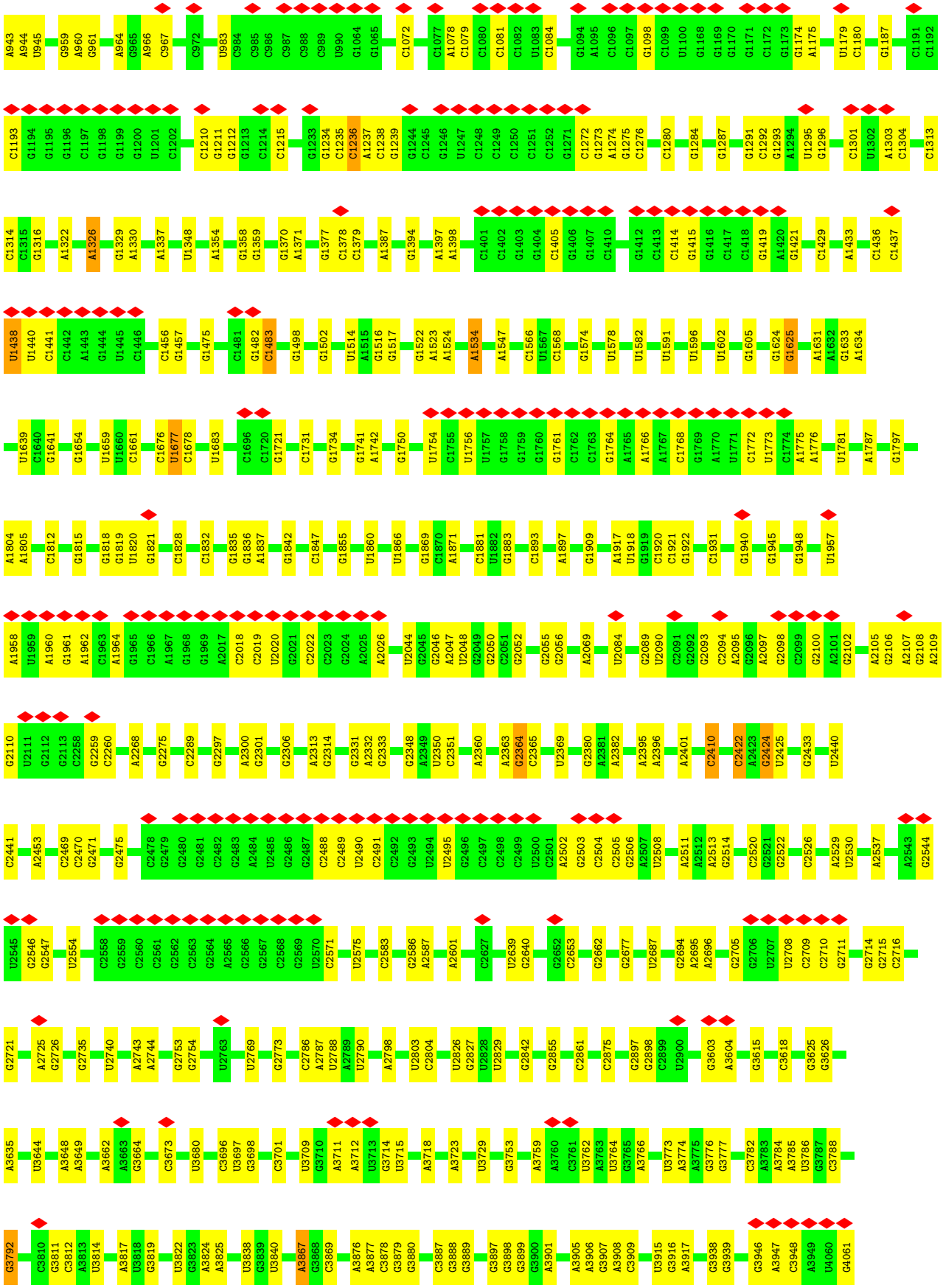


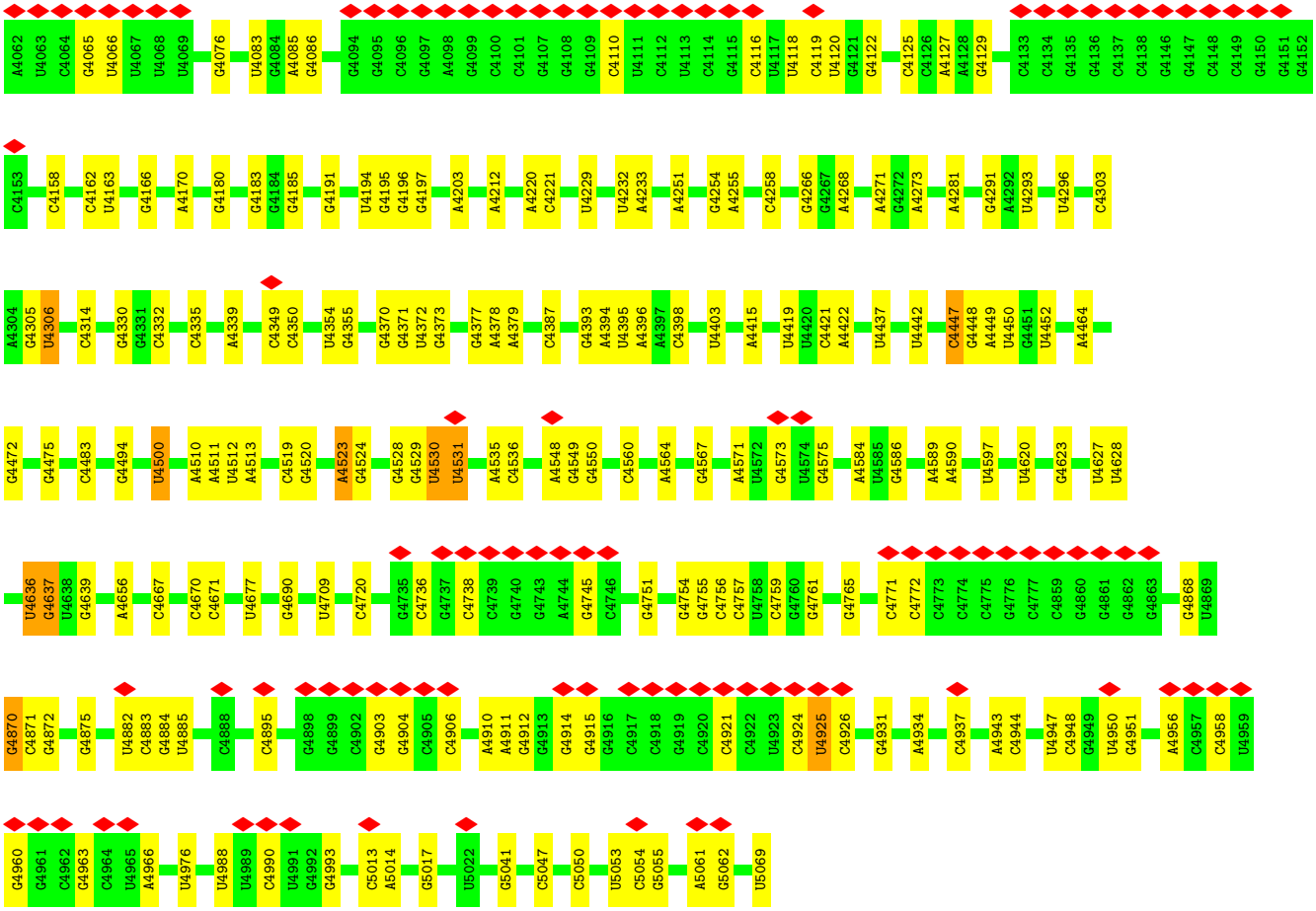






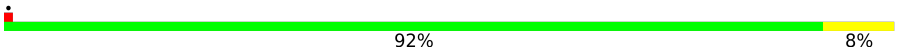


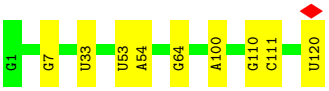




• Molecule 4: 5S rRNA

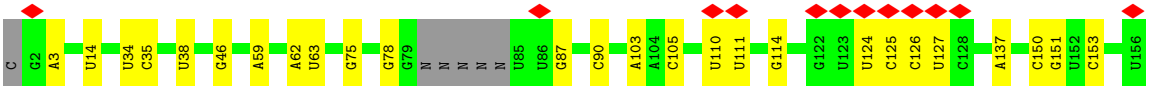
Chain 7:





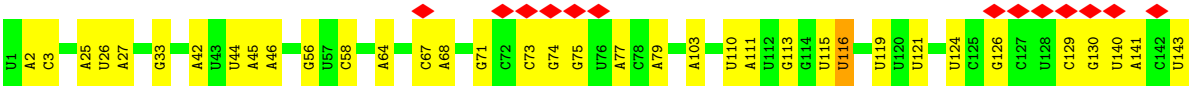
• Molecule 5: 5.8S rRNA

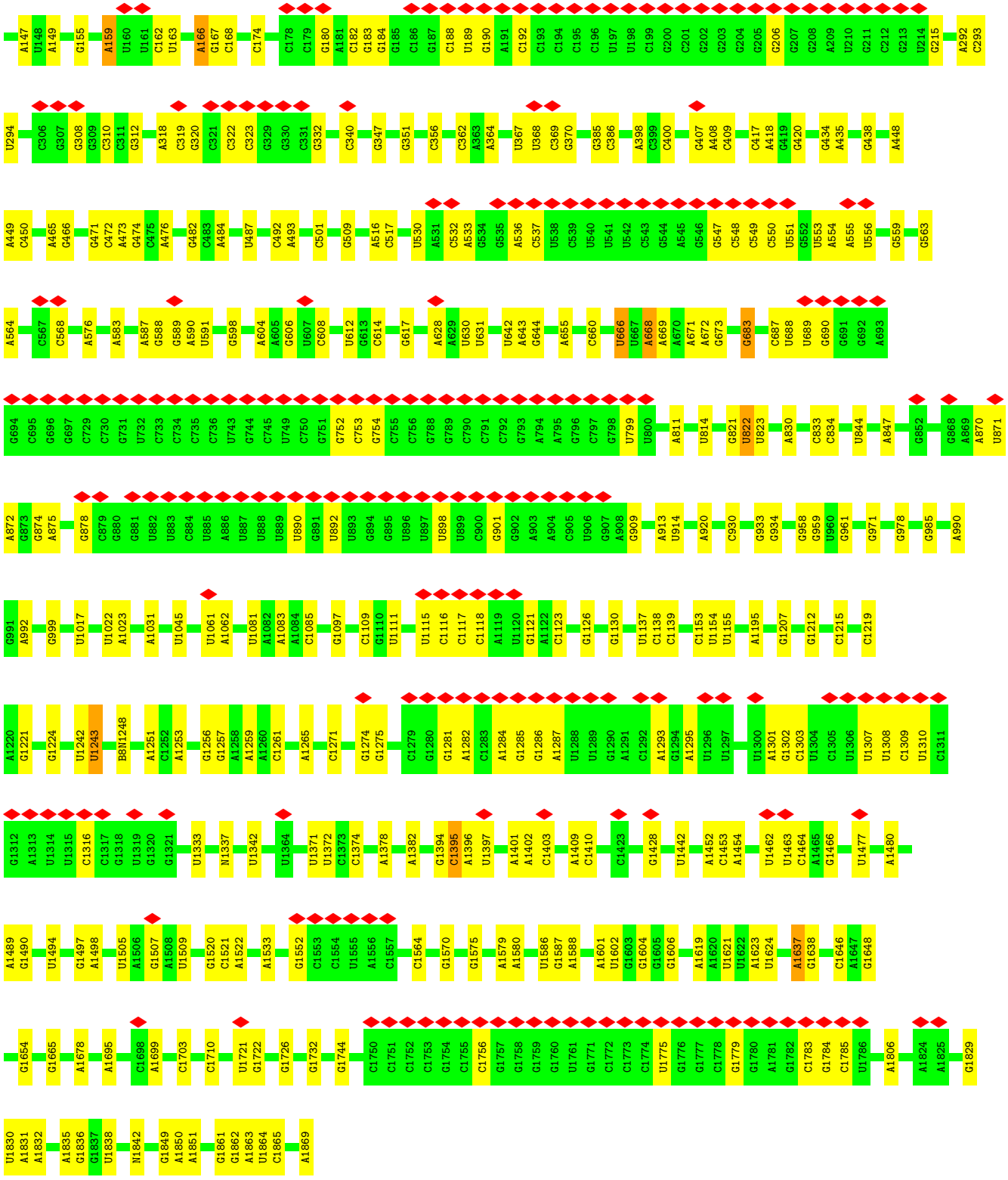
Chain 8:



• Molecule 6: 18S rRNA

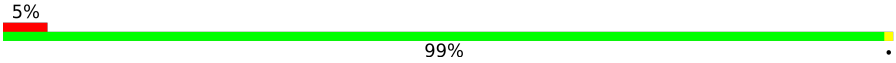
Chain 9:

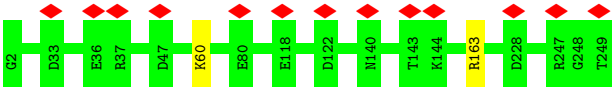




• Molecule 7: 60S ribosomal protein L8

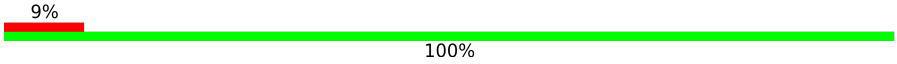
Chain A:

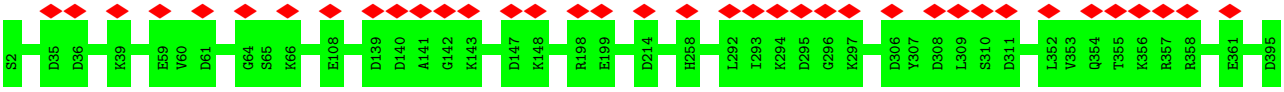




• Molecule 8: 60S ribosomal protein L3

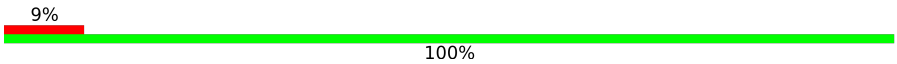
Chain B:

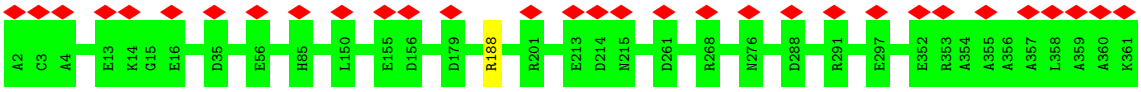




• Molecule 9: 60S ribosomal protein L4

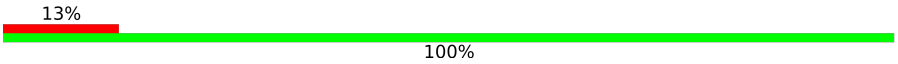
Chain C:

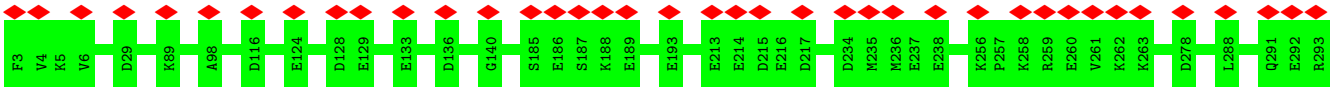




• Molecule 10: Ribosomal_L18_c domain-containing protein

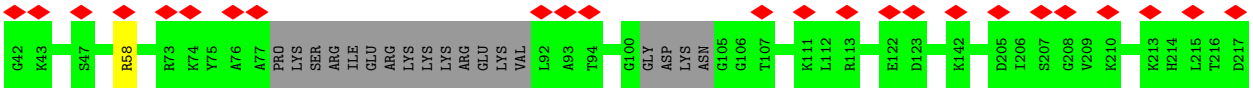
Chain D:

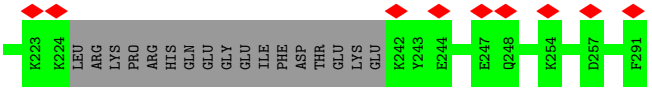




• Molecule 11: 60S ribosomal protein L6

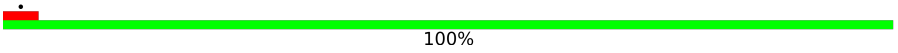
Chain E:

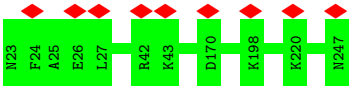




• Molecule 12: 60S ribosomal protein L7

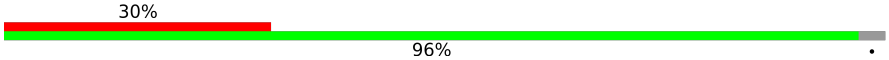
Chain F:

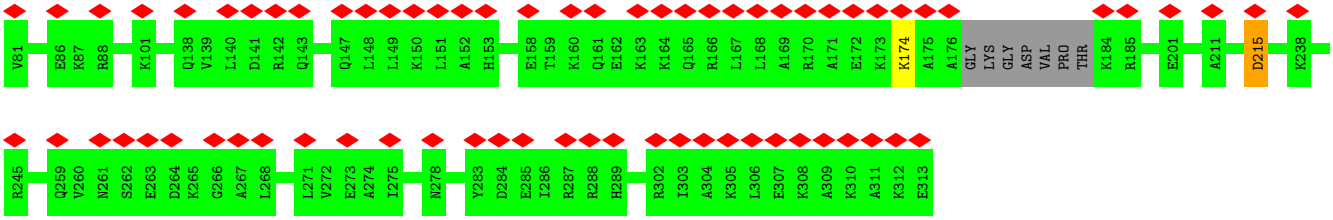




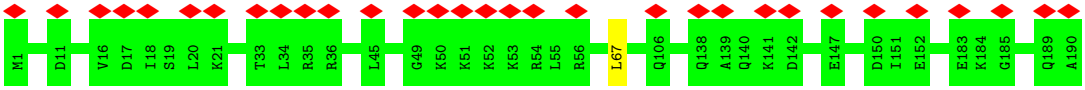
• Molecule 13: 60S ribosomal protein L7a

