Full wwPDB EM Validation Report ⓘ

Jan 21, 2025 – 01:54 PM EST

PDB ID	:	6OLF
EMDB ID	:	EMD-0599
Title	:	Human ribosome nascent chain complex (CDH1-RNC) stalled by a drug-like molecule with AA and PE tRNAs
Authors	:	Li, W.; Cate, J.H.D.
Deposited on	:	2019-04-16
Resolution	:	3.90 Å(reported)

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

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

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

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

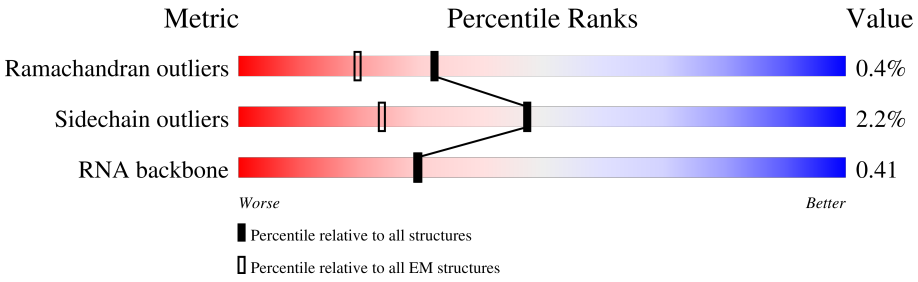
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	S2	1714	13% 59% 37%
2	SA	221	39% 96%
3	SB	214	47% 97%
4	SD	226	60% 99%
5	SE	259	47% 98%
6	SF	189	65% 98%
7	SH	189	54% 97%
8	SI	204	43% 98%

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Mol	Chain	Length	Quality of chain
9	SK	98	67% 97%
10	SL	153	39% 95% 5%
11	SP	127	43% 98%
12	SQ	146	54% 97%
13	SR	134	66% 99%
14	SS	145	54% 99%
15	ST	143	53% 97%
16	SU	104	61% 94% 6%
17	SV	82	37% 96%
18	SX	141	30% 98%
19	Sa	102	25% 97%
20	Sc	64	67% 100%
21	Sd	55	27% 89% 11%
22	Sg	312	78% 98%
23	SC	220	33% 98%
24	SG	237	63% 97%
25	SJ	185	50% 95% 5%
26	SM	118	97% 97%
27	SN	150	29% 99%
28	SO	137	45% 100%
29	SW	129	23% 98%
30	SY	131	44% 98%
31	SZ	73	77% 95% 5%
32	Sb	82	54% 100%
33	Se	57	54% 98%

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Mol	Chain	Length	Quality of chain
34	Sf	67	93% 96%
35	A	252	8% 98%
36	B	397	14% 98%
37	C	363	11% 96%
38	D	157	11% 71% 26%
39	E	119	80% 20%
40	F	294	17% 97%
41	G	247	26% 92%
42	H	225	8% 97%
43	I	234	24% 100%
44	J	191	24% 97%
45	K	211	18% 96%
46	L	169	21% 99%
47	M	205	20% 97%
48	N	139	12% 99%
49	O	203	6% 98%
50	P	195	8% 96%
51	Q	153	5% 97%
52	R	187	11% 96%
53	S	181	22% 97%
54	T	175	12% 98%
55	U	157	12% 97%
56	V	99	23% 94% 6%
57	W	129	18% 100%
58	X	121	56% 98%

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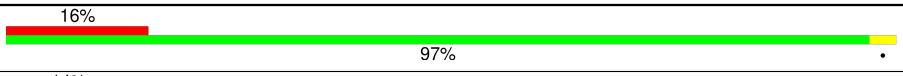
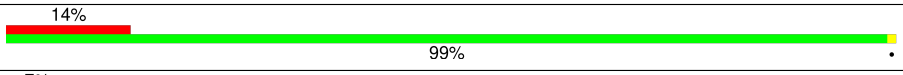
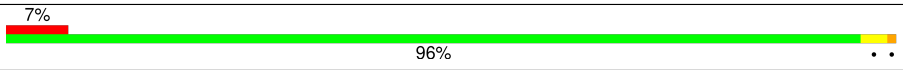
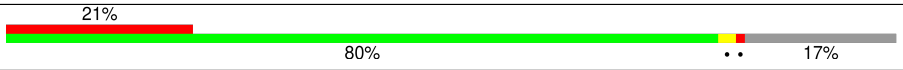
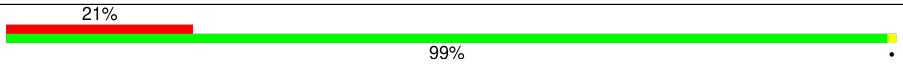
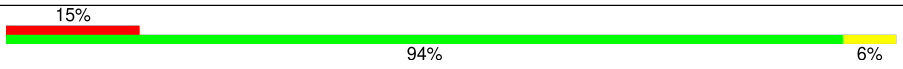
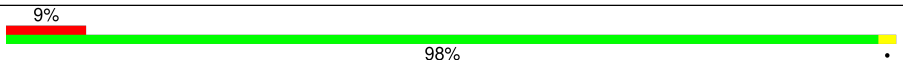
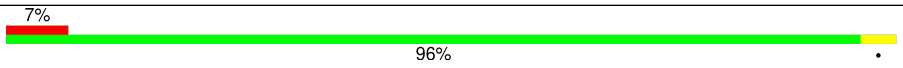
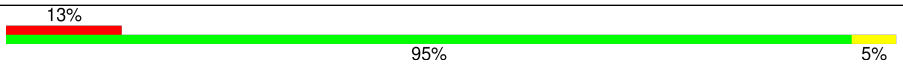
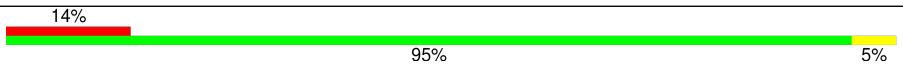
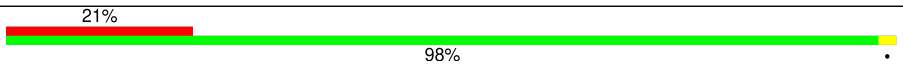
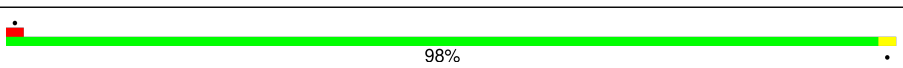
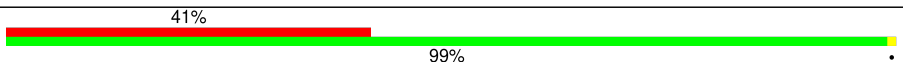
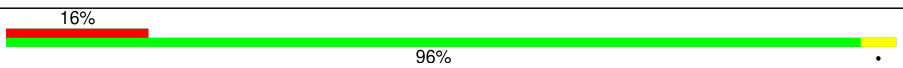
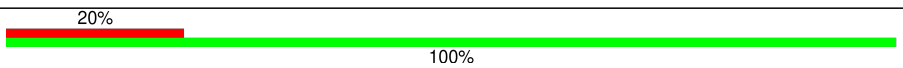
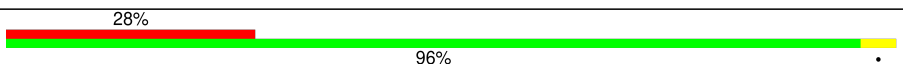
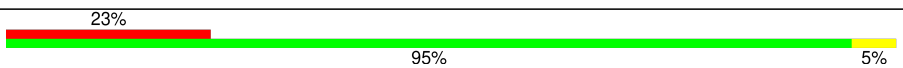
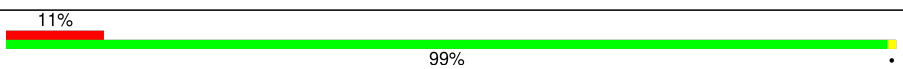
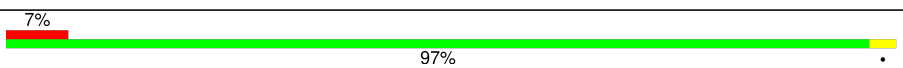
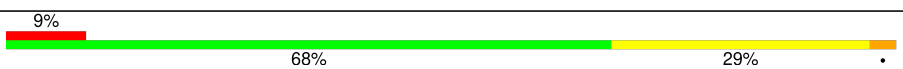
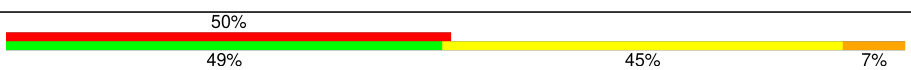
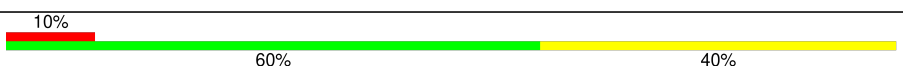
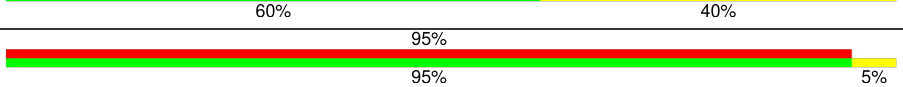
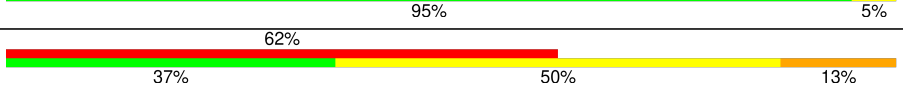
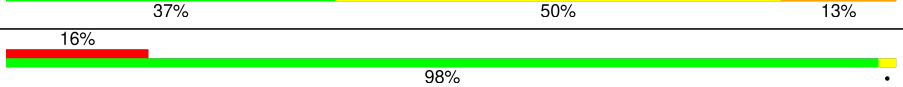
Mol	Chain	Length	Quality of chain
59	Y	117	
60	Z	134	
61	b	147	
62	c	121	
63	d	103	
64	e	106	
65	f	129	
66	g	109	
67	h	114	
68	i	122	
69	j	97	
70	k	84	
71	l	69	
72	m	50	
73	n	50	
74	o	25	
75	p	105	
76	q	91	
77	r	122	
78	t	3607	
79	v	76	
80	w	10	
81	y	39	
82	u	76	
83	a	134	

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 215429 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	S2	1714	36501	16306	6533	11949	1713	0	0

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SA	221	1741	1106	305	322	8	0	0

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	SB	214	1738	1103	310	311	14	0	0

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SD	226	1757	1120	316	314	7	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SE	259	2059	1316	383	352	8	0	0

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SF	189	1495	934	284	270	7	0	0

- Molecule 7 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SI	204	Total	C	N	O	S	0	0
			1673	1050	329	289	5		

- Molecule 9 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 10 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SL	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 11 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SP	127	Total	C	N	O	S	0	0
			1045	663	198	177	7		

- Molecule 12 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SQ	146	Total	C	N	O	S	0	0
			1158	736	218	200	4		

- Molecule 13 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SR	134	Total	C	N	O	S	0	0
			1082	680	201	197	4		

- Molecule 14 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 15 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	ST	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 16 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 17 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SV	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 18 is a protein called 40S ribosomal protein S23.

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

- Molecule 19 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Sa	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 20 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 21 is a protein called 40S ribosomal protein S29.

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

- Molecule 22 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Sg	312	Total	C	N	O	S	0	0
			2429	1531	423	463	12		

- Molecule 23 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SC	220	Total	C	N	O	S	1	0
			1715	1109	296	300	10		

- Molecule 24 is a protein called 40S ribosomal protein S6.

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

- Molecule 25 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SJ	185	Total	C	N	O	S	1	0
			1533	974	309	248	2		

- Molecule 26 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SM	118	Total	C	N	O	S	0	0
			912	571	161	173	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SM	52	GLN	LEU	conflict	UNP P25398
SM	69	LEU	CYS	conflict	UNP P25398
SM	99	ASN	LYS	conflict	UNP P25398

- Molecule 27 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 28 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SO	137	Total	C	N	O	S	0	0
			1024	627	200	191	6		

- Molecule 29 is a protein called 40S ribosomal protein S15a.

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

- Molecule 30 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SY	131	Total	C	N	O	S	1	0
			1073	678	212	178	5		

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SZ	73	Total	C	N	O	S	0	0
			579	372	106	100	1		

- Molecule 32 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Sb	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 33 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Se	57	Total	C	N	O	S	0	0
			452	281	99	71	1		

- Molecule 34 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Sf	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 35 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	A	252	Total	C	N	O	S	0	0
			1930	1209	395	320	6		

- Molecule 36 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B	397	Total	C	N	O	S	0	0
			3202	2039	602	547	14		

- Molecule 37 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	C	363	Total	C	N	O	S	0	0
			2888	1817	577	480	14		

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	D	157	Total	C	N	O	P	0	0
			3337	1489	587	1104	157		

- Molecule 39 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	E	119	Total	C	N	O	P	0	0
			2541	1132	454	836	119		

- Molecule 40 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	F	294	Total	C	N	O	S	0	0
			2392	1510	436	432	14		

- Molecule 41 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	G	236	Total	C	N	O	S	0	0
			1904	1222	361	317	4		

- Molecule 42 is a protein called 60S ribosomal protein L7.

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

- Molecule 43 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	I	234	Total	C	N	O	S	0	0
			1880	1197	362	317	4		

- Molecule 44 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	J	191	Total	C	N	O	S	0	0
			1526	960	285	275	6		

- Molecule 45 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	K	208	Total	C	N	O	S	0	0
			1692	1074	327	278	13		

- Molecule 46 is a protein called 60S ribosomal protein L11.

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

- Molecule 47 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	M	205	Total	C	N	O	S	0	0
			1657	1036	344	273	4		

- Molecule 48 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	N	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 49 is a protein called 60S ribosomal protein L15.

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

- Molecule 50 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	P	195	Total	C	N	O	S	0	0
			1606	1034	315	252	5		

- Molecule 51 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Q	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 52 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	R	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 53 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S	181	Total	C	N	O	S	0	0
			1517	938	329	241	9		

- Molecule 54 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	T	175	Total	C	N	O	S	0	0
			1449	921	283	234	11		

- Molecule 55 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	U	157	Total	C	N	O	S	0	0
			1284	815	250	214	5		

- Molecule 56 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	V	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 57 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	W	129	Total	C	N	O	S	0	0
			969	613	182	169	5		

- Molecule 58 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	X	121	Total	C	N	O	S	0	0
			989	617	202	167	3		

- Molecule 59 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Y	117	Total	C	N	O	S	0	0
			958	612	180	165	1		

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

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

- Molecule 61 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	b	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 62 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	c	100	Total	C	N	O	S	0	0
			814	506	179	125	4		

- Molecule 63 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	d	103	Total	C	N	O	S	0	0
			801	508	141	145	7		

- Molecule 64 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	e	106	Total	C	N	O	S	0	0
			879	555	170	152	2		

- Molecule 65 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	f	129	Total	C	N	O	S	0	0
			1064	673	220	166	5		

- Molecule 66 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	g	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 67 is a protein called 60S ribosomal protein L34.

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

- Molecule 68 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	i	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 69 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	j	97	Total	C	N	O	S	0	0
			794	497	168	124	5		

- Molecule 70 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	k	84	Total	C	N	O	S	0	0
			689	423	152	109	5		

- Molecule 71 is a protein called 60S ribosomal protein L38.

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

- Molecule 72 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	m	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 73 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	n	50	Total	C	N	O	S	0	0
			411	254	87	64	6		

- Molecule 74 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	o	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

- Molecule 75 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	p	105	Total	C	N	O	S	0	0
			863	542	175	140	6		

- Molecule 76 is a protein called 60S ribosomal protein L37a.