Chain G:

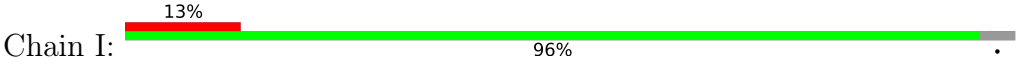


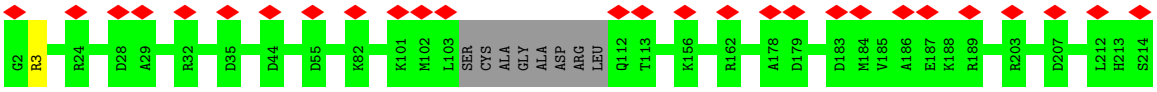


• Molecule 14: 60S ribosomal protein L9

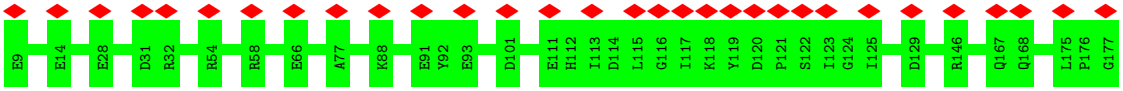


• Molecule 15: Ribosomal protein L10

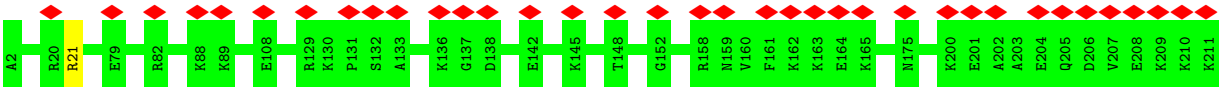




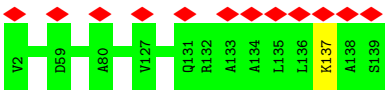
• Molecule 16: 60S ribosomal protein L11



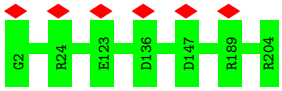
• Molecule 17: 60S ribosomal protein L13



• Molecule 18: 60S ribosomal protein L14

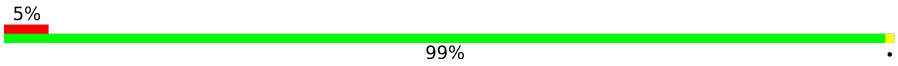


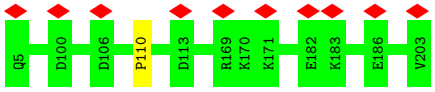
• Molecule 19: 60S ribosomal protein L15



• Molecule 20: 60S ribosomal protein L13a

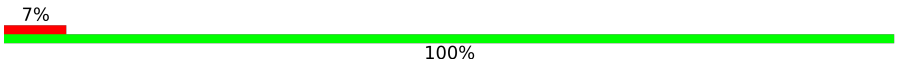
Chain O:

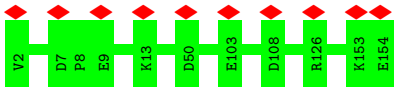




• Molecule 21: 60S ribosomal protein L17

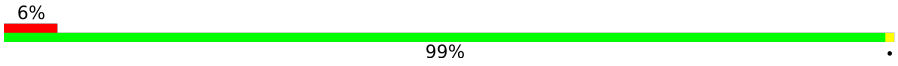
Chain P:

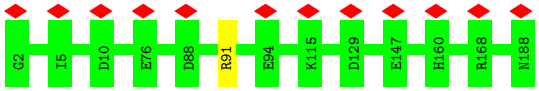




• Molecule 22: 60S ribosomal protein L18

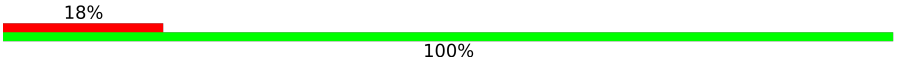
Chain Q:

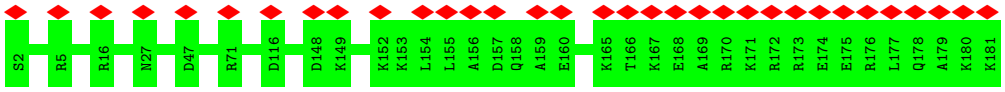




• Molecule 23: 60S ribosomal protein L19

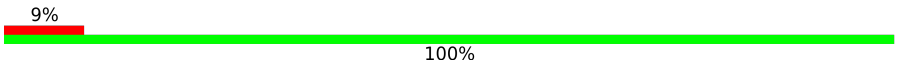
Chain R:

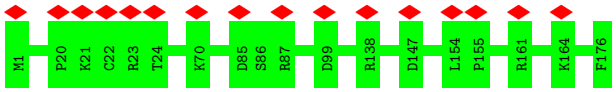




• Molecule 24: 60S ribosomal protein L18a

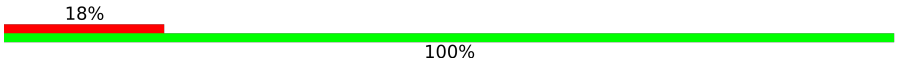
Chain S:

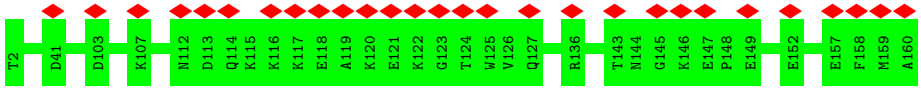




• Molecule 25: 60S ribosomal protein L21

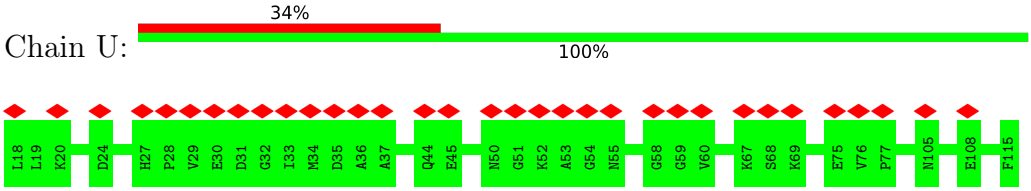
Chain T:





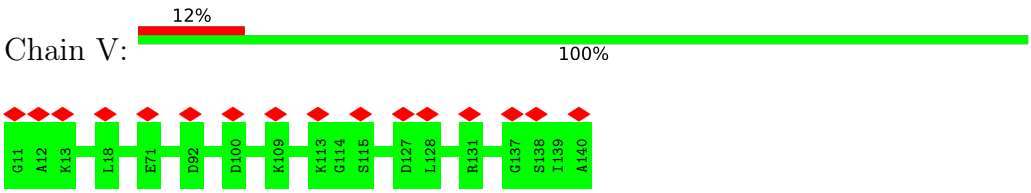
• Molecule 26: 60S ribosomal protein L22

Chain U:



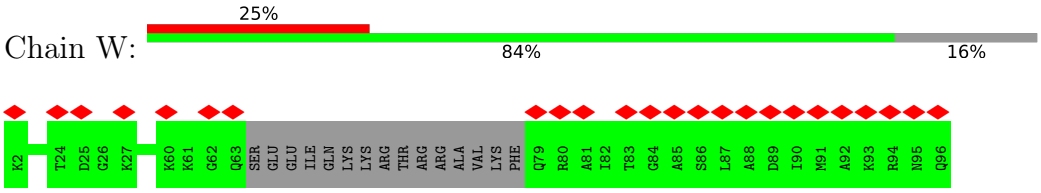
• Molecule 27: 60S ribosomal protein L23

Chain V:



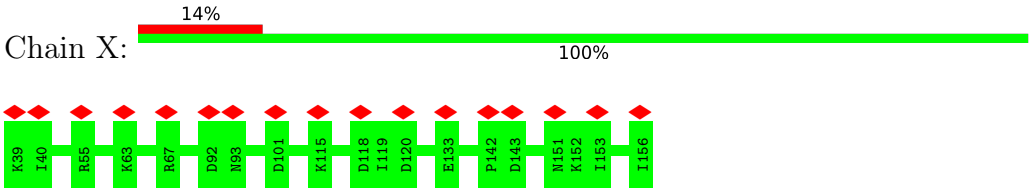
• Molecule 28: Ribosomal protein L24

Chain W:



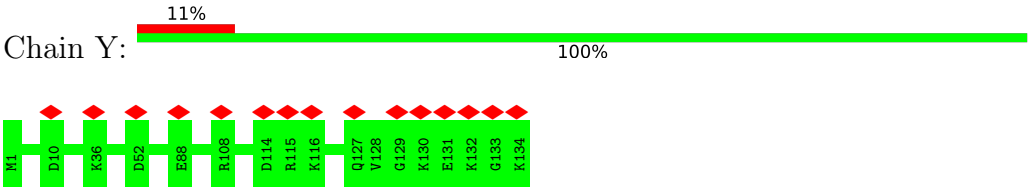
• Molecule 29: 60S ribosomal protein L23a

Chain X:



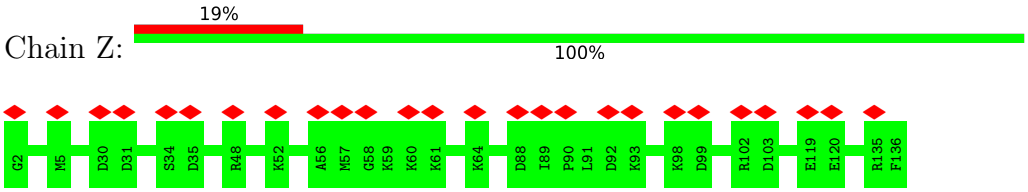
• Molecule 30: 60S ribosomal protein L26

Chain Y:



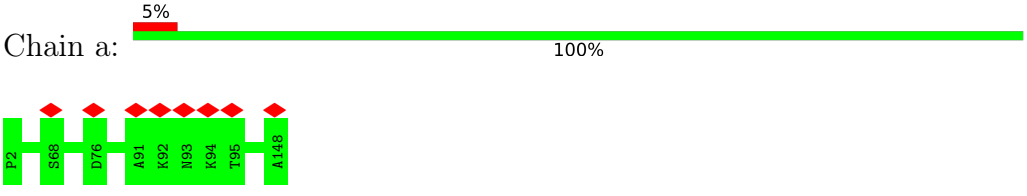
• Molecule 31: 60S ribosomal protein L27

Chain Z:



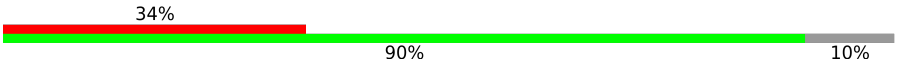
• Molecule 32: 60S ribosomal protein L27a

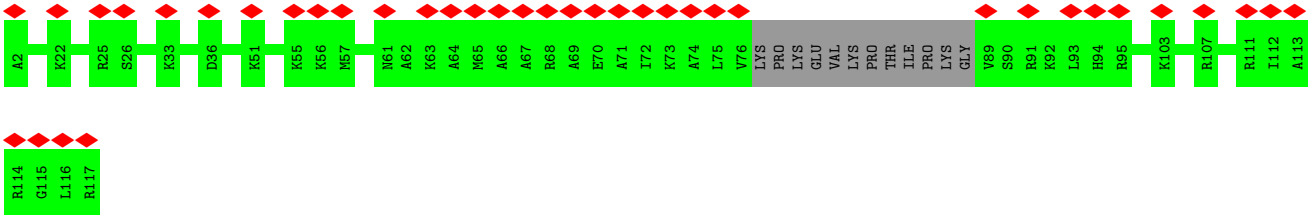
Chain a:



• Molecule 33: 60S ribosomal protein L29

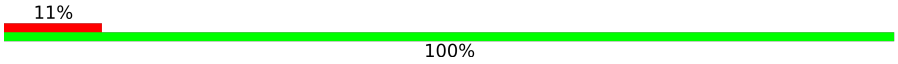
Chain b:

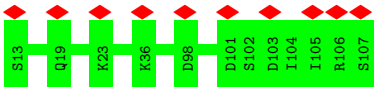




• Molecule 34: 60S ribosomal protein L30

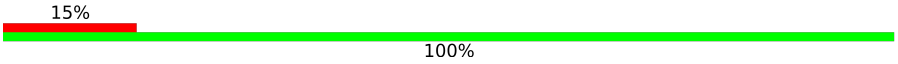
Chain c:

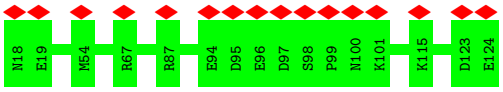




• Molecule 35: 60S ribosomal protein L31

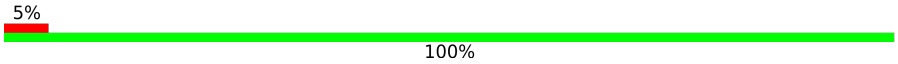
Chain d:

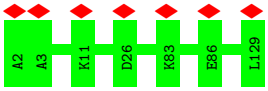




• Molecule 36: 60S ribosomal protein L32

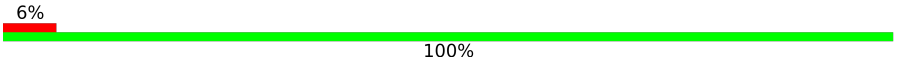
Chain e:

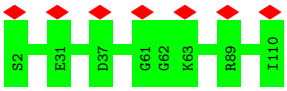




• Molecule 37: 60S ribosomal protein L35a

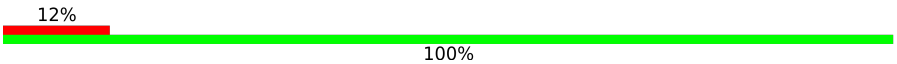
Chain f:

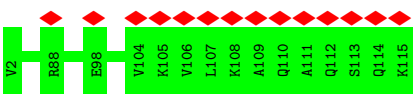




• Molecule 38: 60S ribosomal protein L34

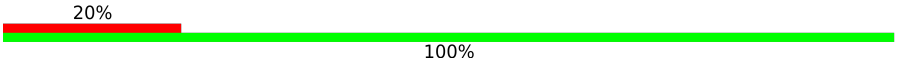
Chain g:

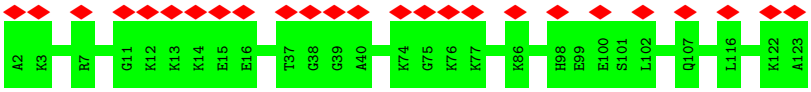




• Molecule 39: 60S ribosomal protein L35

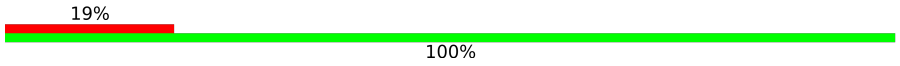
Chain h:

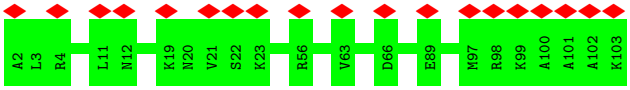




• Molecule 40: 60S ribosomal protein L36

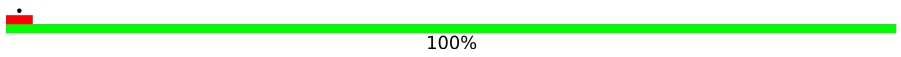
Chain i:

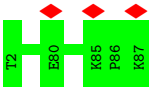




• Molecule 41: 60S ribosomal protein L37

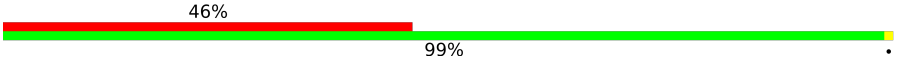
Chain j:

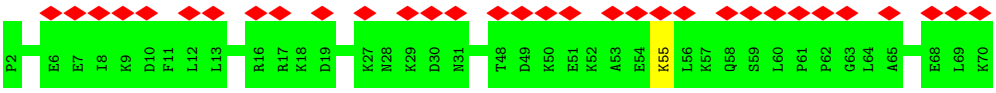




• Molecule 42: 60S ribosomal protein L38

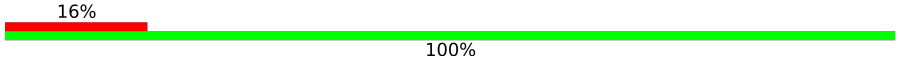
Chain k:

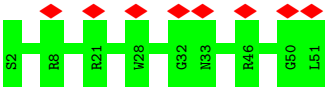




• Molecule 43: 60S ribosomal protein L39

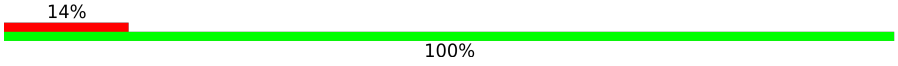
Chain l:

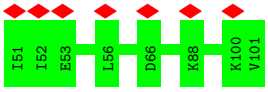




• Molecule 44: 60S ribosomal protein L40

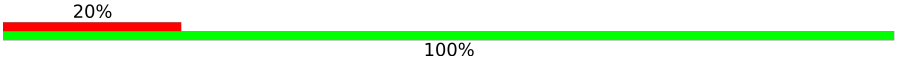
Chain m:

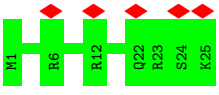




• Molecule 45: eL41

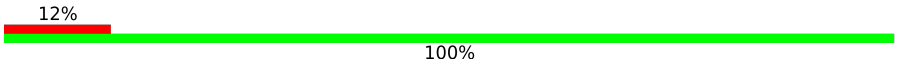
Chain n:

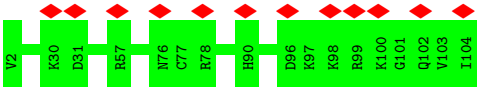




• Molecule 46: 60S ribosomal protein L36a

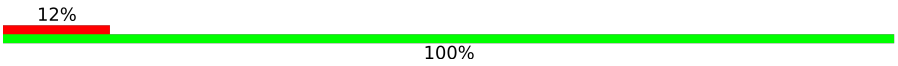
Chain o:

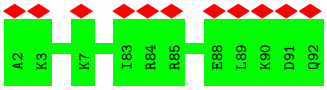




• Molecule 47: 60S ribosomal protein L37a

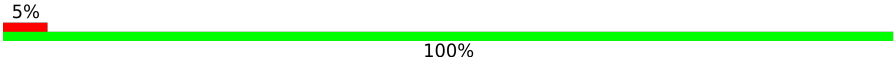
Chain p:

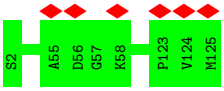




• Molecule 48: 60S ribosomal protein L28

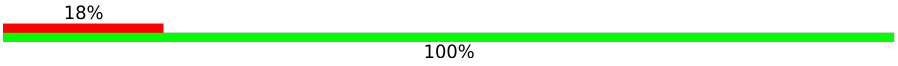
Chain r:

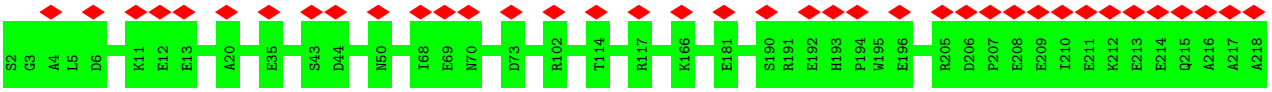




• Molecule 49: 40S_SA_C domain-containing protein

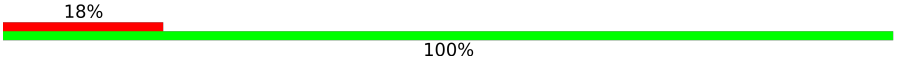
Chain AA:

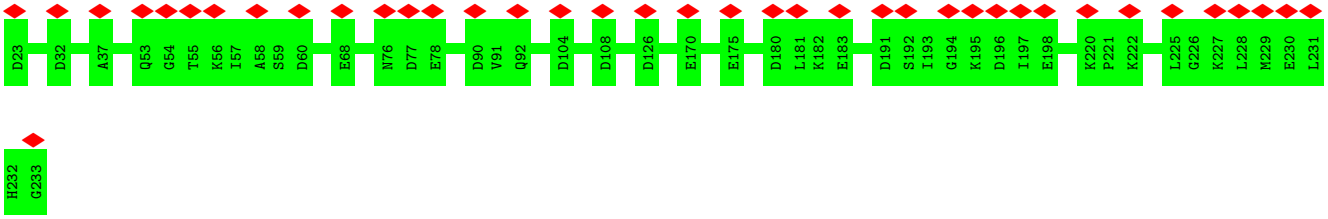




• Molecule 50: 40S ribosomal protein S3a

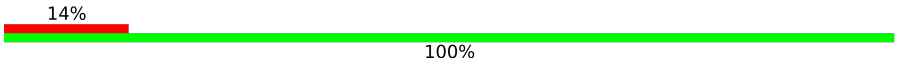
Chain BB:

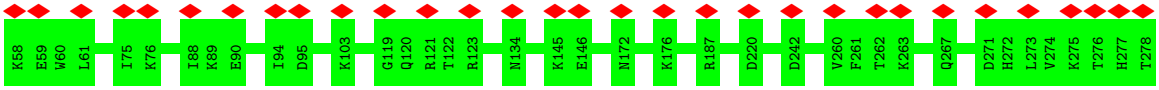




• Molecule 51: 40S ribosomal protein S2

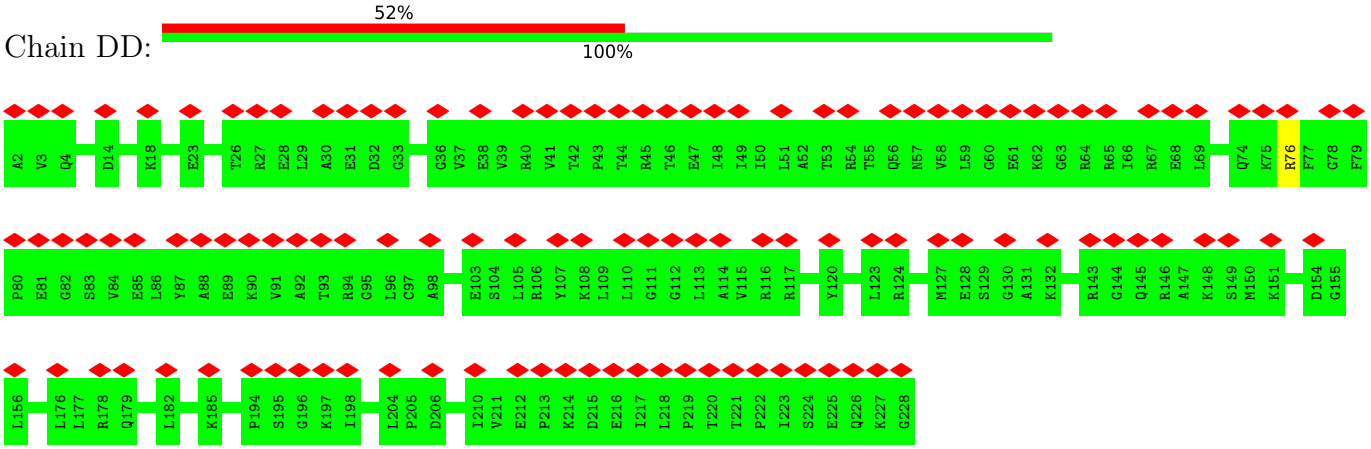
Chain CC:





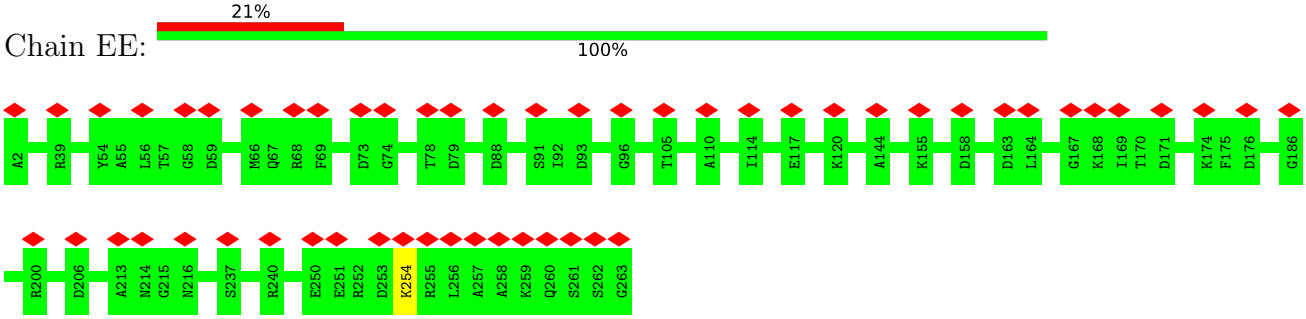
• Molecule 52: 40S ribosomal protein S3

Chain DD:



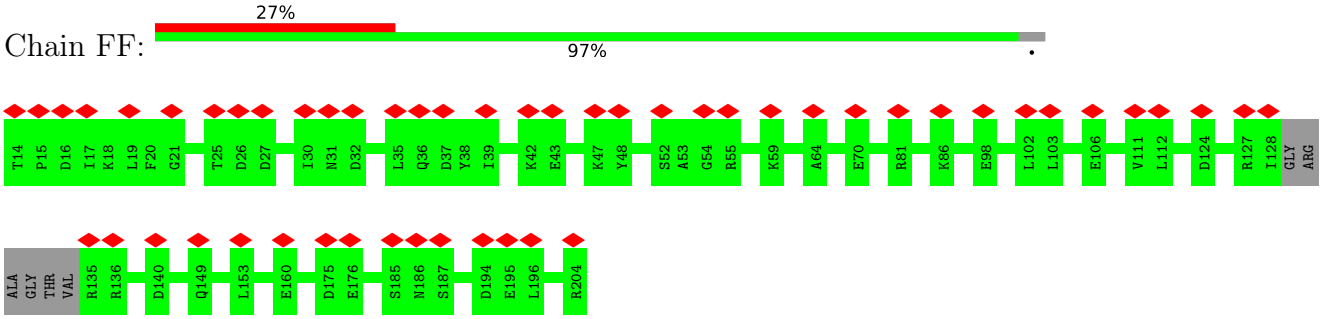
• Molecule 53: 40S ribosomal protein S4

Chain EE:



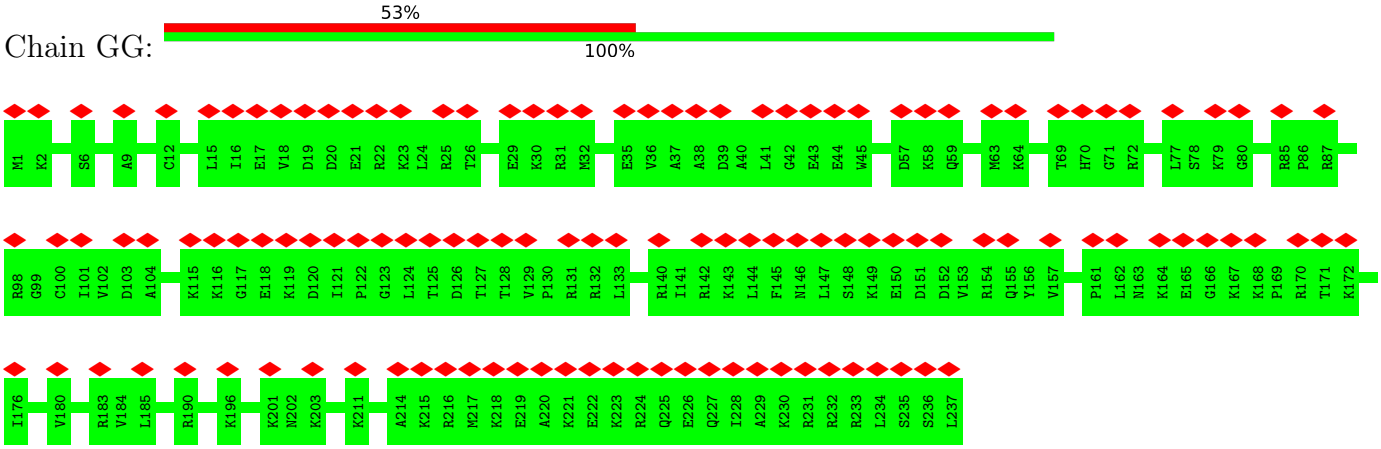
• Molecule 54: Ribosomal protein S5

Chain FF:



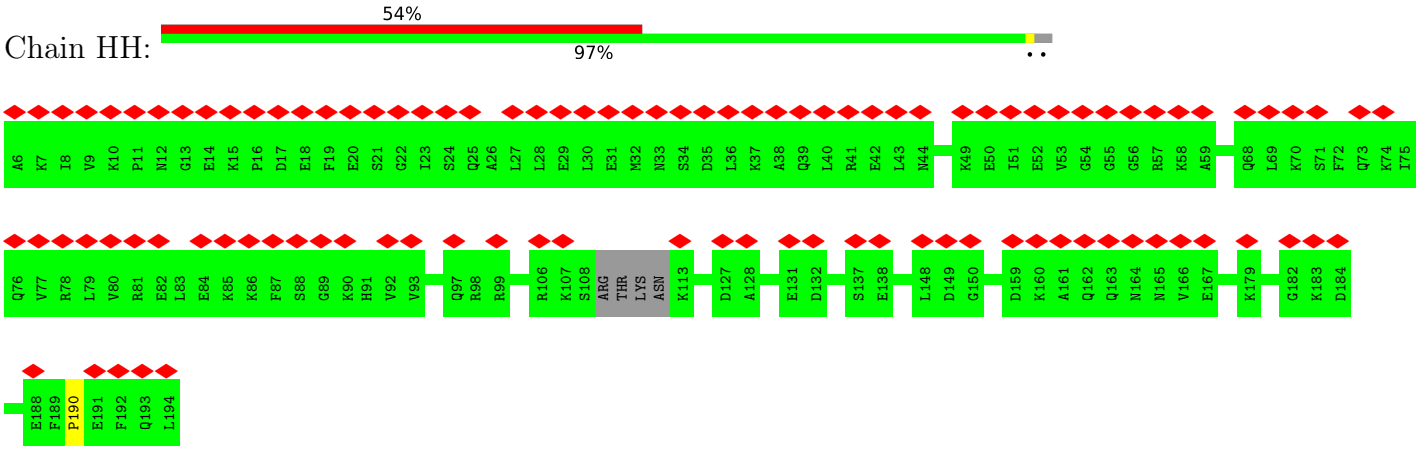
• Molecule 55: 40S ribosomal protein S6

Chain GG:



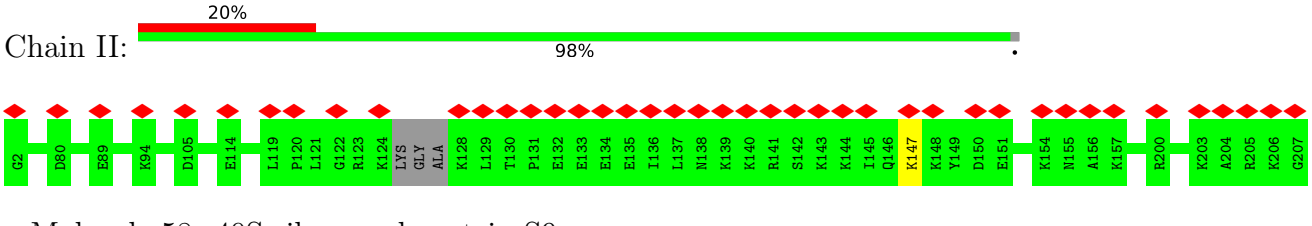
• Molecule 56: 40S ribosomal protein S7

Chain HH:



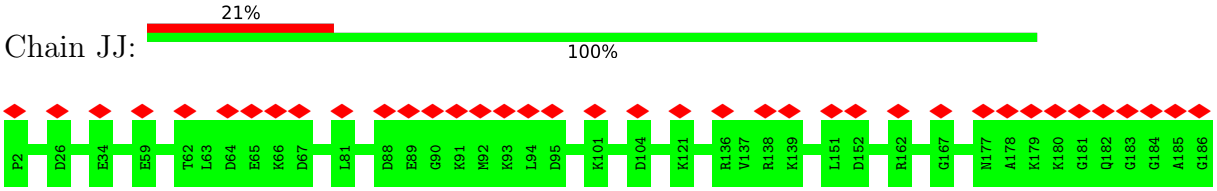
• Molecule 57: 40S ribosomal protein S8

Chain II:



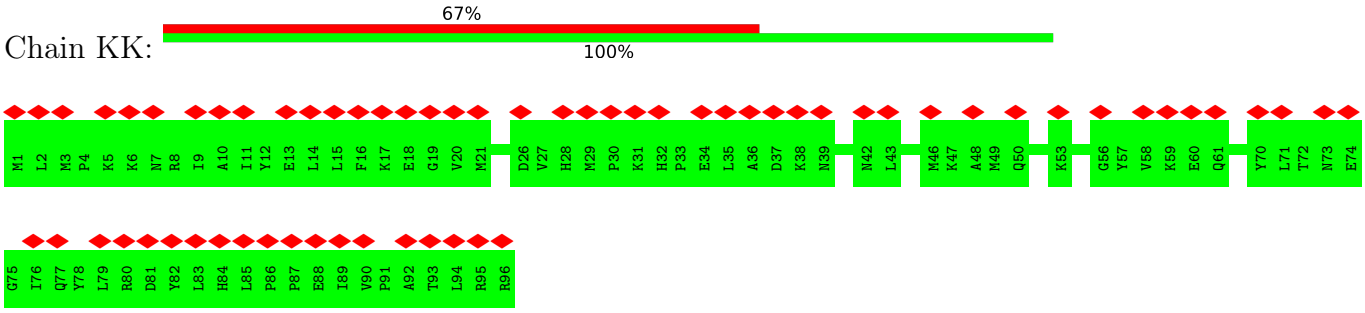
• Molecule 58: 40S ribosomal protein S9

Chain JJ:



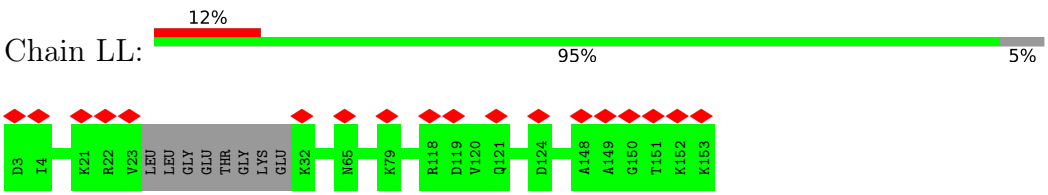
• Molecule 59: 40S ribosomal protein S10

Chain KK:



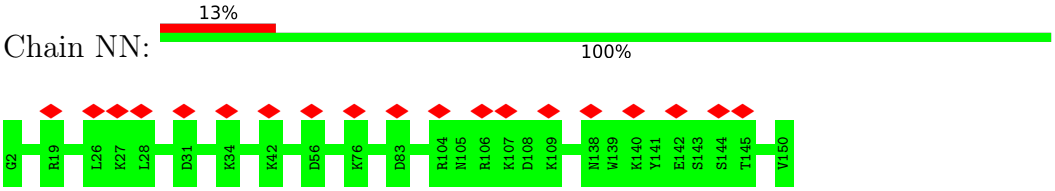
• Molecule 60: 40S ribosomal protein S11

Chain LL:



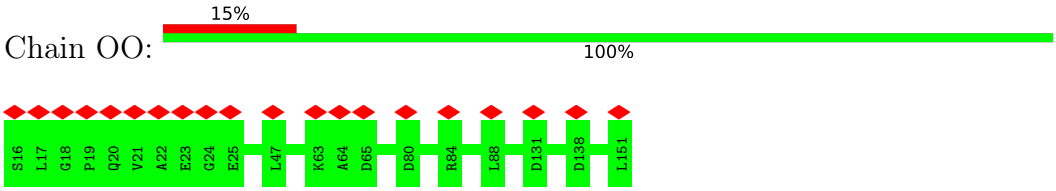
• Molecule 61: 40S ribosomal protein S13

Chain NN:



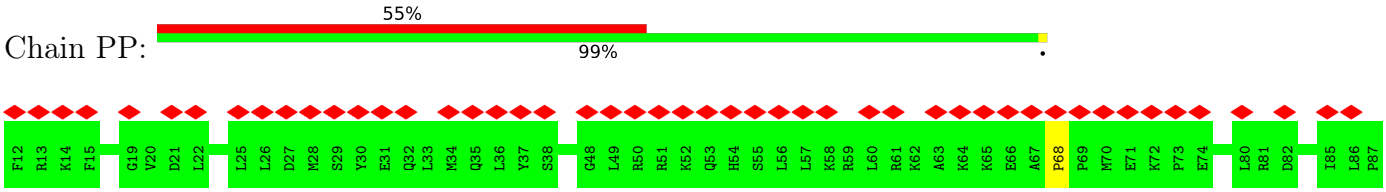
• Molecule 62: 40S ribosomal protein S14

Chain OO:



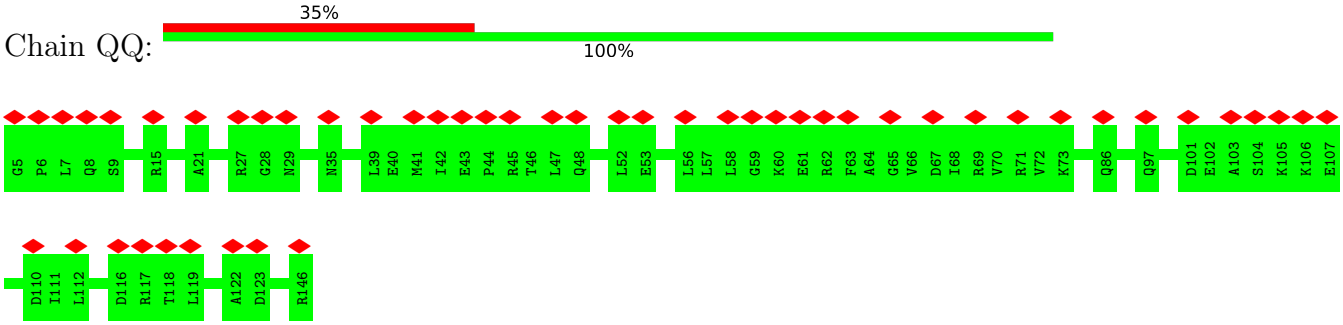
• Molecule 63: 40S ribosomal protein S15

Chain PP:



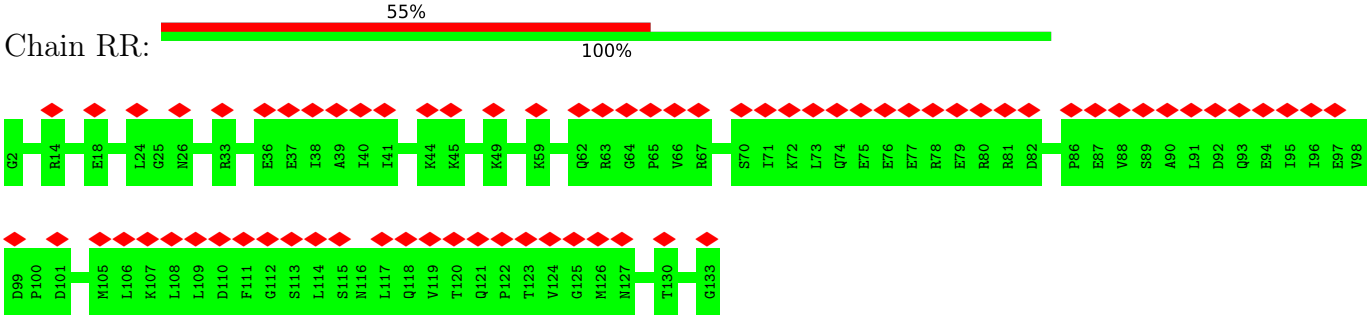
• Molecule 64: 40S ribosomal protein S16

Chain QQ:



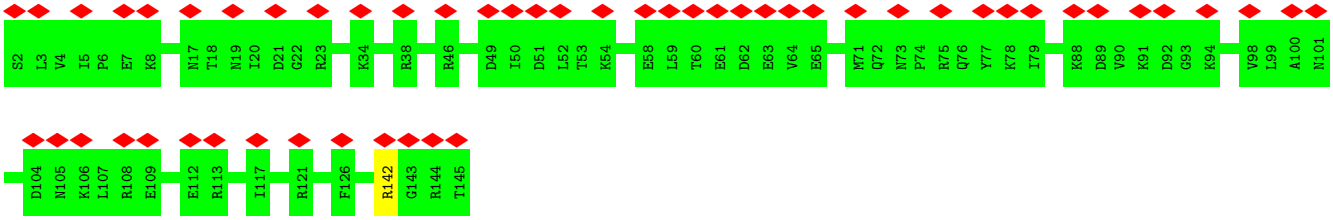
• Molecule 65: 40S ribosomal protein S17

Chain RR:

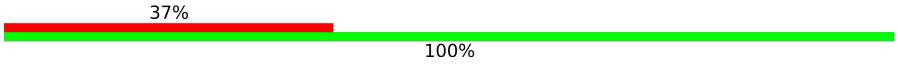


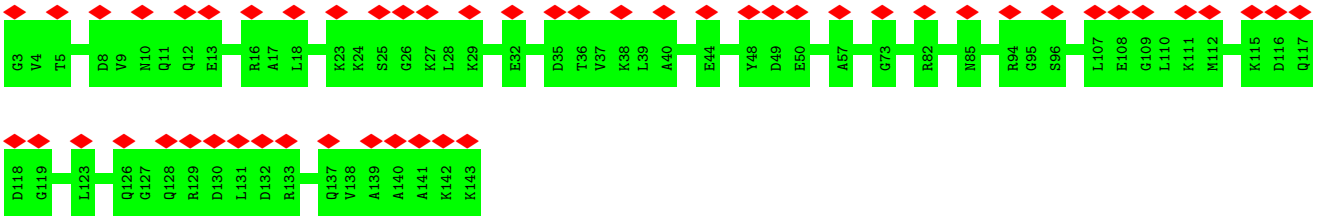
• Molecule 66: 40S ribosomal protein S18

Chain SS:

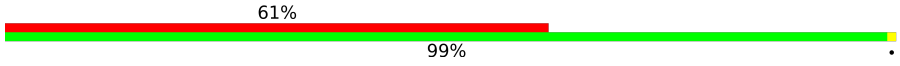


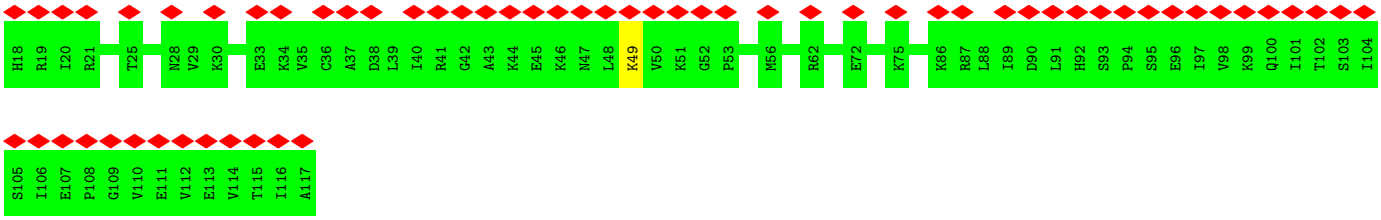
• Molecule 67: 40S ribosomal protein S19



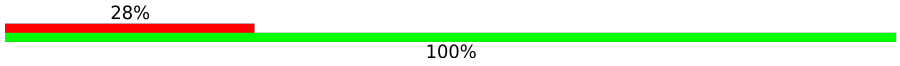


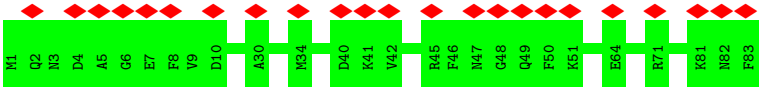
• Molecule 68: 40S ribosomal protein S20



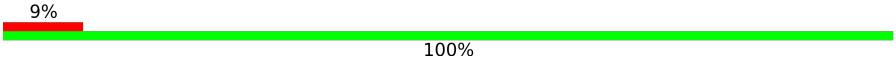


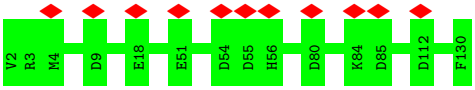
• Molecule 69: eS21



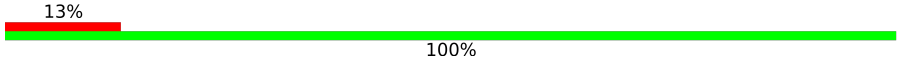


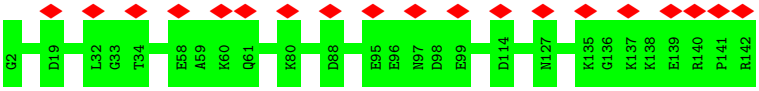
• Molecule 70: 40S ribosomal protein S15a





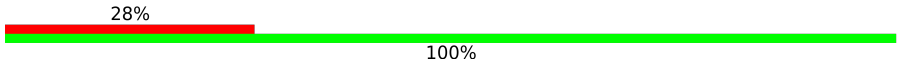
• Molecule 71: 40S ribosomal protein S23

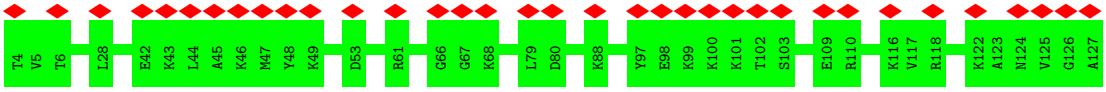




• Molecule 72: 40S ribosomal protein S24

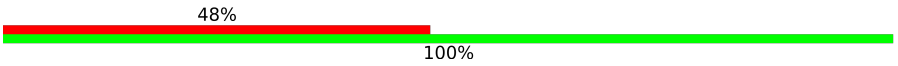
Chain YY:

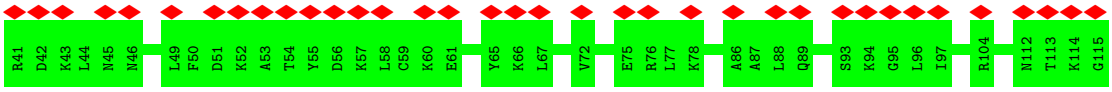




• Molecule 73: 40S ribosomal protein S25

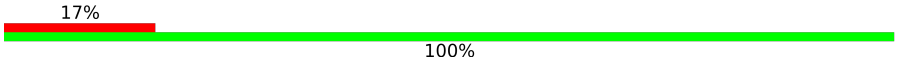
Chain ZZ:

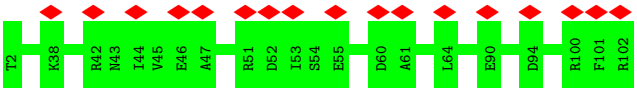




• Molecule 74: eS26

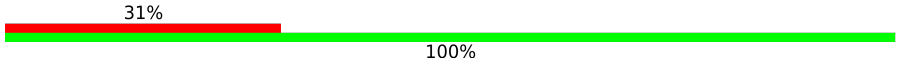
Chain Aa:

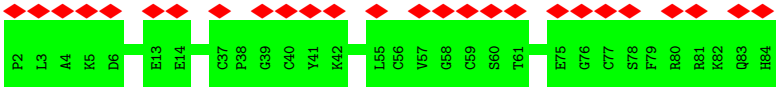




• Molecule 75: 40S ribosomal protein S27

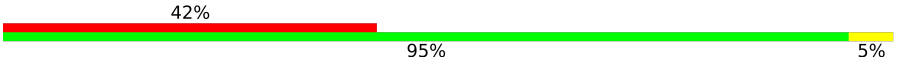
Chain Bb:

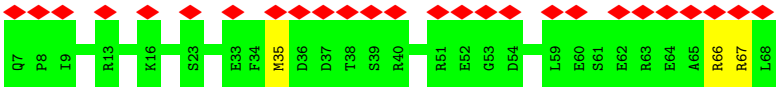




• Molecule 76: 40S ribosomal protein S28

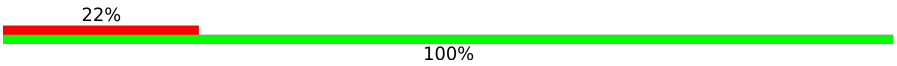
Chain Cc:

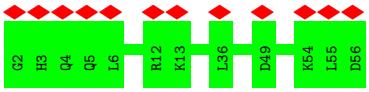




• Molecule 77: 40S ribosomal protein S29

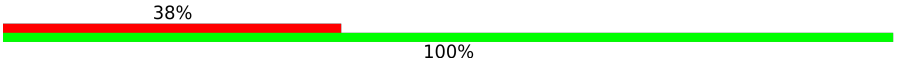
Chain Dd:

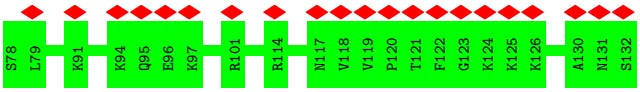




• Molecule 78: 40S ribosomal protein S30

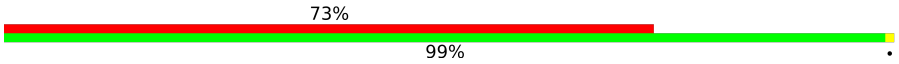
Chain Ee:

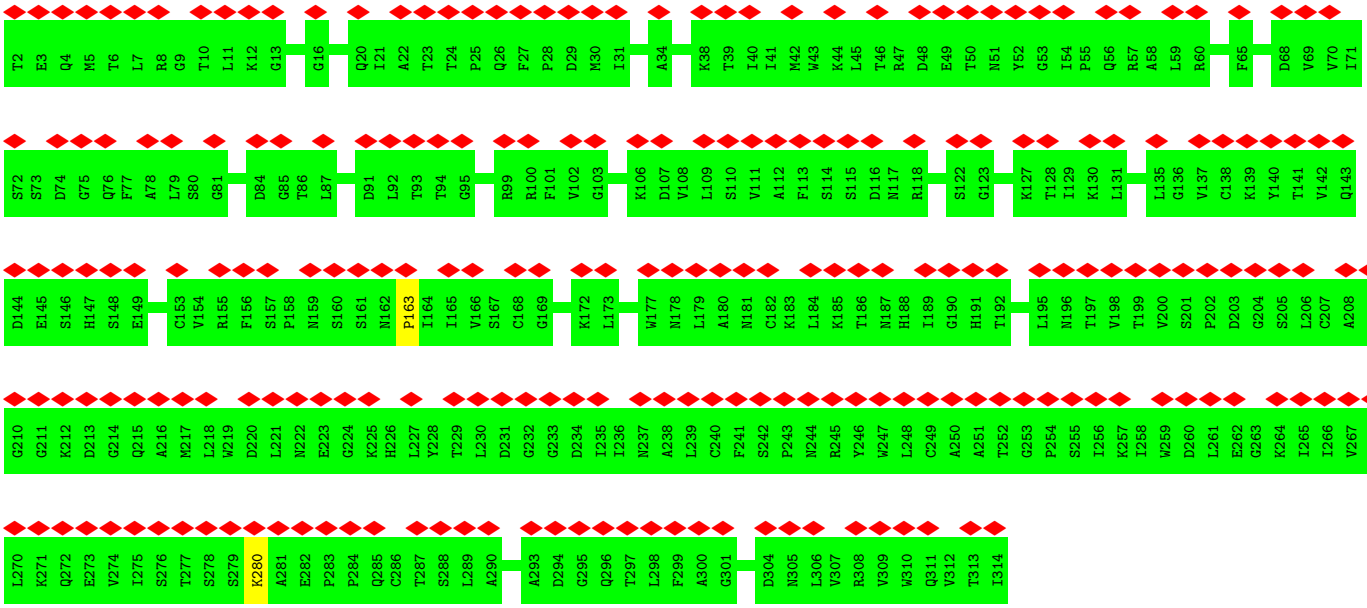




• Molecule 79: Receptor of activated protein C kinase 1

Chain Gg:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52555	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.224	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.037	Depositor
Map size (Å)	651.84, 651.84, 651.84	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.358, 1.358, 1.358	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B9H, B8H, ZN, T6A, OMU, BGH, 6MZ, B8W, UR3, B8N, I4U, M7A, MHG, 7MG, 5MC, 4AC, A2M, PSU, OMG, MA6, B8K, E6G, E7G, B9B, 2MG, B8Q, P7G, 5MU, MQ6, OMC, MLZ, 1MA, B8T, MG, P4U, MMX

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	2	0.28	0/1698	0.83	2/2640 (0.1%)
2	1	0.25	0/145	0.77	0/224
3	5	0.36	0/81475	0.80	34/126990 (0.0%)
4	7	0.34	0/2858	0.73	0/4455
5	8	0.33	0/3540	0.75	0/5513
6	9	0.32	0/39730	0.80	27/61898 (0.0%)
7	A	0.29	0/1936	0.58	0/2596
8	B	0.28	0/3240	0.53	0/4339
9	C	0.28	0/2913	0.56	0/3913
10	D	0.29	0/2427	0.52	0/3250
11	E	0.27	0/1753	0.55	0/2351
12	F	0.29	0/1911	0.53	0/2549
13	G	0.28	0/1861	0.55	1/2504 (0.0%)
14	H	0.27	0/1535	0.57	1/2063 (0.0%)
15	I	0.28	0/1702	0.55	0/2272
16	J	0.28	0/1376	0.59	0/1841
17	L	0.27	0/1733	0.59	0/2316
18	M	0.28	0/1158	0.55	0/1547
19	N	0.29	0/1746	0.58	0/2338
20	O	0.30	0/1662	0.56	0/2222
21	P	0.27	0/1268	0.52	0/1700
22	Q	0.28	0/1539	0.60	0/2054
23	R	0.26	0/1524	0.59	0/2013
24	S	0.29	0/1501	0.55	0/2012
25	T	0.30	0/1326	0.54	0/1770
26	U	0.28	0/814	0.54	0/1092
27	V	0.29	0/987	0.54	0/1324
28	W	0.28	0/666	0.56	0/886
29	X	0.27	0/984	0.55	0/1323
30	Y	0.28	0/1132	0.56	0/1504