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

- Molecule 77 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	r	122	Total	C	N	O	S	0	0
			980	607	204	165	4		

- Molecule 78 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	t	3607	Total	C	N	O	P	0	0
			77332	34436	14150	25139	3607		

- Molecule 79 is a RNA chain called PE tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	v	76	Total	C	N	O	P	0	0
			1618	721	287	534	76		

- Molecule 80 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	w	10	Total	C	N	O	P	0	0
			213	95	37	72	9		

- Molecule 81 is a protein called Cadherin-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
81	y	39	Total	C	N	O	0	0
			262	180	40	42		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	6	ALA	-	insertion	UNP P12830

- Molecule 82 is a RNA chain called AA tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	u	76	Total	C	N	O	P	0	0
			1613	720	283	535	75		

- Molecule 83 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	a	134	Total	C	N	O	S	0	0
			1103	712	207	181	3		

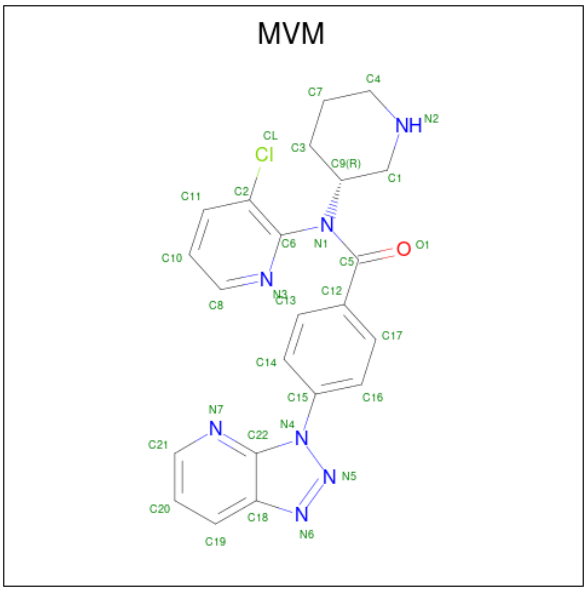
- Molecule 84 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
84	S2	1	Total	Zn	0
			1	1	
84	Sa	1	Total	Zn	0
			1	1	
84	Sf	1	Total	Zn	0
			1	1	
84	k	1	Total	Zn	0
			1	1	
84	p	1	Total	Zn	0
			1	1	
84	q	1	Total	Zn	0
			1	1	

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
85	S2	3	Total	Mg	0
			3	3	
85	D	6	Total	Mg	0
			6	6	
85	E	9	Total	Mg	0
			9	9	
85	b	2	Total	Mg	0
			2	2	
85	t	11	Total	Mg	0
			11	11	

- Molecule 86 is N-(3-chloropyridin-2-yl)-N-[(3R)-piperidin-3-yl]-4-(3H-[1,2,3]triazolo[4,5-b]pyridin-3-yl)benzamide (three-letter code: MVM) (formula: $C_{22}H_{20}ClN_7O$).



Mol	Chain	Residues	Atoms					AltConf
86	t	1	Total	C	Cl	N	O	0
			31	22	1	7	1	

- Molecule 87 is water.

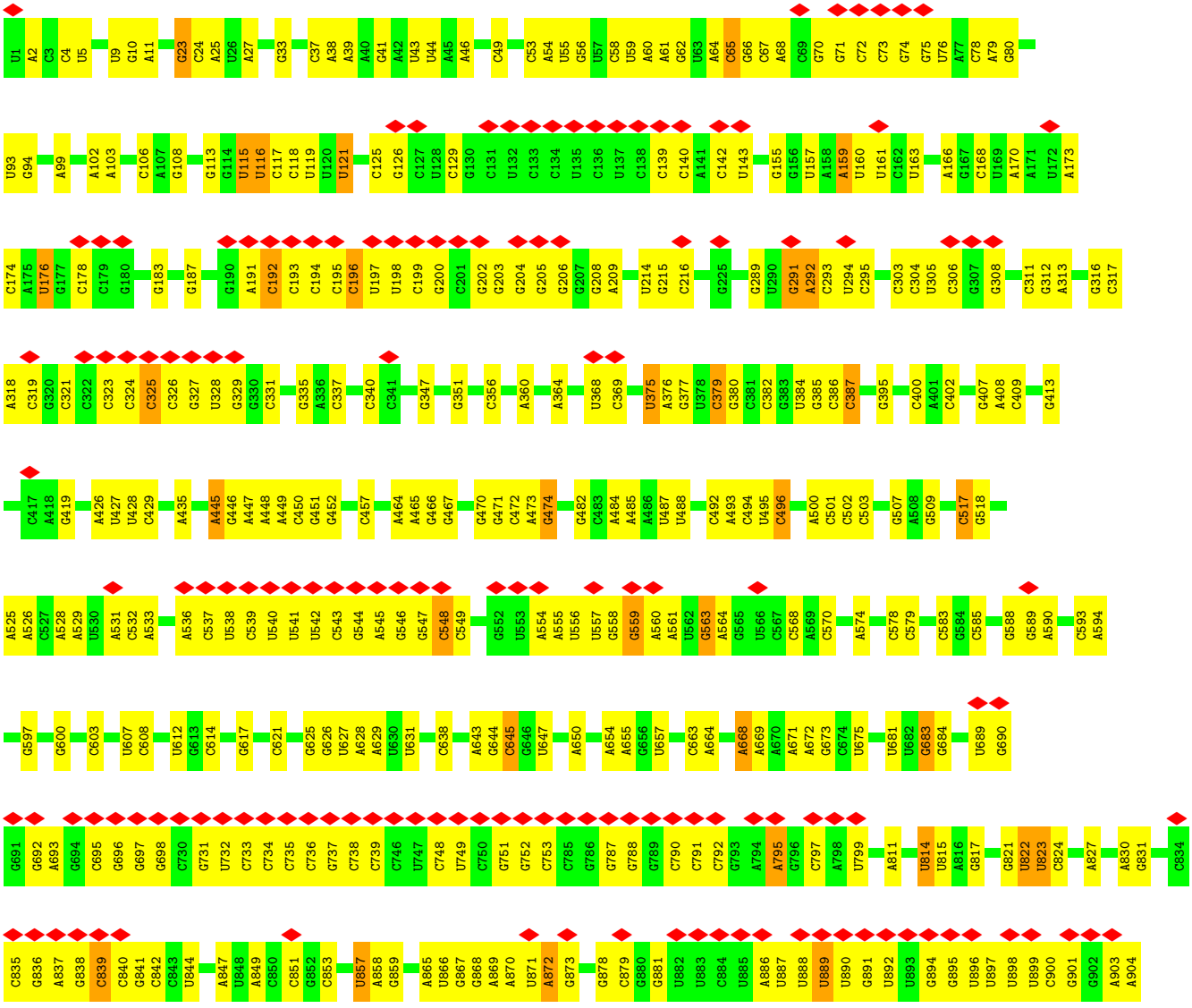
Mol	Chain	Residues	Atoms		AltConf
87	S2	5	Total	O	0
			5	5	
87	SP	1	Total	O	0
			1	1	
87	SQ	1	Total	O	0
			1	1	
87	SR	1	Total	O	0
			1	1	
87	SS	2	Total	O	0
			2	2	
87	SV	1	Total	O	0
			1	1	
87	SN	1	Total	O	0
			1	1	
87	Sf	1	Total	O	0
			1	1	
87	u	1	Total	O	0
			1	1	

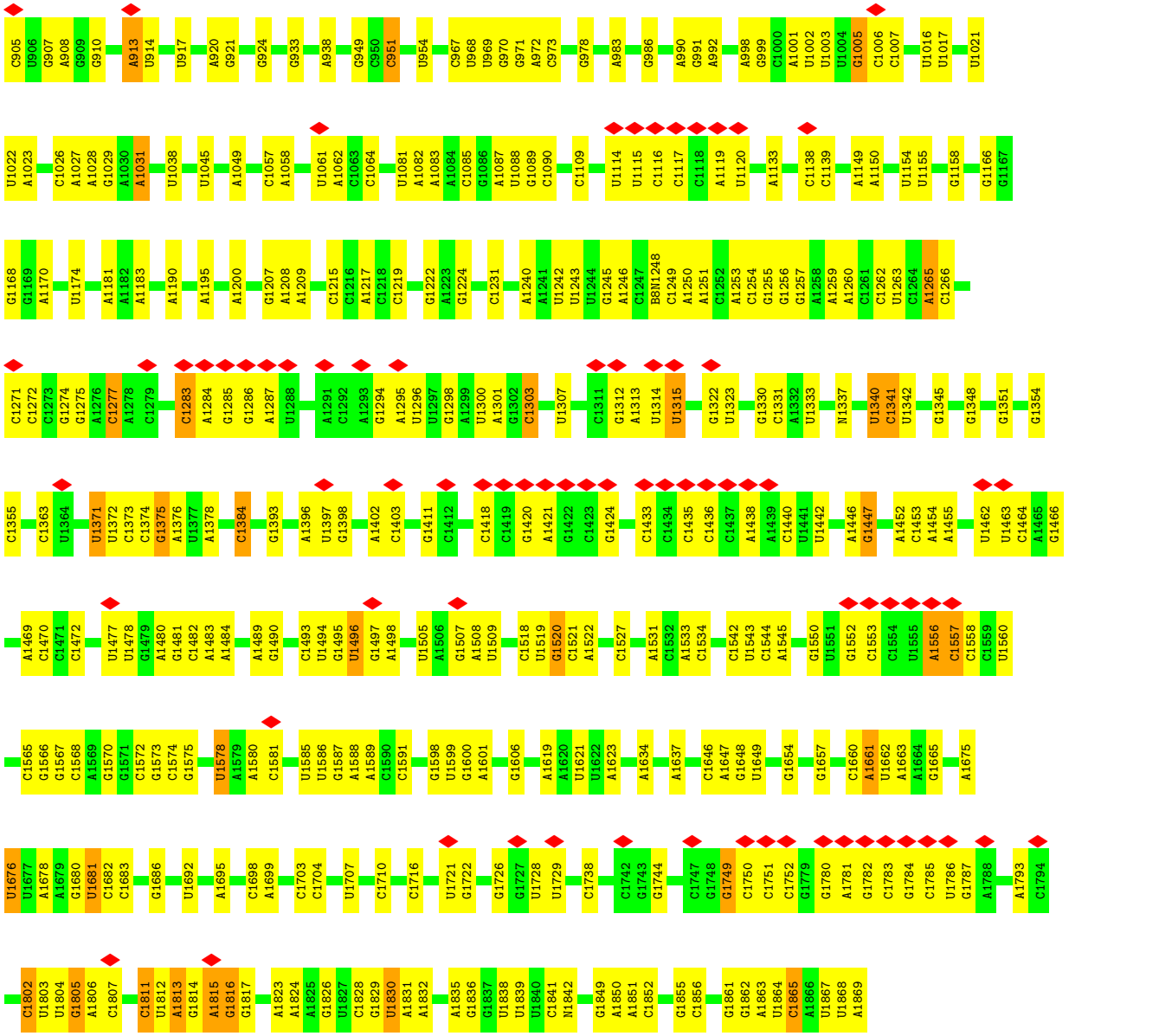
3 Residue-property plots (i)