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	Z	0.29	0/1130	0.51	0/1507
32	a	0.30	0/1191	0.54	0/1590
33	b	0.26	0/861	0.55	0/1138
34	c	0.30	0/748	0.52	0/1003
35	d	0.27	0/903	0.55	0/1216
36	e	0.28	0/1071	0.53	0/1429
37	f	0.29	0/895	0.58	0/1198
38	g	0.28	0/916	0.58	0/1220
39	h	0.26	0/1021	0.57	0/1348
40	i	0.27	0/841	0.58	0/1112
41	j	0.29	0/720	0.61	0/952
42	k	0.27	0/575	0.53	0/761
43	l	0.25	0/459	0.57	0/608
44	m	0.27	0/415	0.56	0/550
45	n	0.26	0/240	0.69	0/305
46	o	0.27	0/855	0.53	0/1128
47	p	0.29	0/718	0.52	0/953
48	r	0.27	0/1010	0.57	0/1354
49	AA	0.26	0/1747	0.51	0/2374
50	BB	0.27	0/1742	0.51	0/2330
51	CC	0.28	0/1753	0.51	0/2369
52	DD	0.27	0/1788	0.52	0/2407
53	EE	0.27	0/2118	0.54	0/2849
54	FF	0.25	0/1492	0.50	0/2005
55	GG	0.25	0/1946	0.56	0/2590
56	HH	0.37	1/1510 (0.1%)	0.63	3/2022 (0.1%)
57	II	0.26	0/1696	0.54	0/2261
58	JJ	0.26	0/1550	0.57	0/2069
59	KK	0.26	0/834	0.55	0/1125
60	LL	0.29	0/1195	0.54	0/1597
61	NN	0.26	0/1226	0.55	0/1649
62	OO	0.27	0/1029	0.58	0/1380
63	PP	0.32	0/1017	0.63	2/1358 (0.1%)
64	QQ	0.27	0/1146	0.55	0/1534
65	RR	0.26	0/1082	0.52	0/1452
66	SS	0.26	0/1208	0.57	0/1618
67	TT	0.25	0/1115	0.50	0/1493
68	UU	0.25	0/805	0.58	0/1081
69	VV	0.27	0/643	0.54	0/860
70	WW	0.27	0/1051	0.53	0/1406
71	XX	0.27	0/1116	0.52	0/1490
72	YY	0.27	0/1028	0.54	0/1366
73	ZZ	0.27	0/604	0.57	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
74	Aa	0.28	0/828	0.57	0/1109
75	Bb	0.26	0/665	0.51	0/891
76	Cc	0.25	0/490	0.61	0/656
77	Dd	0.27	0/470	0.57	0/623
78	Ee	0.26	0/447	0.57	0/587
79	Gg	0.40	2/2493 (0.1%)	0.63	3/3394 (0.1%)
All	All	0.32	3/220543 (0.0%)	0.71	73/323626 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	G	0	1
20	O	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	Gg	163	PRO	CG-CD	-14.27	1.03	1.50
56	HH	190	PRO	CG-CD	-9.09	1.20	1.50
79	Gg	163	PRO	N-CD	6.23	1.56	1.47

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
79	Gg	163	PRO	N-CD-CG	-15.55	79.87	103.20
56	HH	190	PRO	N-CD-CG	-11.94	85.29	103.20
79	Gg	163	PRO	CA-N-CD	-10.33	97.03	111.50
56	HH	190	PRO	CA-N-CD	-8.84	99.13	111.50
3	5	133	C	N1-C2-O2	8.52	124.01	118.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	G	215	ASP	Peptide
20	O	110	PRO	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	
7	A	246/248 (99%)	235 (96%)	11 (4%)	0	100	100
8	B	392/394 (100%)	383 (98%)	9 (2%)	0	100	100
9	C	357/360 (99%)	342 (96%)	15 (4%)	0	100	100
10	D	289/291 (99%)	277 (96%)	12 (4%)	0	100	100
11	E	207/250 (83%)	200 (97%)	7 (3%)	0	100	100
12	F	223/225 (99%)	218 (98%)	5 (2%)	0	100	100
13	G	222/233 (95%)	214 (96%)	8 (4%)	0	100	100
14	H	188/190 (99%)	182 (97%)	6 (3%)	0	100	100
15	I	201/213 (94%)	195 (97%)	6 (3%)	0	100	100
16	J	167/169 (99%)	162 (97%)	5 (3%)	0	100	100
17	L	208/210 (99%)	204 (98%)	4 (2%)	0	100	100
18	M	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
19	N	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
20	O	197/199 (99%)	192 (98%)	5 (2%)	0	100	100
21	P	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
22	Q	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
23	R	178/180 (99%)	175 (98%)	3 (2%)	0	100	100
24	S	174/176 (99%)	165 (95%)	9 (5%)	0	100	100
25	T	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
26	U	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
27	V	128/130 (98%)	126 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	W	76/95 (80%)	74 (97%)	2 (3%)	0	100	100
29	X	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
30	Y	132/134 (98%)	131 (99%)	1 (1%)	0	100	100
31	Z	133/135 (98%)	129 (97%)	4 (3%)	0	100	100
32	a	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
33	b	100/116 (86%)	96 (96%)	4 (4%)	0	100	100
34	c	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
35	d	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
36	e	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
37	f	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
38	g	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
39	h	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
40	i	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
41	j	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
42	k	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
43	l	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
44	m	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
45	n	23/25 (92%)	23 (100%)	0	0	100	100
46	o	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
47	p	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
48	r	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
49	AA	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
50	BB	209/211 (99%)	200 (96%)	9 (4%)	0	100	100
51	CC	219/221 (99%)	215 (98%)	4 (2%)	0	100	100
52	DD	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
53	EE	260/262 (99%)	256 (98%)	4 (2%)	0	100	100
54	FF	181/191 (95%)	169 (93%)	12 (7%)	0	100	100
55	GG	235/237 (99%)	232 (99%)	3 (1%)	0	100	100
56	HH	181/189 (96%)	174 (96%)	7 (4%)	0	100	100
57	II	199/206 (97%)	193 (97%)	6 (3%)	0	100	100
58	JJ	183/185 (99%)	179 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	KK	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
60	LL	139/151 (92%)	136 (98%)	3 (2%)	0	100	100
61	NN	147/149 (99%)	144 (98%)	3 (2%)	0	100	100
62	OO	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
63	PP	118/120 (98%)	108 (92%)	10 (8%)	0	100	100
64	QQ	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
65	RR	130/132 (98%)	129 (99%)	1 (1%)	0	100	100
66	SS	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
67	TT	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
68	UU	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
69	VV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
70	WW	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
71	XX	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
72	YY	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
73	ZZ	73/75 (97%)	73 (100%)	0	0	100	100
74	Aa	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
75	Bb	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
76	Cc	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
77	Dd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
78	Ee	53/55 (96%)	53 (100%)	0	0	100	100
79	Gg	311/313 (99%)	289 (93%)	22 (7%)	0	100	100
All	All	10937/11205 (98%)	10582 (97%)	355 (3%)	0	100	100

There are no Ramachandran outliers to report.

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
7	A	190/190 (100%)	188 (99%)	2 (1%)	73 89
8	B	342/342 (100%)	342 (100%)	0	100 100
9	C	299/299 (100%)	298 (100%)	1 (0%)	92 96
10	D	247/247 (100%)	247 (100%)	0	100 100
11	E	189/222 (85%)	188 (100%)	1 (0%)	88 94
12	F	196/196 (100%)	196 (100%)	0	100 100
13	G	195/200 (98%)	194 (100%)	1 (0%)	88 94
14	H	169/169 (100%)	169 (100%)	0	100 100
15	I	175/180 (97%)	174 (99%)	1 (1%)	86 94
16	J	142/142 (100%)	142 (100%)	0	100 100
17	L	175/175 (100%)	174 (99%)	1 (1%)	86 94
18	M	117/117 (100%)	116 (99%)	1 (1%)	78 91
19	N	171/171 (100%)	171 (100%)	0	100 100
20	O	171/171 (100%)	171 (100%)	0	100 100
21	P	134/134 (100%)	134 (100%)	0	100 100
22	Q	164/164 (100%)	163 (99%)	1 (1%)	86 94
23	R	159/159 (100%)	159 (100%)	0	100 100
24	S	157/157 (100%)	157 (100%)	0	100 100
25	T	139/139 (100%)	139 (100%)	0	100 100
26	U	88/88 (100%)	88 (100%)	0	100 100
27	V	100/100 (100%)	100 (100%)	0	100 100
28	W	67/81 (83%)	67 (100%)	0	100 100
29	X	106/106 (100%)	106 (100%)	0	100 100
30	Y	124/124 (100%)	124 (100%)	0	100 100
31	Z	117/117 (100%)	117 (100%)	0	100 100
32	a	119/119 (100%)	119 (100%)	0	100 100
33	b	84/95 (88%)	84 (100%)	0	100 100
34	c	81/81 (100%)	81 (100%)	0	100 100
35	d	98/98 (100%)	98 (100%)	0	100 100
36	e	114/114 (100%)	114 (100%)	0	100 100
37	f	88/88 (100%)	88 (100%)	0	100 100
38	g	98/98 (100%)	98 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	h	109/109 (100%)	109 (100%)	0	100	100
40	i	86/86 (100%)	86 (100%)	0	100	100
41	j	73/73 (100%)	73 (100%)	0	100	100
42	k	64/64 (100%)	63 (98%)	1 (2%)	62	84
43	l	47/47 (100%)	47 (100%)	0	100	100
44	m	46/46 (100%)	46 (100%)	0	100	100
45	n	24/24 (100%)	24 (100%)	0	100	100
46	o	91/91 (100%)	91 (100%)	0	100	100
47	p	74/74 (100%)	74 (100%)	0	100	100
48	r	108/108 (100%)	108 (100%)	0	100	100
49	AA	180/181 (99%)	180 (100%)	0	100	100
50	BB	192/192 (100%)	192 (100%)	0	100	100
51	CC	187/187 (100%)	187 (100%)	0	100	100
52	DD	189/189 (100%)	188 (100%)	1 (0%)	88	94
53	EE	224/224 (100%)	223 (100%)	1 (0%)	91	96
54	FF	158/161 (98%)	158 (100%)	0	100	100
55	GG	207/207 (100%)	207 (100%)	0	100	100
56	HH	165/169 (98%)	165 (100%)	0	100	100
57	II	177/178 (99%)	176 (99%)	1 (1%)	86	94
58	JJ	161/161 (100%)	161 (100%)	0	100	100
59	KK	87/87 (100%)	87 (100%)	0	100	100
60	LL	130/136 (96%)	130 (100%)	0	100	100
61	NN	130/130 (100%)	130 (100%)	0	100	100
62	OO	106/106 (100%)	106 (100%)	0	100	100
63	PP	109/109 (100%)	109 (100%)	0	100	100
64	QQ	117/117 (100%)	117 (100%)	0	100	100
65	RR	119/119 (100%)	119 (100%)	0	100	100
66	SS	125/125 (100%)	124 (99%)	1 (1%)	81	92
67	TT	111/111 (100%)	111 (100%)	0	100	100
68	UU	92/92 (100%)	91 (99%)	1 (1%)	73	89
69	VV	67/67 (100%)	67 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
70	WW	112/112 (100%)	112 (100%)	0	100 100
71	XX	113/113 (100%)	113 (100%)	0	100 100
72	YY	107/107 (100%)	107 (100%)	0	100 100
73	ZZ	66/66 (100%)	66 (100%)	0	100 100
74	Aa	88/88 (100%)	88 (100%)	0	100 100
75	Bb	75/75 (100%)	75 (100%)	0	100 100
76	Cc	55/55 (100%)	52 (94%)	3 (6%)	21 53
77	Dd	48/48 (100%)	48 (100%)	0	100 100
78	Ee	46/46 (100%)	46 (100%)	0	100 100
79	Gg	272/272 (100%)	271 (100%)	1 (0%)	91 96
All	All	9552/9635 (99%)	9533 (100%)	19 (0%)	93 97

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
68	UU	49	LYS
76	Cc	67	ARG
79	Gg	280	LYS
76	Cc	66	ARG
22	Q	91	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 140 such sidechains are listed below:

Mol	Chain	Res	Type
64	QQ	35	ASN
65	RR	48	ASN
71	XX	73	GLN
26	U	94	ASN
25	T	54	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	68/76 (89%)	13 (19%)	0
2	1	5/6 (83%)	2 (40%)	0
3	5	3445/3499 (98%)	627 (18%)	46 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	7	119/120 (99%)	9 (7%)	0
5	8	148/156 (94%)	25 (16%)	1 (0%)
6	9	1678/1698 (98%)	315 (18%)	17 (1%)
All	All	5463/5555 (98%)	991 (18%)	64 (1%)

5 of 991 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	11	G
1	2	13	G
1	2	14	C
1	2	19	G
1	2	37	T6A

5 of 64 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	9	874	G
6	9	1394	G
3	5	1440	U
3	5	1438	U
6	9	1395	C