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: 18S ribosomal RNA

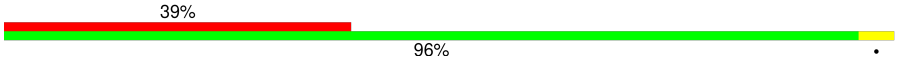
Chain S2:

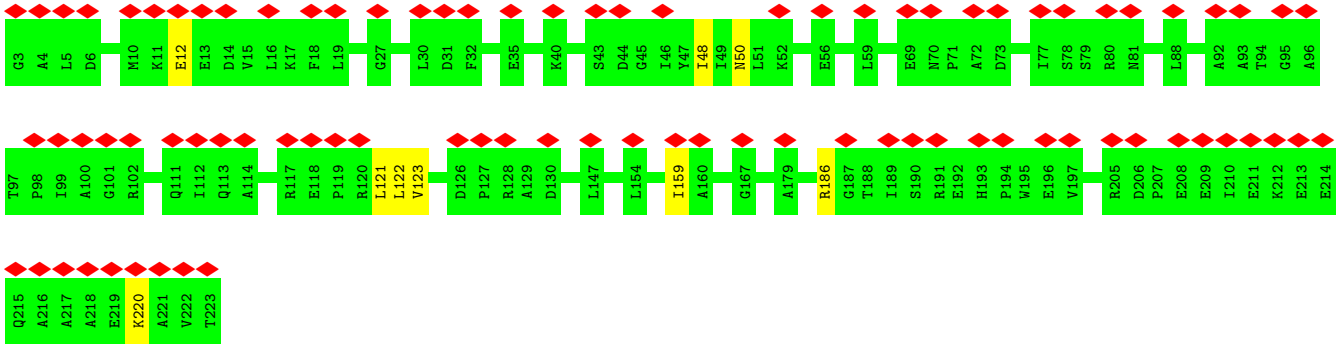




• Molecule 2: 40S ribosomal protein SA

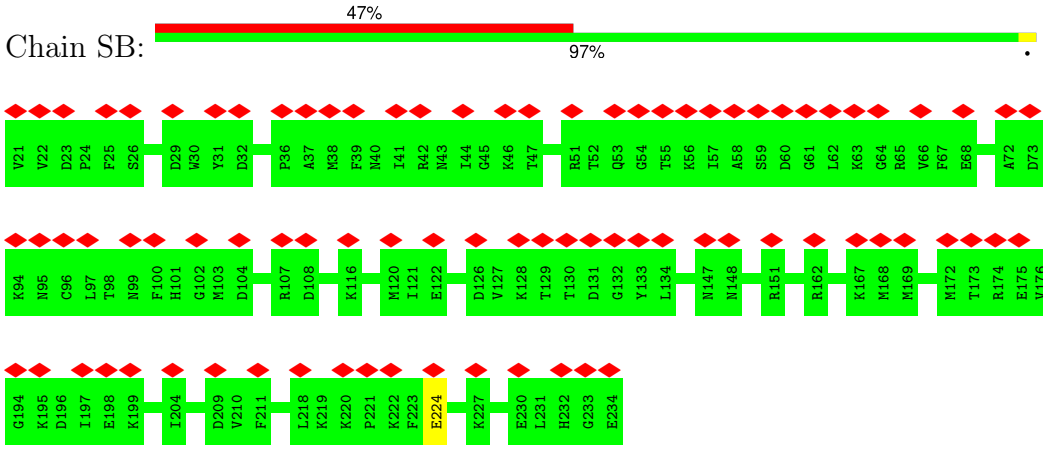
Chain SA:





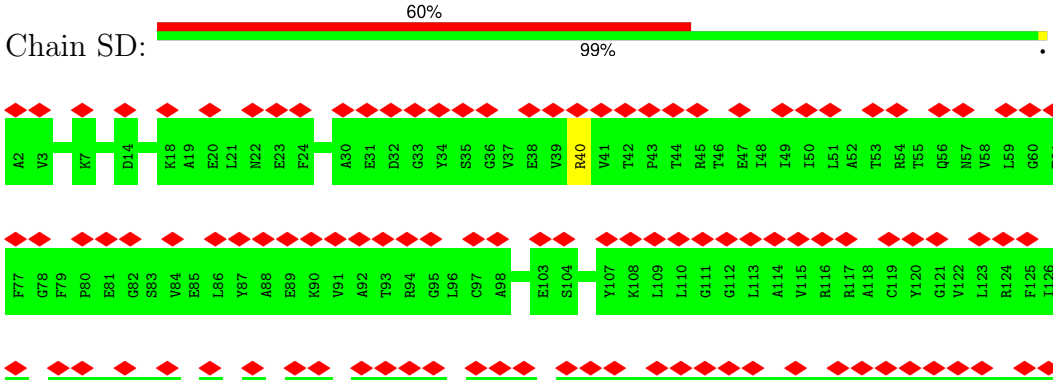
• Molecule 3: 40S ribosomal protein S3a

Chain SB:



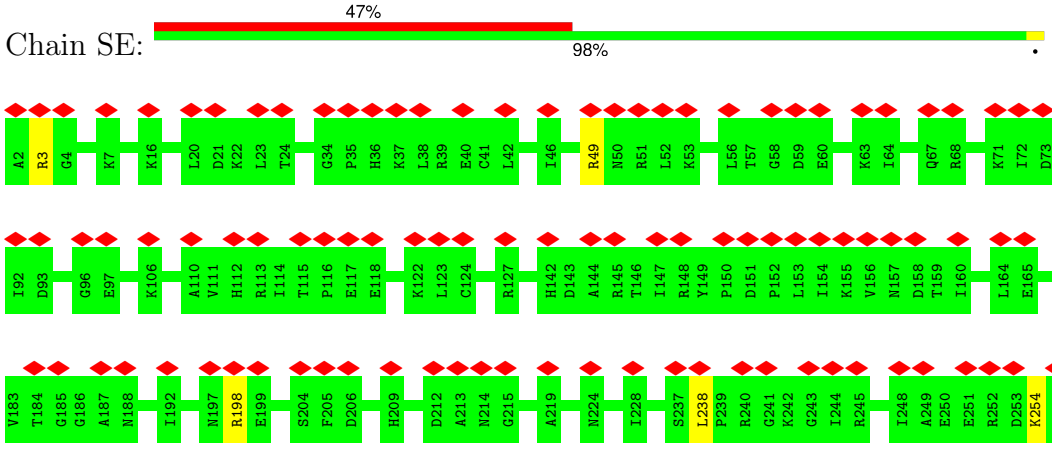
• Molecule 4: 40S ribosomal protein S3

Chain SD:



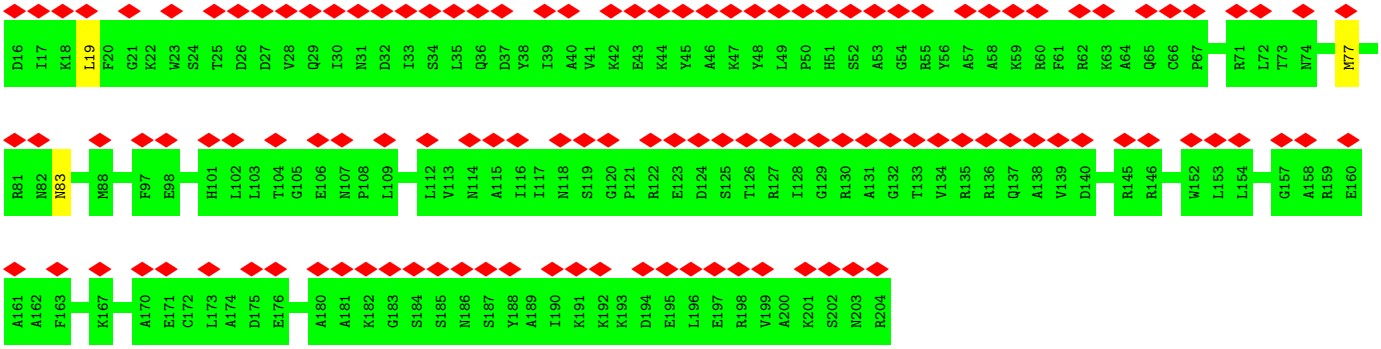
• Molecule 5: 40S ribosomal protein S4, X isoform

Chain SE:



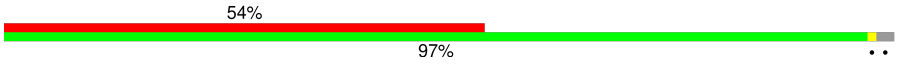
• Molecule 6: 40S ribosomal protein S5

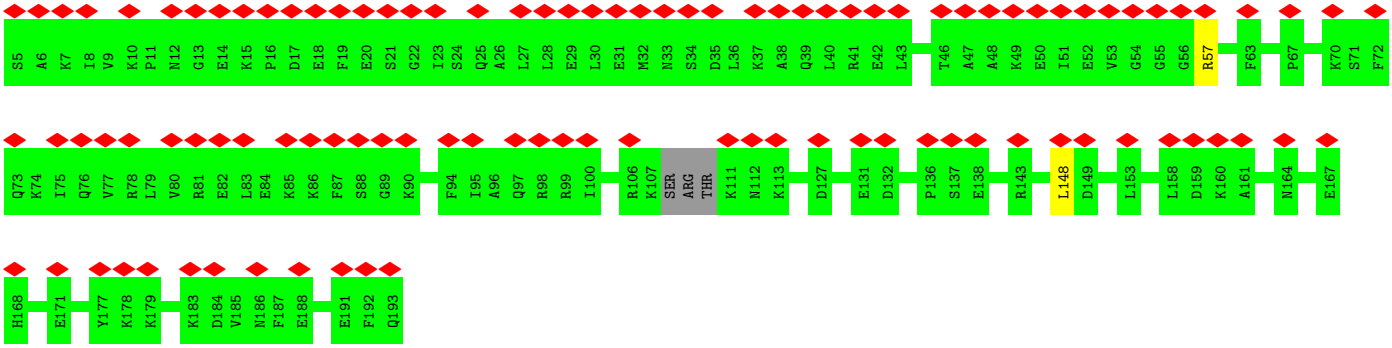
Chain SF:



• Molecule 7: 40S ribosomal protein S7

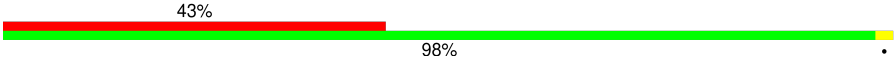
Chain SH:

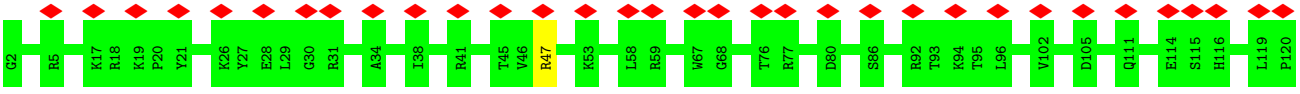




• Molecule 8: 40S ribosomal protein S8

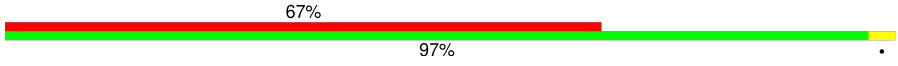
Chain SI:

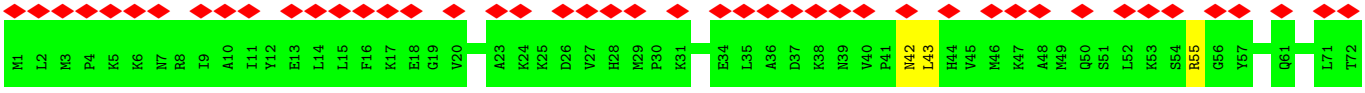


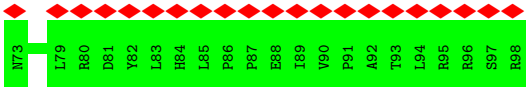


• Molecule 9: 40S ribosomal protein S10

Chain SK:

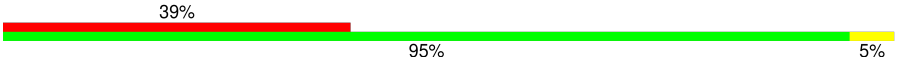


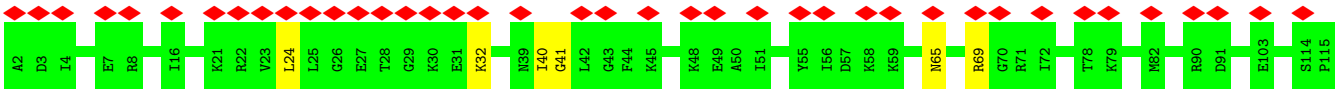


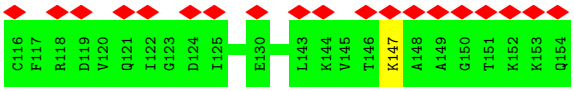


• Molecule 10: 40S ribosomal protein S11

Chain SL:

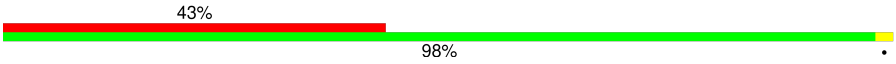


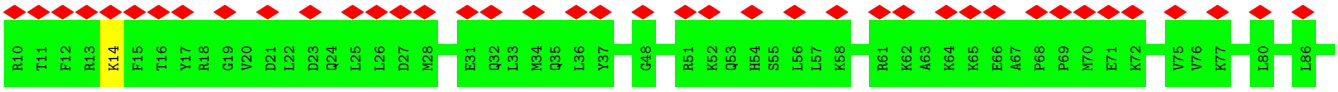


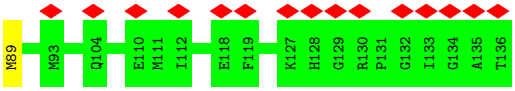


• Molecule 11: 40S ribosomal protein S15

Chain SP:

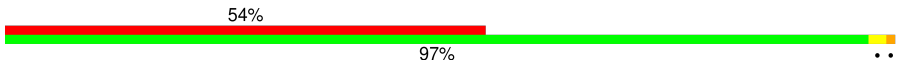


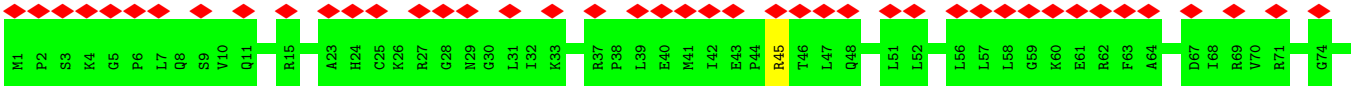


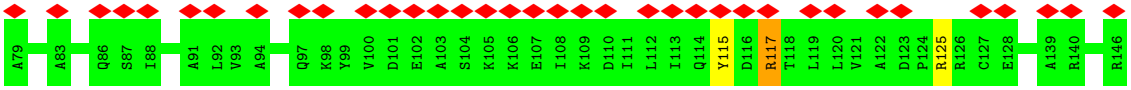


• Molecule 12: 40S ribosomal protein S16

Chain SQ:

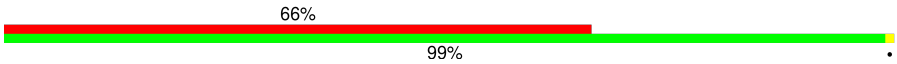


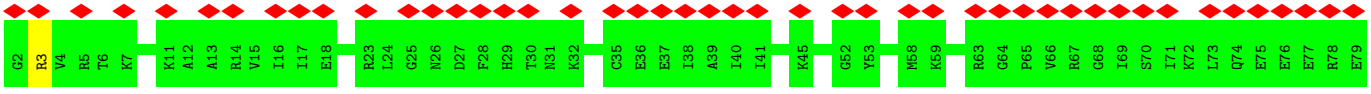


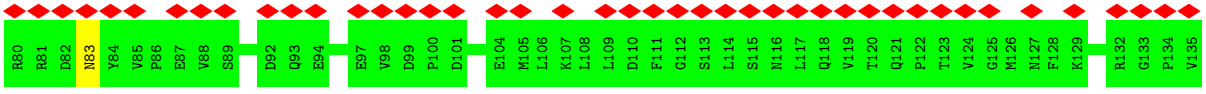


• Molecule 13: 40S ribosomal protein S17

Chain SR:

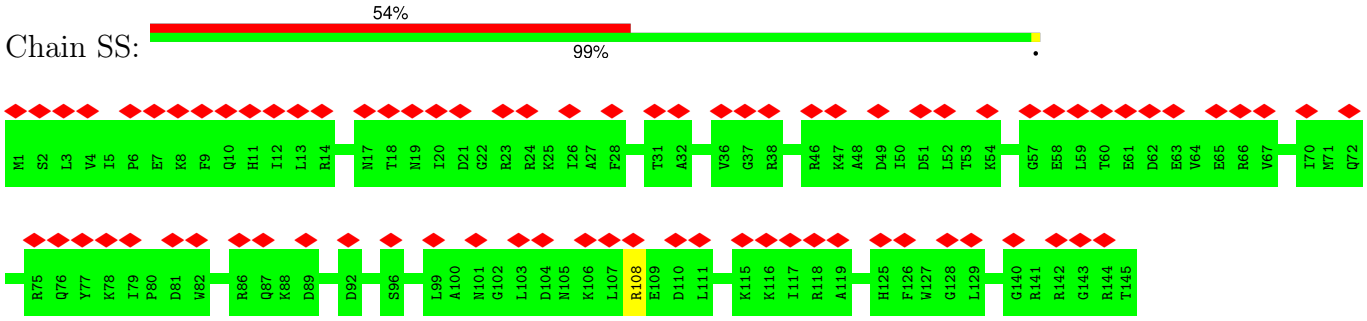






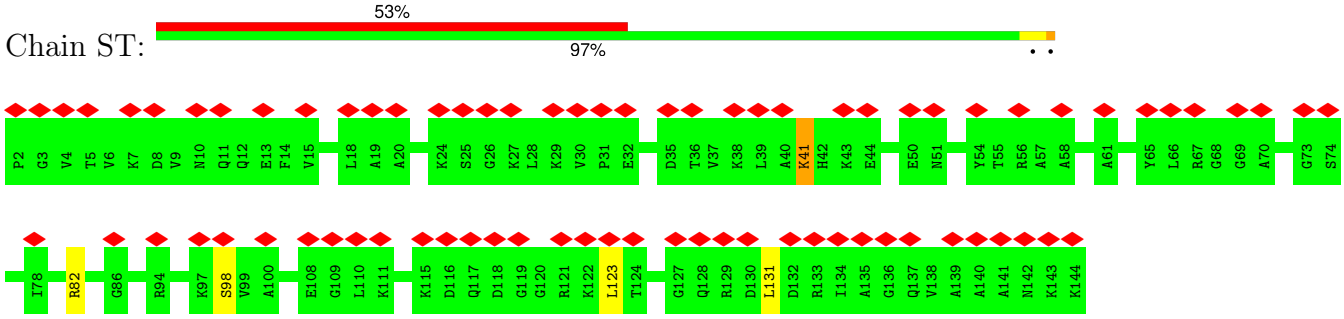
• Molecule 14: 40S ribosomal protein S18

Chain SS:



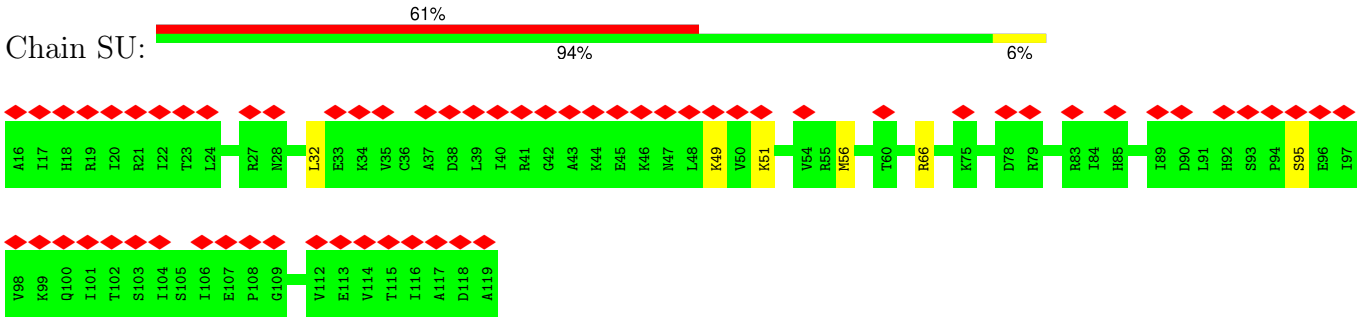
• Molecule 15: 40S ribosomal protein S19

Chain ST:



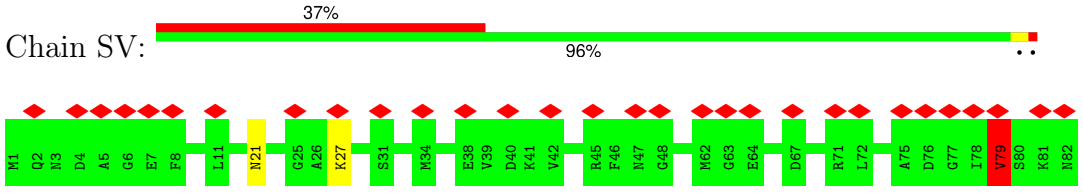
• Molecule 16: 40S ribosomal protein S20

Chain SU:



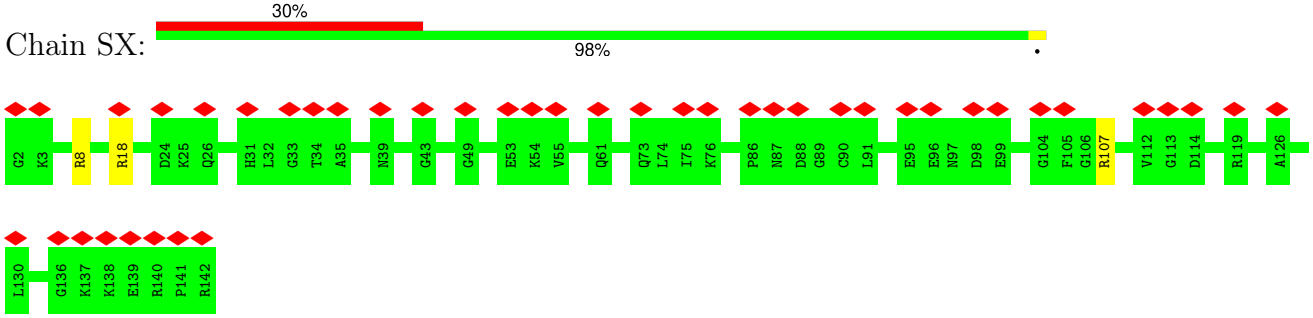
• Molecule 17: 40S ribosomal protein S21

Chain SV:



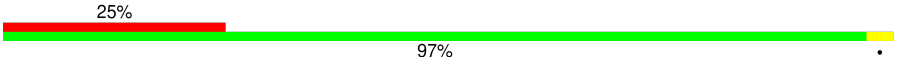
• Molecule 18: 40S ribosomal protein S23