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

138 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	$\#\|Z\| > 2$
3	I4U	5	1659	3	21,24,25	3.47	9 (42%)	27,34,37	0.94	1 (3%)
3	OMC	5	3909	3	19,22,23	2.95	8 (42%)	26,31,34	0.92	1 (3%)
3	B9B	5	237	3	21,28,29	1.98	3 (14%)	23,40,43	6.24	5 (21%)
6	4AC	9	1842	6	21,24,25	3.17	10 (47%)	29,34,37	1.12	4 (13%)
3	7MG	5	4550	3	22,26,27	3.70	10 (45%)	29,39,42	2.04	9 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	M7A	9	1806	6	20,25,26	2.01	3 (15%)	28,37,40	3.98	8 (28%)
3	B8Q	5	1456	3	17,22,23	2.86	5 (29%)	22,32,35	2.08	4 (18%)
3	A2M	5	2401	3,80	18,25,26	3.61	8 (44%)	18,36,39	3.36	4 (22%)
3	B8W	5	4129	3	18,26,27	2.10	2 (11%)	21,38,41	2.44	7 (33%)
3	OMC	5	2804	3	19,22,23	2.96	8 (42%)	26,31,34	0.65	0
3	PSU	5	3729	3	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
3	1MA	5	4415	3	16,25,26	4.32	5 (31%)	18,37,40	1.78	3 (16%)
3	B8H	5	3762	3	19,22,23	6.80	6 (31%)	22,32,35	2.34	5 (22%)
6	A2M	9	27	6,80	18,25,26	3.60	8 (44%)	18,36,39	3.27	3 (16%)
3	OMG	5	2424	3	18,26,27	2.48	8 (44%)	19,38,41	1.51	4 (21%)
3	OMG	5	1625	3	18,26,27	2.47	8 (44%)	19,38,41	1.53	4 (21%)
3	5MC	5	4447	3	18,22,23	3.50	7 (38%)	26,32,35	1.06	1 (3%)
3	B8T	5	4483	3	19,22,23	3.55	8 (42%)	26,31,34	0.90	1 (3%)
3	5MC	5	4335	3	18,22,23	3.58	7 (38%)	26,32,35	1.08	1 (3%)
3	OMG	5	373	3	18,26,27	2.47	8 (44%)	19,38,41	1.55	4 (21%)
3	I4U	5	4194	3	21,24,25	3.43	9 (42%)	27,34,37	1.02	1 (3%)
3	A2M	5	398	3	18,25,26	3.60	8 (44%)	18,36,39	3.36	3 (16%)
3	B8K	5	4690	14,3	24,28,29	3.40	11 (45%)	30,42,45	2.35	11 (36%)
6	PSU	9	119	6	18,21,22	1.02	1 (5%)	22,30,33	1.69	4 (18%)
3	2MG	5	4872	18,3	18,26,27	2.53	7 (38%)	16,38,41	1.58	4 (25%)
3	2MG	5	729	3	18,26,27	2.45	7 (38%)	16,38,41	1.37	3 (18%)
3	A2M	5	2363	3,80	18,25,26	3.62	8 (44%)	18,36,39	3.37	4 (22%)
6	B8Q	9	1219	6,80	17,22,23	2.95	4 (23%)	22,32,35	2.35	7 (31%)
3	E7G	5	1797	3	24,27,28	3.98	11 (45%)	30,40,43	2.28	10 (33%)
3	2MG	5	1517	3	18,26,27	2.43	7 (38%)	16,38,41	1.45	4 (25%)
6	5MC	9	1374	6	18,22,23	3.55	7 (38%)	26,32,35	1.07	2 (7%)
3	PSU	5	4531	3	18,21,22	1.08	1 (5%)	22,30,33	1.82	5 (22%)
3	OMG	5	3792	3	18,26,27	2.48	8 (44%)	19,38,41	1.50	4 (21%)
6	OMG	9	644	6	18,26,27	2.44	8 (44%)	19,38,41	1.49	4 (21%)
3	P7G	5	1909	3	24,28,29	4.06	11 (45%)	27,41,44	1.56	2 (7%)
3	OMC	5	3869	3	19,22,23	3.00	8 (42%)	26,31,34	0.73	0
3	PSU	5	4500	3	18,21,22	1.06	1 (5%)	22,30,33	1.86	5 (22%)
6	PSU	9	823	6	18,21,22	1.08	1 (5%)	22,30,33	1.84	5 (22%)
3	B8K	5	3897	3	24,28,29	3.34	11 (45%)	30,42,45	2.33	10 (33%)
3	B9H	5	2786	3	20,25,26	3.09	3 (15%)	22,35,38	1.46	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	OMC	5	3701	3,80	19,22,23	2.96	8 (42%)	26,31,34	0.69	0
6	OMU	9	116	6	19,22,23	3.00	8 (42%)	26,31,34	1.69	5 (19%)
3	OMG	5	2364	3	18,26,27	2.43	8 (44%)	19,38,41	1.50	4 (21%)
6	PSU	9	822	6	18,21,22	1.07	1 (5%)	22,30,33	1.84	6 (27%)
1	T6A	2	37	1	27,34,35	0.98	1 (3%)	29,49,52	2.48	7 (24%)
3	A2M	5	1326	3	18,25,26	3.61	8 (44%)	18,36,39	3.37	4 (22%)
3	OMG	5	4637	3	18,26,27	2.47	8 (44%)	19,38,41	1.52	4 (21%)
6	MA6	9	1851	6	19,26,27	1.37	3 (15%)	18,38,41	4.33	3 (16%)
6	PSU	9	1081	6	18,21,22	0.99	1 (5%)	22,30,33	1.76	4 (18%)
3	B8T	5	4671	3	19,22,23	3.58	8 (42%)	26,31,34	0.89	1 (3%)
3	OMG	5	4196	3	18,26,27	2.45	8 (44%)	19,38,41	1.53	4 (21%)
3	OMG	5	1883	3	18,26,27	2.50	8 (44%)	19,38,41	1.59	4 (21%)
3	P7G	5	3880	3	24,28,29	3.93	11 (45%)	27,41,44	1.69	3 (11%)
3	A2M	5	4571	3	18,25,26	3.63	8 (44%)	18,36,39	3.38	3 (16%)
3	B8W	5	4529	3,80	18,26,27	2.10	2 (11%)	21,38,41	2.43	9 (42%)
3	OMC	5	4536	3	19,22,23	2.95	8 (42%)	26,31,34	0.69	0
3	PSU	5	4293	3	18,21,22	1.04	1 (5%)	22,30,33	1.78	4 (18%)
3	A2M	5	4523	3,80	18,25,26	3.60	7 (38%)	18,36,39	3.28	3 (16%)
3	A2M	5	3785	3	18,25,26	3.65	8 (44%)	18,36,39	3.41	5 (27%)
3	OMG	5	4623	3	18,26,27	2.47	8 (44%)	19,38,41	1.53	4 (21%)
6	5MU	9	814	6	19,22,23	4.91	7 (36%)	28,32,35	3.60	9 (32%)
3	PSU	5	1582	3	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
3	A2M	5	3825	3	18,25,26	3.60	7 (38%)	18,36,39	3.30	3 (16%)
3	PSU	5	4628	3	18,21,22	1.06	1 (5%)	22,30,33	1.86	4 (18%)
3	OMC	5	2861	3	19,22,23	3.01	8 (42%)	26,31,34	0.78	0
3	UR3	5	4597	3	19,22,23	2.82	6 (31%)	26,32,35	1.19	2 (7%)
6	MMX	9	568	6	19,23,24	3.94	5 (26%)	22,33,36	2.84	5 (22%)
3	PSU	5	1677	3	18,21,22	1.06	1 (5%)	22,30,33	1.84	4 (18%)
6	6MZ	9	1832	6,80	18,25,26	1.83	3 (16%)	16,36,39	3.52	4 (25%)
6	OMC	9	1710	6	19,22,23	3.00	8 (42%)	26,31,34	0.73	0
6	A2M	9	159	6	18,25,26	3.60	8 (44%)	18,36,39	3.45	4 (22%)
9	MLZ	C	333	9	8,9,10	0.81	0	4,9,11	0.63	0
3	MHG	5	4371	3	29,32,33	3.81	11 (37%)	34,46,49	2.38	11 (32%)
6	OMC	9	174	6	19,22,23	3.04	8 (42%)	26,31,34	0.72	0
3	M7A	5	4564	3	20,25,26	1.98	3 (15%)	28,37,40	3.89	8 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	6MZ	5	4220	3	18,25,26	1.90	3 (16%)	16,36,39	3.59	3 (18%)
3	B8W	5	2380	3	18,26,27	2.10	2 (11%)	21,38,41	2.42	7 (33%)
3	A2M	5	3723	3	18,25,26	3.59	8 (44%)	18,36,39	3.26	4 (22%)
3	P4U	5	1348	3	21,24,25	3.55	8 (38%)	27,33,36	1.00	1 (3%)
6	UR3	9	1830	6	19,22,23	2.83	6 (31%)	26,32,35	1.39	3 (11%)
3	OMG	5	1316	3	18,26,27	2.46	8 (44%)	19,38,41	1.54	4 (21%)
3	5MU	5	4083	3	19,22,23	4.90	7 (36%)	28,32,35	3.55	9 (32%)
3	B8H	5	4296	3	19,22,23	6.81	6 (31%)	22,32,35	2.38	5 (22%)
6	A2M	9	484	6	18,25,26	3.62	8 (44%)	18,36,39	3.37	4 (22%)
3	OMG	5	4370	3	18,26,27	2.48	8 (44%)	19,38,41	1.52	4 (21%)
3	B8W	5	4185	3	18,26,27	2.10	2 (11%)	21,38,41	2.42	7 (33%)
44	MLZ	m	72	44	8,9,10	0.77	0	4,9,11	0.58	0
6	A2M	9	166	6	18,25,26	3.62	8 (44%)	18,36,39	3.42	5 (27%)
6	OMU	9	121	6	19,22,23	3.00	8 (42%)	26,31,34	1.73	5 (19%)
3	E7G	5	2297	3	24,27,28	3.99	11 (45%)	30,40,43	2.22	10 (33%)
3	OMU	5	4620	3	19,22,23	2.98	8 (42%)	26,31,34	1.76	5 (19%)
3	A2M	5	3718	3	18,25,26	3.61	8 (44%)	18,36,39	3.29	4 (22%)
3	PSU	5	4442	3	18,21,22	1.08	2 (11%)	22,30,33	1.87	6 (27%)
3	PSU	5	2508	3	18,21,22	1.05	1 (5%)	22,30,33	1.82	4 (18%)
3	UR3	5	1866	3	19,22,23	2.84	7 (36%)	26,32,35	1.29	2 (7%)
6	OMC	9	1703	6	19,22,23	2.95	8 (42%)	26,31,34	0.70	0
3	A2M	5	3867	3	18,25,26	3.62	8 (44%)	18,36,39	3.35	4 (22%)
6	OMC	9	517	6	19,22,23	3.01	8 (42%)	26,31,34	0.75	0
3	7MG	5	2522	3	22,26,27	3.68	10 (45%)	29,39,42	2.03	9 (31%)
3	A2M	5	1871	3,80	18,25,26	3.60	7 (38%)	18,36,39	3.36	3 (16%)
3	PSU	5	4450	3,80	18,21,22	1.05	1 (5%)	22,30,33	1.79	5 (22%)
3	OMC	5	2422	3,80	19,22,23	2.99	8 (42%)	26,31,34	0.75	0
3	OMG	5	2773	3	18,26,27	2.51	8 (44%)	19,38,41	1.53	4 (21%)
3	A2M	5	1524	3	18,25,26	3.60	7 (38%)	18,36,39	3.36	4 (22%)
3	OMG	5	4494	3	18,26,27	2.47	8 (44%)	19,38,41	1.52	4 (21%)
3	B9B	5	2754	3	21,28,29	1.99	3 (14%)	23,40,43	6.49	5 (21%)
6	OMG	9	509	6,80	18,26,27	2.46	8 (44%)	19,38,41	1.51	4 (21%)
3	1MA	5	1322	3,80	16,25,26	4.22	5 (31%)	18,37,40	1.88	3 (16%)
6	A2M	9	668	6,80	18,25,26	3.64	9 (50%)	18,36,39	3.41	3 (16%)
3	PSU	5	4636	3	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PSU	5	4403	3	18,21,22	1.07	1 (5%)	22,30,33	1.69	5 (22%)
6	OMG	9	683	6	18,26,27	2.49	8 (44%)	19,38,41	1.55	4 (21%)
3	OMC	5	2365	3	19,22,23	2.97	8 (42%)	26,31,34	0.74	0
6	PSU	9	1243	6	18,21,22	1.05	1 (5%)	22,30,33	1.75	4 (18%)
6	A2M	9	1031	6	18,25,26	3.60	8 (44%)	18,36,39	3.40	3 (16%)
3	OMG	5	1522	3	18,26,27	2.45	8 (44%)	19,38,41	1.51	4 (21%)
6	PSU	9	612	6	18,21,22	1.03	1 (5%)	22,30,33	1.75	5 (22%)
6	A2M	9	1678	6	18,25,26	3.56	8 (44%)	18,36,39	3.36	3 (16%)
3	UR3	5	4530	3	19,22,23	2.79	7 (36%)	26,32,35	1.26	2 (7%)
6	MA6	9	1850	6	19,26,27	1.42	3 (15%)	18,38,41	4.20	3 (16%)
3	A2M	5	1534	3,80	18,25,26	3.61	8 (44%)	18,36,39	3.36	3 (16%)
3	E6G	5	4355	3	20,27,28	2.81	3 (15%)	22,39,42	3.07	7 (31%)
6	4AC	9	1337	6	21,24,25	3.23	9 (42%)	29,34,37	1.06	3 (10%)
3	PSU	5	1683	3	18,21,22	1.04	1 (5%)	22,30,33	1.78	4 (18%)
3	B9B	5	1574	3	21,28,29	2.00	3 (14%)	23,40,43	6.43	5 (21%)
3	OMG	5	2050	3	18,26,27	2.44	8 (44%)	19,38,41	1.51	4 (21%)
3	BGH	5	3899	3,80	25,29,30	4.49	19 (76%)	31,43,46	2.31	12 (38%)
3	PSU	5	3764	3	18,21,22	1.04	1 (5%)	22,30,33	1.70	4 (18%)
5	OMU	8	14	5,3	19,22,23	2.98	8 (42%)	26,31,34	1.70	5 (19%)
3	5MC	5	3782	3	18,22,23	3.51	7 (38%)	26,32,35	1.06	2 (7%)
3	B8H	5	1860	3	19,22,23	6.81	6 (31%)	22,32,35	2.34	5 (22%)
3	7MG	5	1605	3	22,26,27	3.73	10 (45%)	29,39,42	2.06	9 (31%)
3	OMU	5	4306	3	19,22,23	2.98	8 (42%)	26,31,34	1.73	5 (19%)
3	OMC	5	3887	3	19,22,23	2.98	8 (42%)	26,31,34	0.75	0
3	B8W	5	4472	3	18,26,27	2.10	2 (11%)	21,38,41	2.39	7 (33%)
6	B8N	9	1248	6	24,29,30	3.06	7 (29%)	29,42,45	1.72	5 (17%)
3	PSU	5	3715	3	18,21,22	1.03	1 (5%)	22,30,33	1.75	4 (18%)
3	OMG	5	4870	3	18,26,27	2.51	8 (44%)	19,38,41	1.54	4 (21%)

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
3	I4U	5	1659	3	-	1/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	5	3909	3	-	2/9/27/28	0/2/2/2
3	B9B	5	237	3	-	5/7/29/30	0/3/3/3
6	4AC	9	1842	6	-	0/11/29/30	0/2/2/2
3	7MG	5	4550	3	-	0/7/37/38	0/3/3/3
6	M7A	9	1806	6	-	2/7/37/38	0/3/3/3
3	B8Q	5	1456	3	-	0/7/42/43	0/2/2/2
3	A2M	5	2401	3,80	-	0/5/27/28	0/3/3/3
3	B8W	5	4129	3	-	2/5/27/28	0/3/3/3
3	OMC	5	2804	3	-	0/9/27/28	0/2/2/2
3	PSU	5	3729	3	-	2/7/25/26	0/2/2/2
3	1MA	5	4415	3	-	1/3/25/26	0/3/3/3
3	B8H	5	3762	3	-	2/7/25/26	0/2/2/2
6	A2M	9	27	6,80	-	1/5/27/28	0/3/3/3
3	OMG	5	2424	3	-	2/5/27/28	0/3/3/3
3	OMG	5	1625	3	-	2/5/27/28	0/3/3/3
3	5MC	5	4447	3	-	0/7/25/26	0/2/2/2
3	B8T	5	4483	3	-	0/7/27/28	0/2/2/2
3	5MC	5	4335	3	-	0/7/25/26	0/2/2/2
3	OMG	5	373	3	-	0/5/27/28	0/3/3/3
3	I4U	5	4194	3	-	2/9/29/30	0/2/2/2
3	A2M	5	398	3	-	2/5/27/28	0/3/3/3
3	B8K	5	4690	14,3	-	0/11/41/42	0/3/3/3
6	PSU	9	119	6	-	0/7/25/26	0/2/2/2
3	2MG	5	4872	18,3	-	0/5/27/28	0/3/3/3
3	2MG	5	729	3	-	1/5/27/28	0/3/3/3
3	A2M	5	2363	3,80	-	0/5/27/28	0/3/3/3
6	B8Q	9	1219	6,80	-	2/7/42/43	0/2/2/2
3	E7G	5	1797	3	-	2/9/39/40	0/3/3/3
3	2MG	5	1517	3	-	0/5/27/28	0/3/3/3
6	5MC	9	1374	6	-	0/7/25/26	0/2/2/2
3	PSU	5	4531	3	-	1/7/25/26	0/2/2/2
3	OMG	5	3792	3	-	2/5/27/28	0/3/3/3
6	OMG	9	644	6	-	3/5/27/28	0/3/3/3
3	P7G	5	1909	3	-	1/10/40/41	0/3/3/3
3	OMC	5	3869	3	-	0/9/27/28	0/2/2/2
3	PSU	5	4500	3	-	3/7/25/26	0/2/2/2
6	PSU	9	823	6	-	0/7/25/26	0/2/2/2
3	B8K	5	3897	3	-	3/11/41/42	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	B9H	5	2786	3	-	1/12/47/48	0/2/2/2
3	OMC	5	3701	3,80	-	4/9/27/28	0/2/2/2
6	OMU	9	116	6	-	2/9/27/28	0/2/2/2
3	OMG	5	2364	3	-	3/5/27/28	0/3/3/3
6	PSU	9	822	6	-	0/7/25/26	0/2/2/2
1	T6A	2	37	1	-	4/19/41/42	0/3/3/3
3	A2M	5	1326	3	-	1/5/27/28	0/3/3/3
3	OMG	5	4637	3	-	2/5/27/28	0/3/3/3
6	MA6	9	1851	6	-	2/7/29/30	0/3/3/3
6	PSU	9	1081	6	-	0/7/25/26	0/2/2/2
3	B8T	5	4671	3	-	1/7/27/28	0/2/2/2
3	OMG	5	4196	3	-	0/5/27/28	0/3/3/3
3	OMG	5	1883	3	-	2/5/27/28	0/3/3/3
3	P7G	5	3880	3	-	2/10/40/41	0/3/3/3
3	A2M	5	4571	3	-	1/5/27/28	0/3/3/3
3	B8W	5	4529	3,80	-	2/5/27/28	0/3/3/3
3	OMC	5	4536	3	-	0/9/27/28	0/2/2/2
3	PSU	5	4293	3	-	0/7/25/26	0/2/2/2
3	A2M	5	4523	3,80	-	2/5/27/28	0/3/3/3
3	A2M	5	3785	3	-	3/5/27/28	0/3/3/3
3	OMG	5	4623	3	-	0/5/27/28	0/3/3/3
6	5MU	9	814	6	-	0/7/25/26	0/2/2/2
3	PSU	5	1582	3	-	0/7/25/26	0/2/2/2
3	A2M	5	3825	3	-	1/5/27/28	0/3/3/3
3	PSU	5	4628	3	-	0/7/25/26	0/2/2/2
3	OMC	5	2861	3	-	1/9/27/28	0/2/2/2
3	UR3	5	4597	3	-	0/7/25/26	0/2/2/2
6	MMX	9	568	6	-	4/9/44/45	0/2/2/2
3	PSU	5	1677	3	-	5/7/25/26	0/2/2/2
6	6MZ	9	1832	6,80	-	0/5/27/28	0/3/3/3
6	OMC	9	1710	6	-	0/9/27/28	0/2/2/2
6	A2M	9	159	6	-	3/5/27/28	0/3/3/3
9	MLZ	C	333	9	-	3/7/8/10	-
3	MHG	5	4371	3	-	6/16/46/47	0/3/3/3
6	OMC	9	174	6	-	1/9/27/28	0/2/2/2
3	M7A	5	4564	3	-	0/7/37/38	0/3/3/3
3	6MZ	5	4220	3	-	1/5/27/28	0/3/3/3
3	B8W	5	2380	3	-	4/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	5	3723	3	-	0/5/27/28	0/3/3/3
3	P4U	5	1348	3	-	3/10/29/30	0/2/2/2
6	UR3	9	1830	6	-	2/7/25/26	0/2/2/2
3	OMG	5	1316	3	-	1/5/27/28	0/3/3/3
3	5MU	5	4083	3	-	0/7/25/26	0/2/2/2
3	B8H	5	4296	3	-	3/7/25/26	0/2/2/2
6	A2M	9	484	6	-	0/5/27/28	0/3/3/3
3	OMG	5	4370	3	-	0/5/27/28	0/3/3/3
3	B8W	5	4185	3	-	2/5/27/28	0/3/3/3
44	MLZ	m	72	44	-	1/7/8/10	-
6	A2M	9	166	6	-	2/5/27/28	0/3/3/3
6	OMU	9	121	6	-	0/9/27/28	0/2/2/2
3	E7G	5	2297	3	-	3/9/39/40	0/3/3/3
3	OMU	5	4620	3	-	1/9/27/28	0/2/2/2
3	A2M	5	3718	3	-	1/5/27/28	0/3/3/3
3	PSU	5	4442	3	-	0/7/25/26	0/2/2/2
3	PSU	5	2508	3	-	0/7/25/26	0/2/2/2
3	UR3	5	1866	3	-	0/7/25/26	0/2/2/2
6	OMC	9	1703	6	-	2/9/27/28	0/2/2/2
3	A2M	5	3867	3	-	3/5/27/28	0/3/3/3
6	OMC	9	517	6	-	0/9/27/28	0/2/2/2
3	7MG	5	2522	3	-	0/7/37/38	0/3/3/3
3	A2M	5	1871	3,80	-	0/5/27/28	0/3/3/3
3	PSU	5	4450	3,80	-	2/7/25/26	0/2/2/2
3	OMC	5	2422	3,80	-	1/9/27/28	0/2/2/2
3	OMG	5	2773	3	-	1/5/27/28	0/3/3/3
3	A2M	5	1524	3	-	0/5/27/28	0/3/3/3
3	OMG	5	4494	3	-	0/5/27/28	0/3/3/3
3	B9B	5	2754	3	-	3/7/29/30	0/3/3/3
6	OMG	9	509	6,80	-	0/5/27/28	0/3/3/3
3	1MA	5	1322	3,80	-	0/3/25/26	0/3/3/3
6	A2M	9	668	6,80	-	3/5/27/28	0/3/3/3
3	PSU	5	4636	3	-	3/7/25/26	0/2/2/2
3	PSU	5	4403	3	-	2/7/25/26	0/2/2/2
6	OMG	9	683	6	-	2/5/27/28	0/3/3/3
3	OMC	5	2365	3	-	0/9/27/28	0/2/2/2
6	PSU	9	1243	6	-	2/7/25/26	0/2/2/2
6	A2M	9	1031	6	-	0/5/27/28	0/3/3/3
3	OMG	5	1522	3	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PSU	9	612	6	-	0/7/25/26	0/2/2/2
6	A2M	9	1678	6	-	1/5/27/28	0/3/3/3
3	UR3	5	4530	3	-	2/7/25/26	0/2/2/2
6	MA6	9	1850	6	-	0/7/29/30	0/3/3/3
3	A2M	5	1534	3,80	-	2/5/27/28	0/3/3/3
3	E6G	5	4355	3	-	4/6/28/29	0/3/3/3
6	4AC	9	1337	6	-	0/11/29/30	0/2/2/2
3	PSU	5	1683	3	-	0/7/25/26	0/2/2/2
3	B9B	5	1574	3	-	3/7/29/30	0/3/3/3
3	OMG	5	2050	3	-	0/5/27/28	0/3/3/3
3	BGH	5	3899	3,80	-	1/13/43/44	0/3/3/3
3	PSU	5	3764	3	-	2/7/25/26	0/2/2/2
5	OMU	8	14	5,3	-	1/9/27/28	0/2/2/2
3	5MC	5	3782	3	-	2/7/25/26	0/2/2/2
3	B8H	5	1860	3	-	0/7/25/26	0/2/2/2
3	7MG	5	1605	3	-	0/7/37/38	0/3/3/3
3	OMU	5	4306	3	-	0/9/27/28	0/2/2/2
3	OMC	5	3887	3	-	1/9/27/28	0/2/2/2
3	B8W	5	4472	3	-	2/5/27/28	0/3/3/3
6	B8N	9	1248	6	-	1/16/34/35	0/2/2/2
3	PSU	5	3715	3	-	0/7/25/26	0/2/2/2
3	OMG	5	4870	3	-	4/5/27/28	0/3/3/3

The worst 5 of 852 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	1860	B8H	C6-C5	-16.61	1.11	1.34
3	5	4296	B8H	C6-C5	-16.58	1.11	1.34
3	5	3762	B8H	C6-C5	-16.51	1.11	1.34
3	5	1860	B8H	C4-N3	-15.74	1.09	1.38
3	5	4296	B8H	C4-N3	-15.74	1.09	1.38

The worst 5 of 564 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	5	2754	B9B	O6-C6-N1	-29.76	94.43	120.12
3	5	1574	B9B	O6-C6-N1	-29.59	94.58	120.12
3	5	237	B9B	O6-C6-N1	-28.62	95.42	120.12
6	9	1851	MA6	N1-C6-N6	-16.50	99.69	117.06
6	9	1850	MA6	N1-C6-N6	-15.83	100.40	117.06

There are no chirality outliers.

5 of 174 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	37	T6A	N6-C10-N11-C12
1	2	37	T6A	O10-C10-N11-C12
3	5	237	B9B	C5-C6-O6-C61
3	5	237	B9B	N1-C6-O6-C61
3	5	237	B9B	C3'-C4'-C5'-O5'

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 (i)

Of 304 ligands modelled in this entry, 303 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
81	MQ6	5	5296	-	39,42,42	1.49	5 (12%)	38,65,65	1.76	6 (15%)

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
81	MQ6	5	5296	-	-	10/26/73/73	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	5	5296	MQ6	O37-C06	-4.94	1.33	1.43
81	5	5296	MQ6	C16-C15	3.44	1.59	1.54
81	5	5296	MQ6	C05-C06	3.20	1.59	1.54
81	5	5296	MQ6	C07-C06	-2.70	1.50	1.53
81	5	5296	MQ6	O38-C02	-2.11	1.39	1.44

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	5	5296	MQ6	O37-C06-C07	5.83	123.04	109.40
81	5	5296	MQ6	O14-C12-C06	5.39	121.28	111.27
81	5	5296	MQ6	C23-C22-C21	-3.05	112.69	119.42
81	5	5296	MQ6	O14-C12-O13	-2.88	118.78	123.97
81	5	5296	MQ6	C28-C29-N25	2.62	107.74	103.95

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

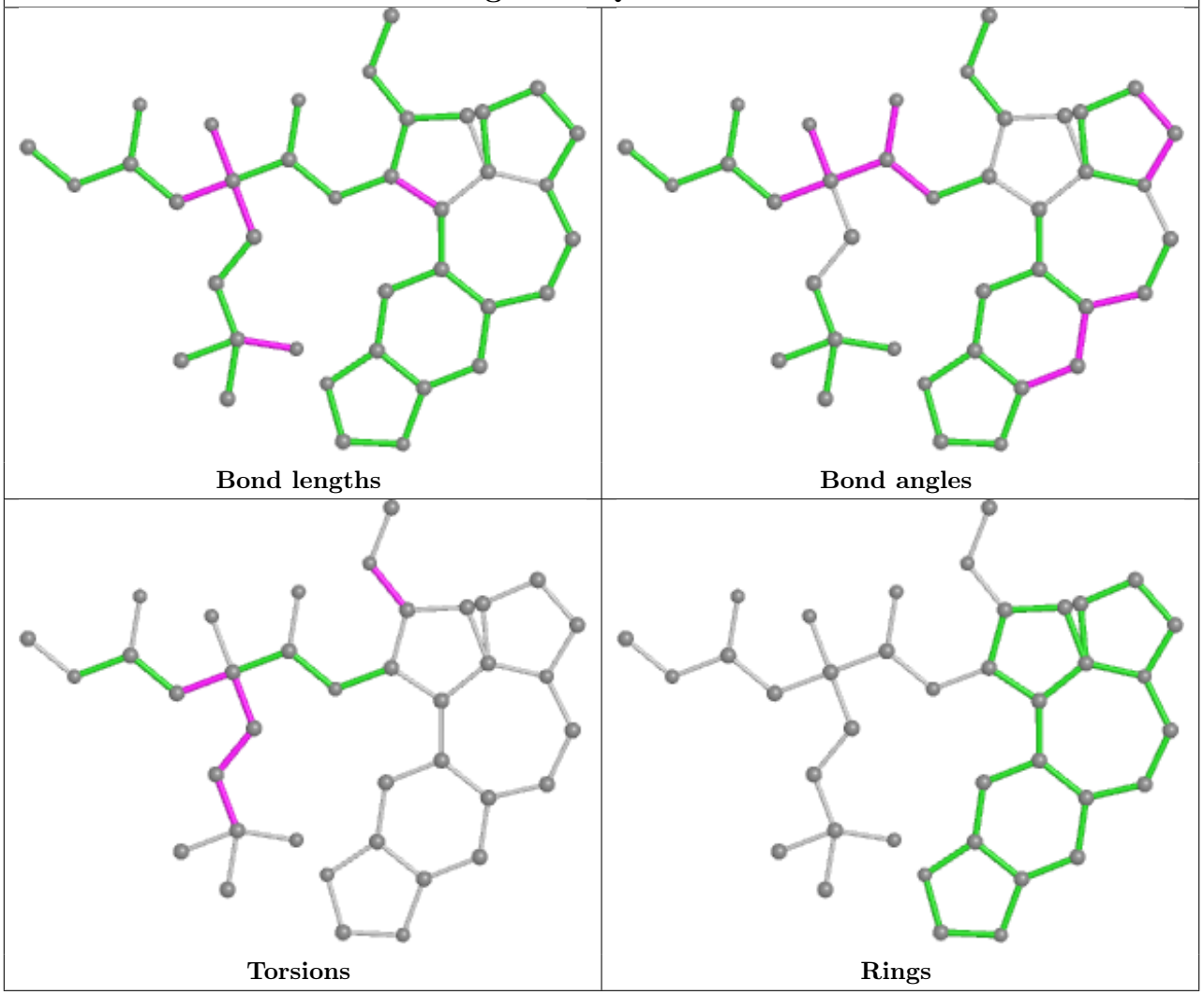
Mol	Chain	Res	Type	Atoms
81	5	5296	MQ6	C04-C05-C06-C07
81	5	5296	MQ6	C04-C05-C06-O37
81	5	5296	MQ6	C15-C31-O32-C33
81	5	5296	MQ6	C30-C31-O32-C33
81	5	5296	MQ6	C12-C06-C07-C08

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 then 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.

Ligand MQ6 5 5296



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	5	25
6	9	11

The worst 5 of 36 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	41.42
1	5	1252:C	O3'	1271:G	P	35.84
1	5	1219:G	O3'	1233:G	P	19.81
1	5	4101:C	O3'	4107:G	P	18.15
1	9	1761:U	O3'	1771:G	P	17.60

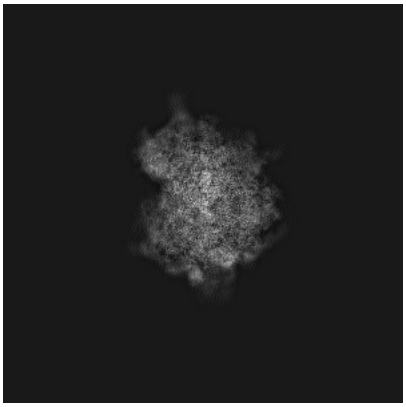
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26444. These allow visual inspection of the internal detail of the map and identification of artifacts.

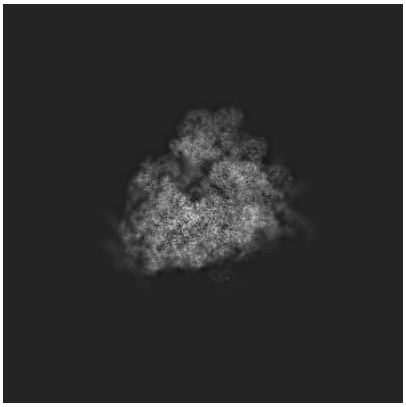
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

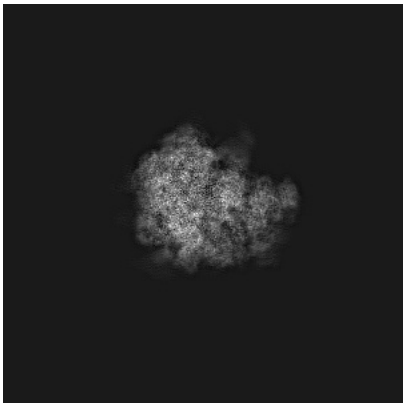
6.1.1 Primary map



X



Y

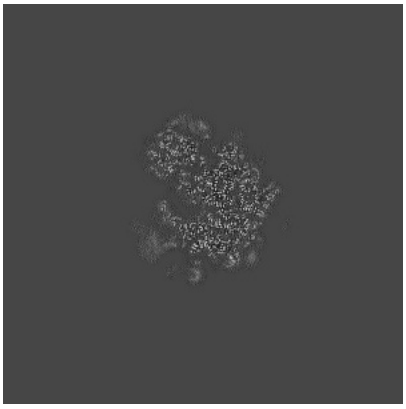


Z

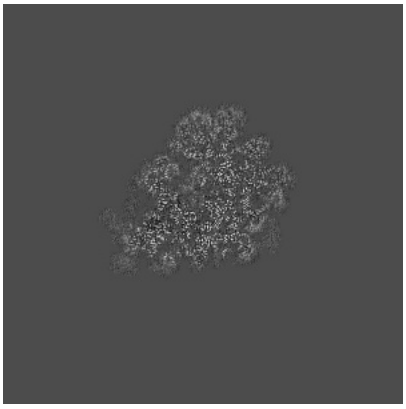
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 240



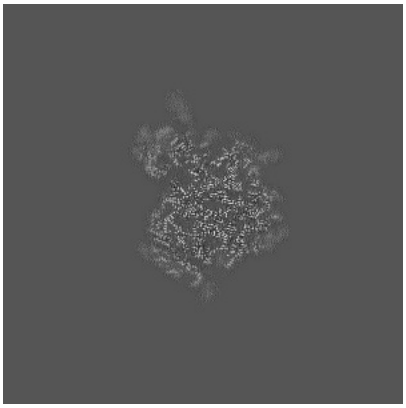
Y Index: 240

Z Index: 240

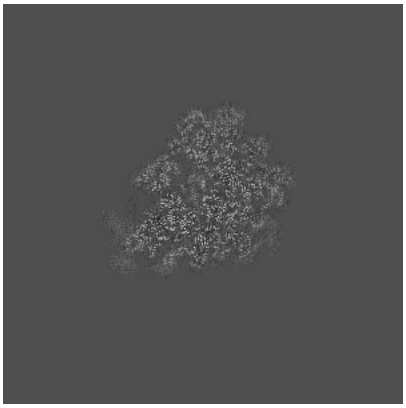
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

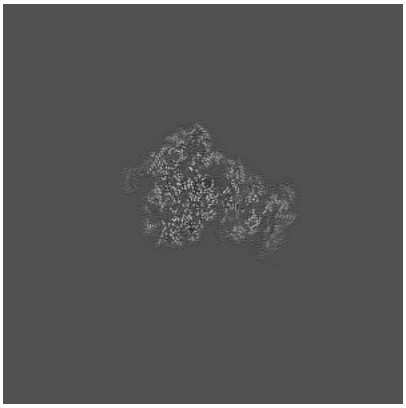
6.3.1 Primary map



X Index: 218



Y Index: 242

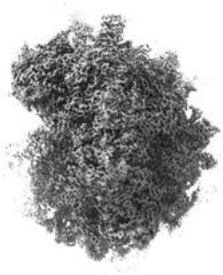


Z Index: 254

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

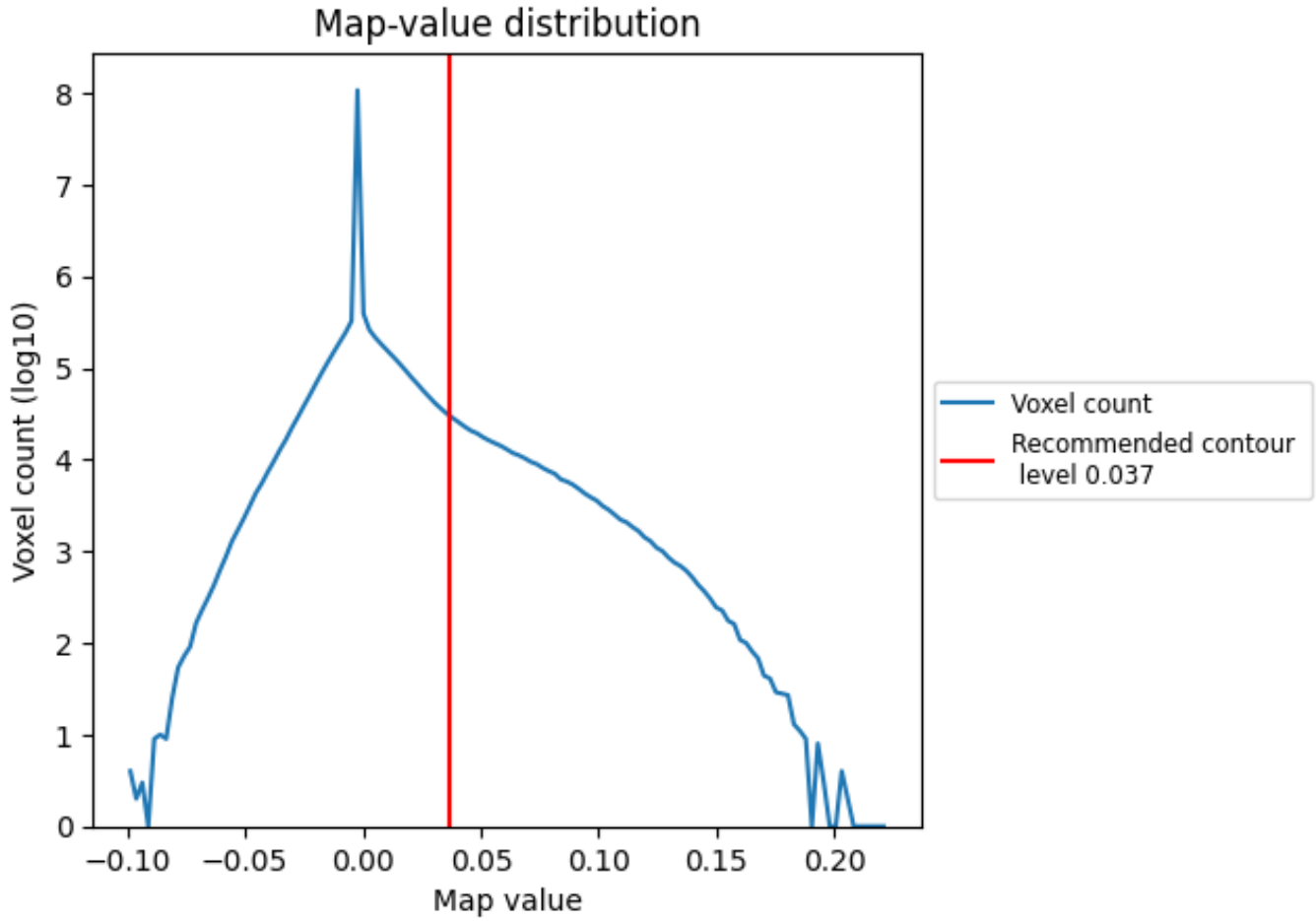
6.5 Mask visualisation (i)

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

7 Map analysis

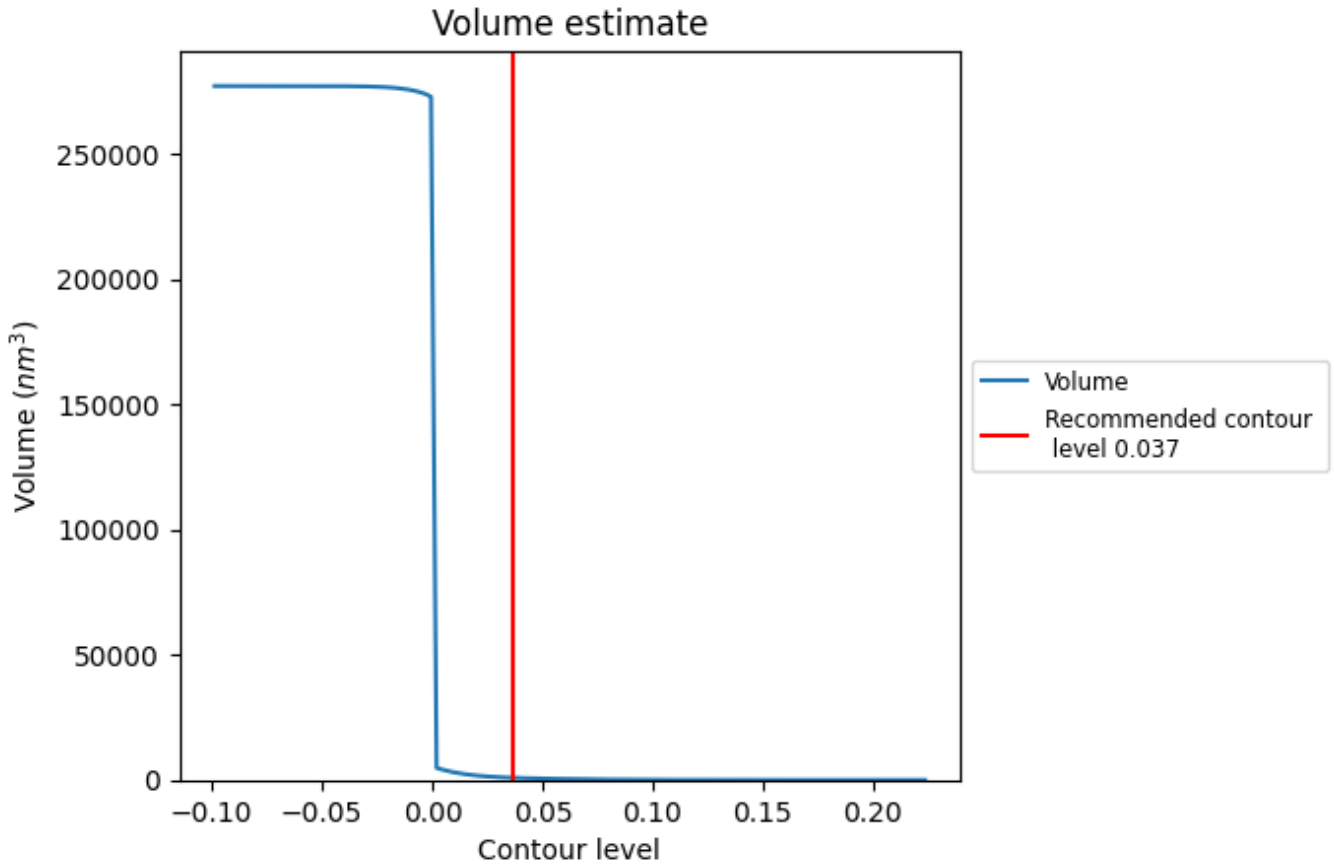
This section contains the results of statistical analysis of the map.

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.

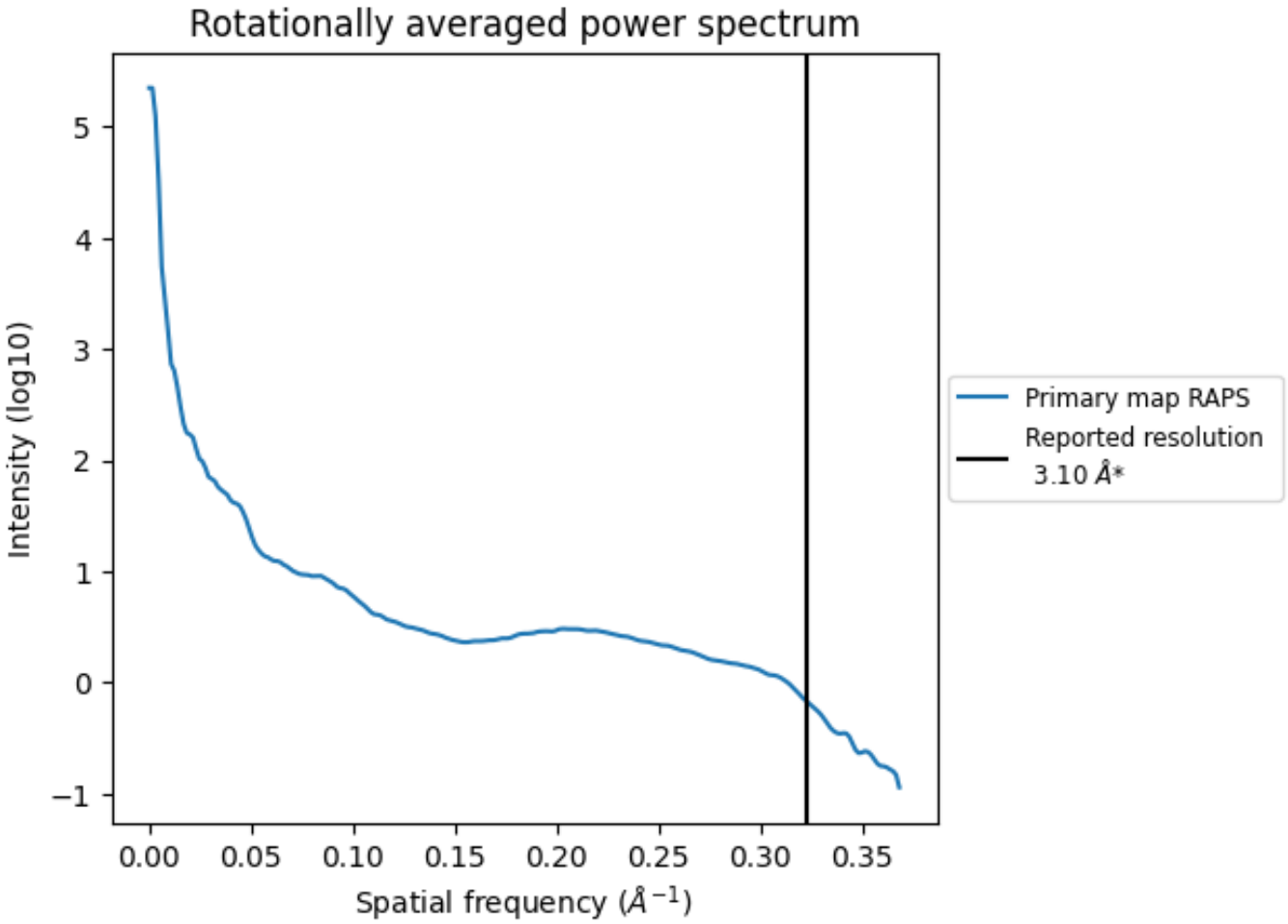
7.2 Volume estimate (i)



The volume at the recommended contour level is 860 nm^3; this corresponds to an approximate mass of 777 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 0.323 Å^{-1}

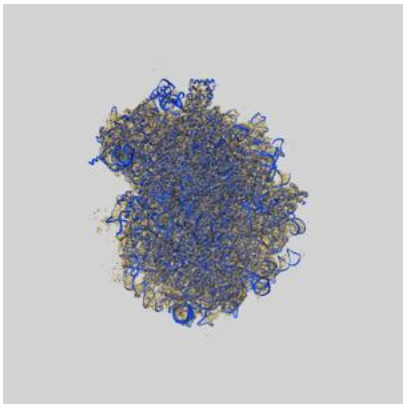
8 Fourier-Shell correlation (i)

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

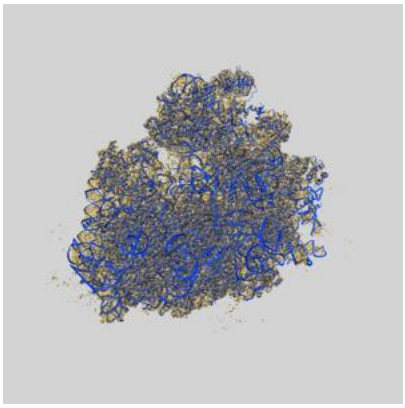
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26444 and PDB model 7UCJ. Per-residue inclusion information can be found in section 3 on page 21.

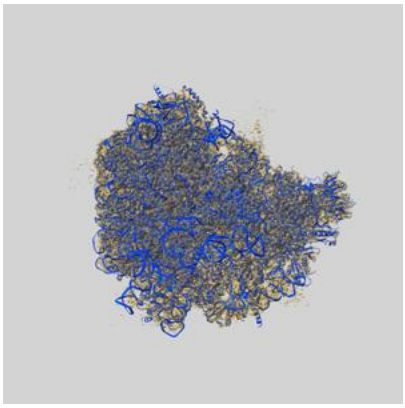
9.1 Map-model overlay



X



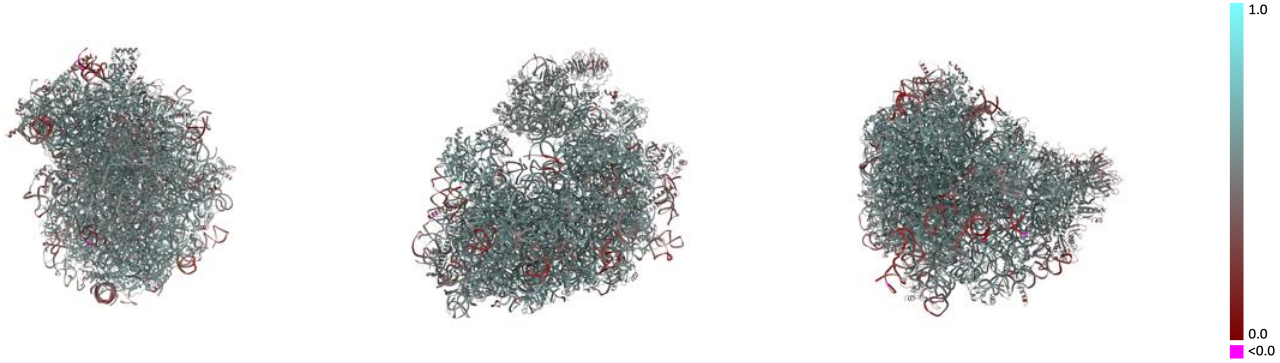
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.037 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.

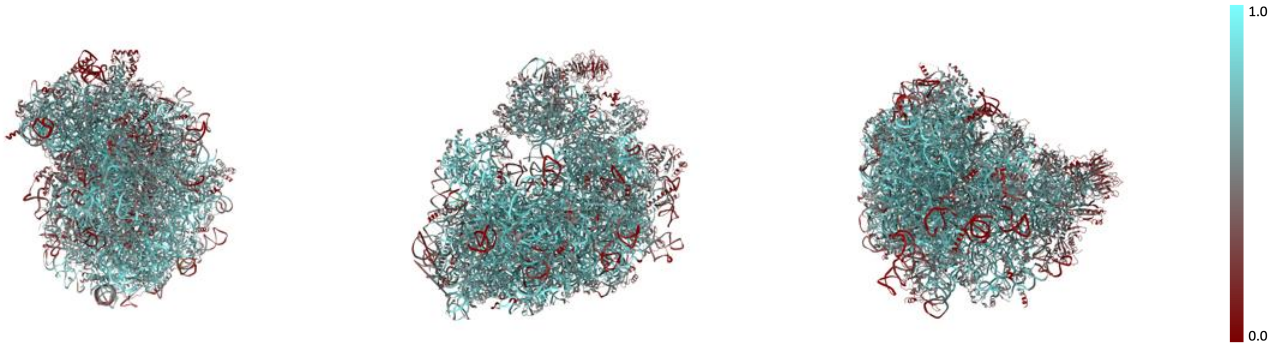
9.2 Q-score mapped to coordinate model (i)



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.

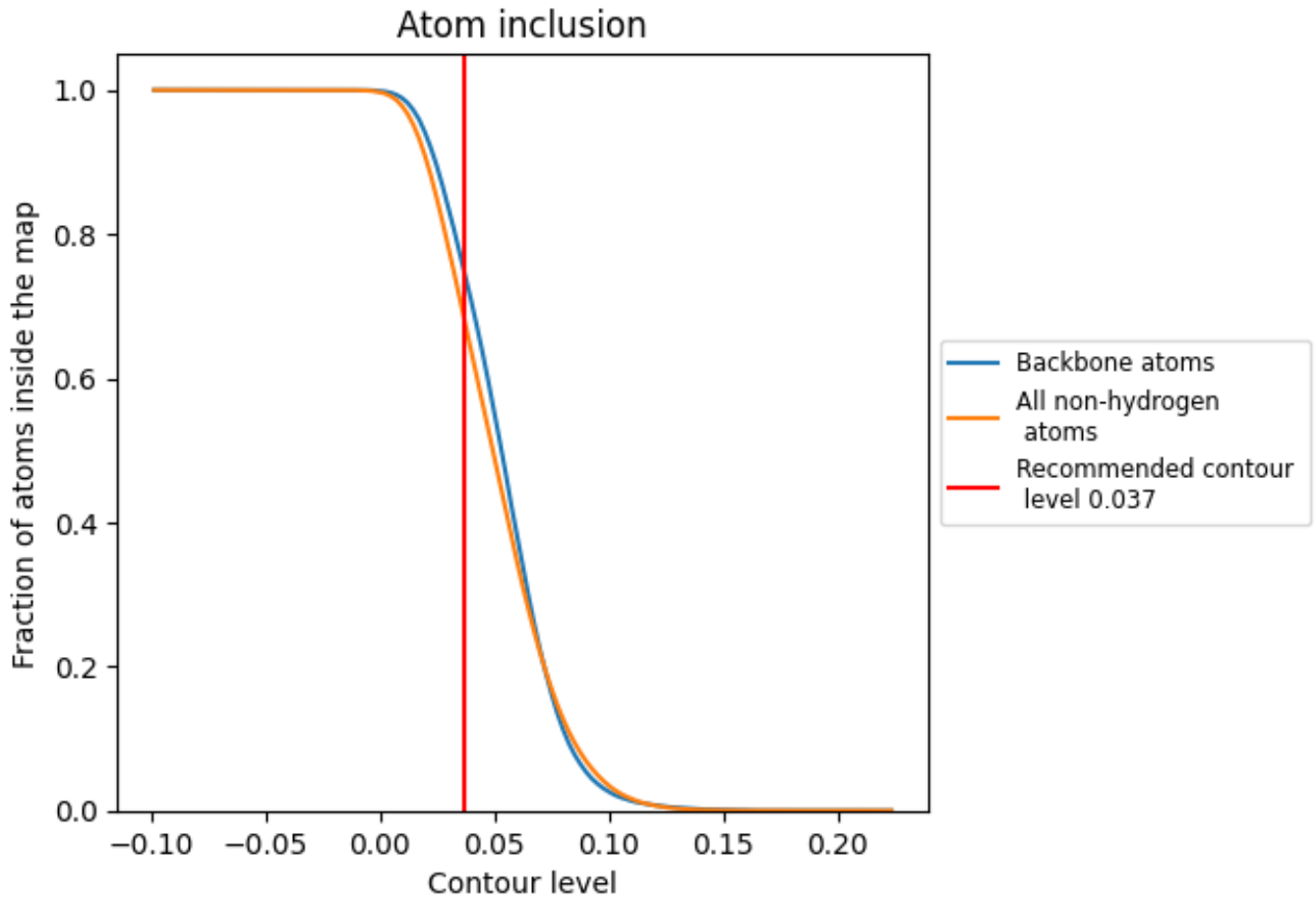
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.037).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 68% 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 (0.037) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6801	0.5390
1	0.5692	0.5540
2	0.3911	0.4900
5	0.7638	0.5420
7	0.8752	0.5830
8	0.7924	0.5570
9	0.7123	0.5210
A	0.7135	0.5930
AA	0.5734	0.5400
Aa	0.6343	0.5590
B	0.6818	0.5770
BB	0.5763	0.5470
Bb	0.5164	0.5230
C	0.7005	0.5780
CC	0.6057	0.5560
Cc	0.4468	0.4960
D	0.6535	0.5540
DD	0.3960	0.4800
Dd	0.5995	0.5400
E	0.6216	0.5500
EE	0.5590	0.5380
Ee	0.4343	0.4930
F	0.7244	0.5820
FF	0.5094	0.5200
G	0.5107	0.5170
GG	0.3876	0.4690
Gg	0.2936	0.4390
H	0.5913	0.5520
HH	0.3785	0.4890
I	0.6601	0.5690
II	0.5817	0.5430
J	0.5854	0.5320
JJ	0.5713	0.5290
KK	0.3380	0.4390
L	0.6132	0.5460

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Chain	Atom inclusion	Q-score
LL	0.6377	0.5690
M	0.6524	0.5510
N	0.7403	0.5920
NN	0.6338	0.5570
O	0.6886	0.5720
OO	0.6079	0.5570
P	0.7042	0.5840
PP	0.4135	0.4740
Q	0.7062	0.5890
QQ	0.5037	0.5210
R	0.6190	0.5560
RR	0.3863	0.4940
S	0.6868	0.5760
SS	0.4795	0.4940
T	0.6405	0.5630
TT	0.4822	0.5130
U	0.4974	0.5010
UU	0.3450	0.4750
V	0.6639	0.5830
VV	0.5113	0.5390
W	0.5689	0.5390
WW	0.6416	0.5680
X	0.6106	0.5530
XX	0.6022	0.5680
Y	0.6364	0.5520
YY	0.5178	0.5120
Z	0.6179	0.5560
ZZ	0.4271	0.4790
a	0.7484	0.5910
b	0.5252	0.5220
c	0.6519	0.5680
d	0.6371	0.5630
e	0.7030	0.5920
f	0.7363	0.5900
g	0.6395	0.5590
h	0.5955	0.5410
i	0.5905	0.5380
j	0.7429	0.5940
k	0.4596	0.4890
l	0.6276	0.5630
m	0.6757	0.5600
n	0.6376	0.5840

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Chain	Atom inclusion	Q-score
o	0.6548	0.5840
p	0.6662	0.5780
r	0.7168	0.5840