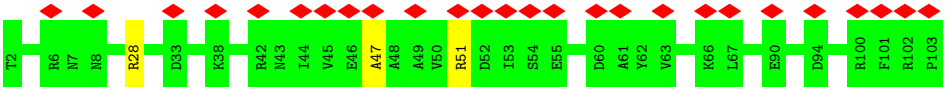
Chain SX:



• Molecule 19: 40S ribosomal protein S26

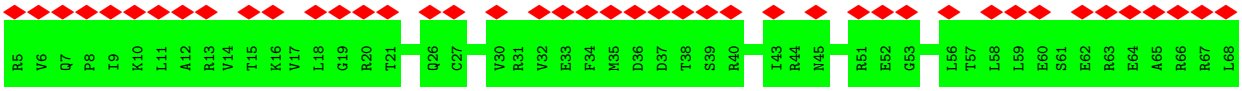
Chain Sa:





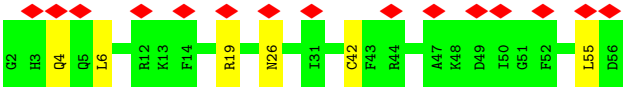
• Molecule 20: 40S ribosomal protein S28

Chain Sc:



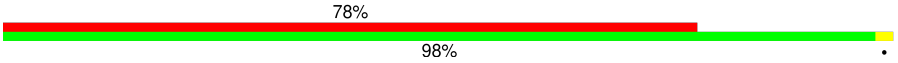
• Molecule 21: 40S ribosomal protein S29

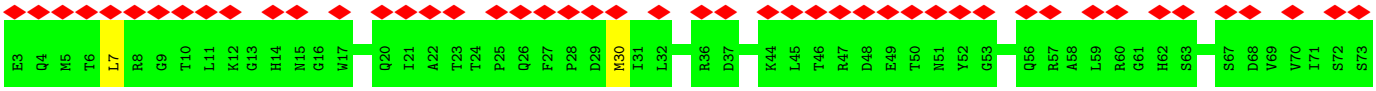
Chain Sd:

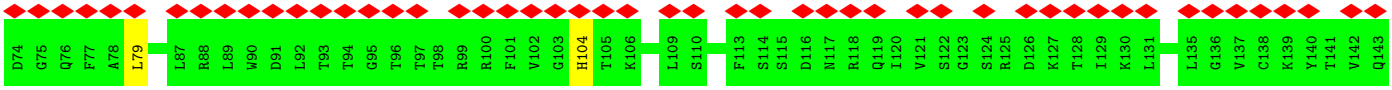


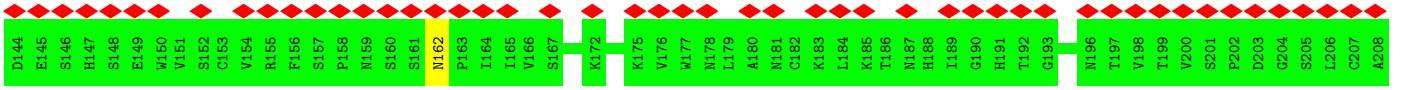
• Molecule 22: Receptor of activated protein C kinase 1

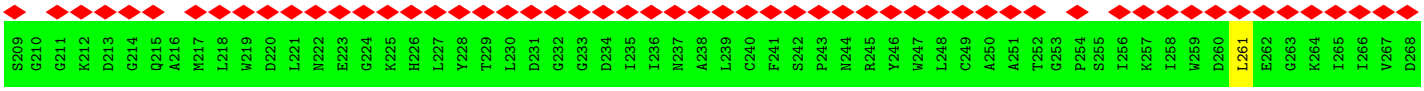
Chain Sg:

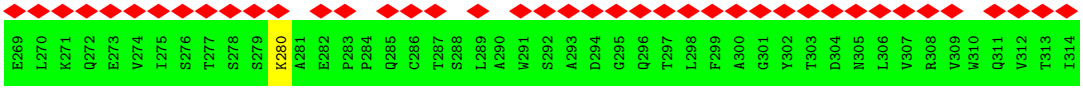






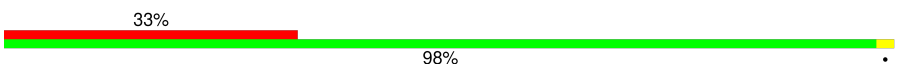


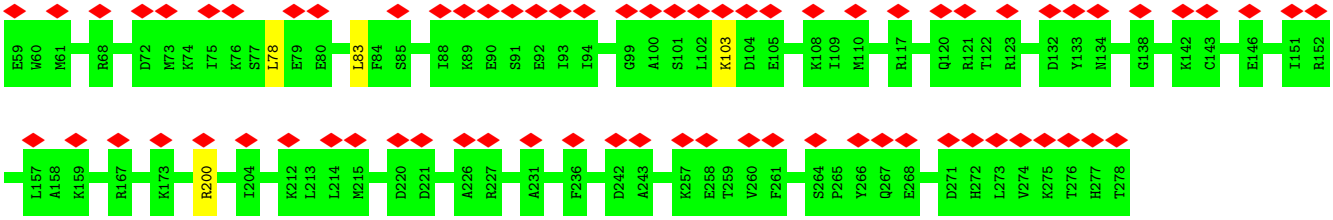




• Molecule 23: 40S ribosomal protein S2

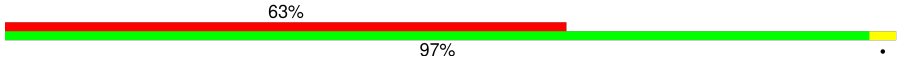
Chain SC:

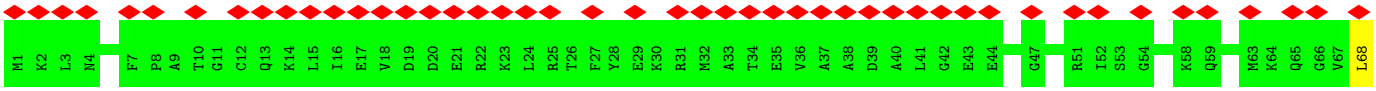




• Molecule 24: 40S ribosomal protein S6

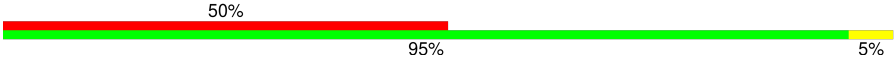
Chain SG:

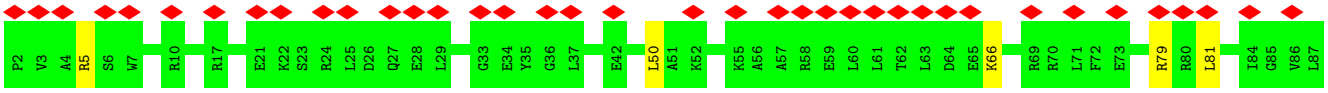


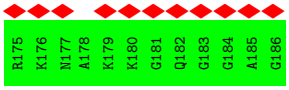


• Molecule 25: 40S ribosomal protein S9

Chain SJ:

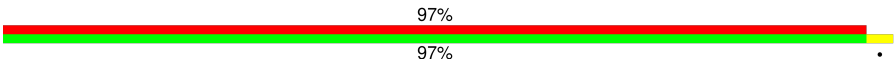


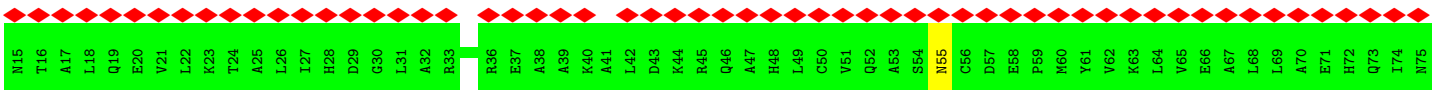


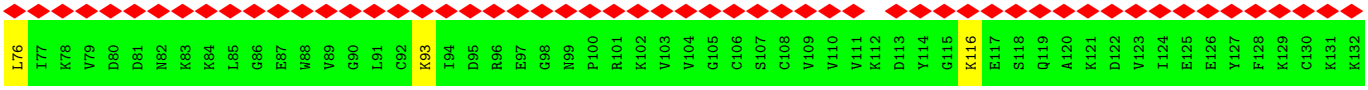


• Molecule 26: 40S ribosomal protein S12

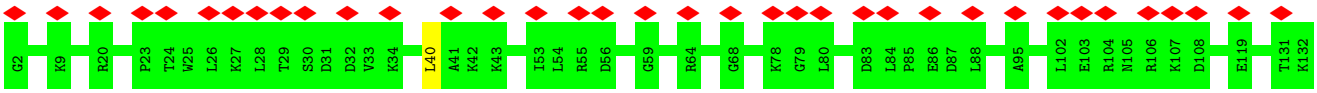
Chain SM:

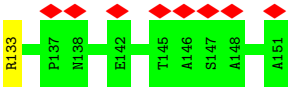




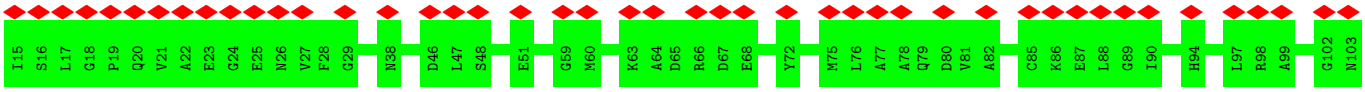


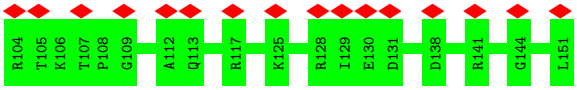
• Molecule 27: 40S ribosomal protein S13



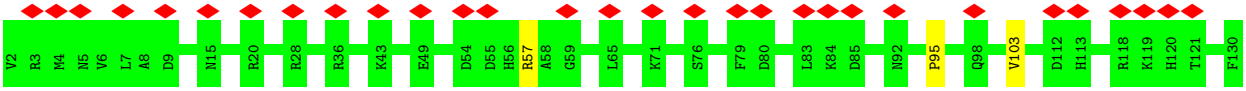


• Molecule 28: 40S ribosomal protein S14

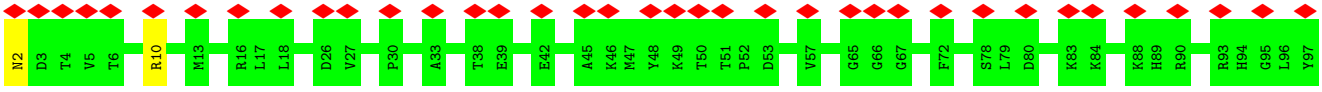


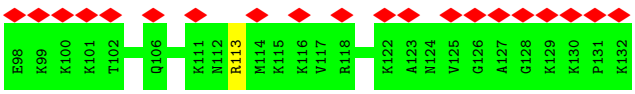


• Molecule 29: 40S ribosomal protein S15a

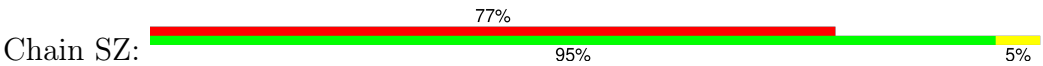


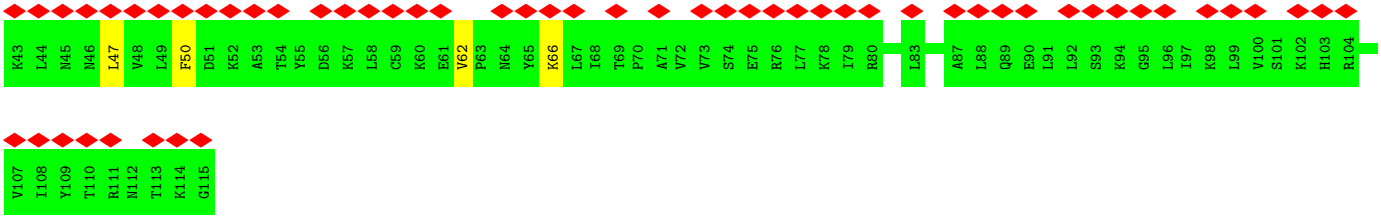
• Molecule 30: 40S ribosomal protein S24





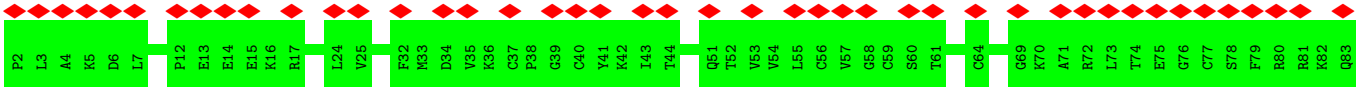
• Molecule 31: 40S ribosomal protein S25





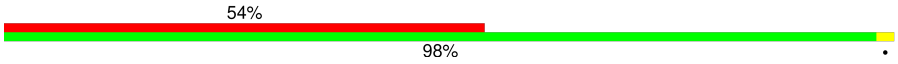
• Molecule 32: 40S ribosomal protein S27

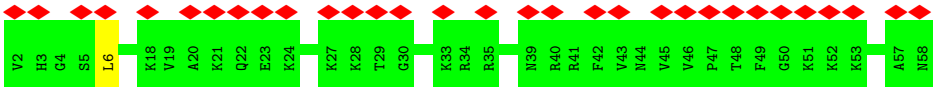
Chain Sb:



• Molecule 33: 40S ribosomal protein S30

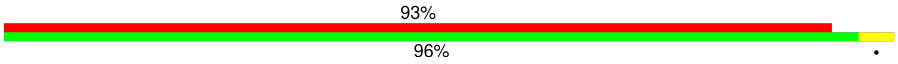
Chain Se:

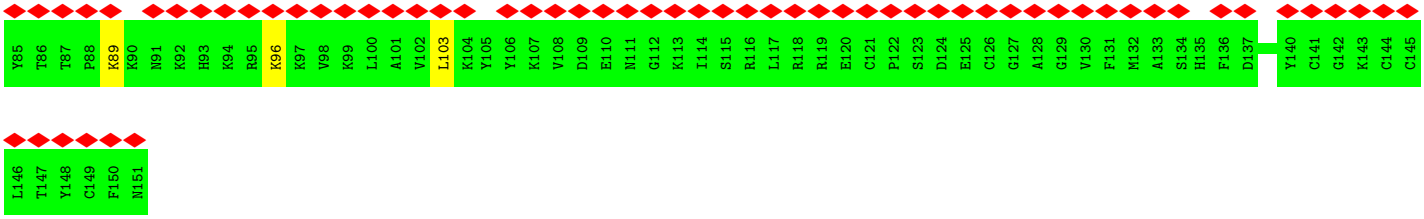




• Molecule 34: 40S ribosomal protein S27a

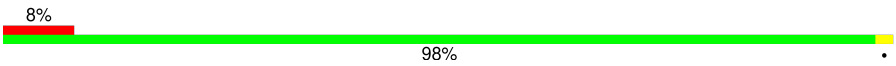
Chain Sf:

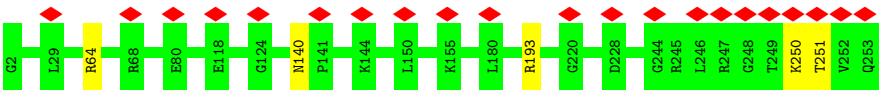




• Molecule 35: 60S ribosomal protein L8

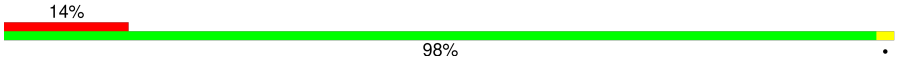
Chain A:

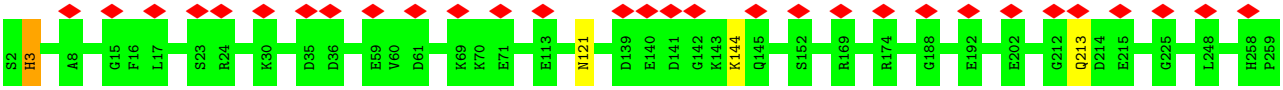


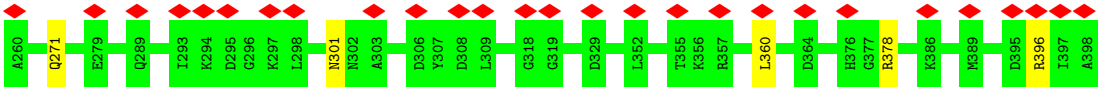


• Molecule 36: 60S ribosomal protein L3

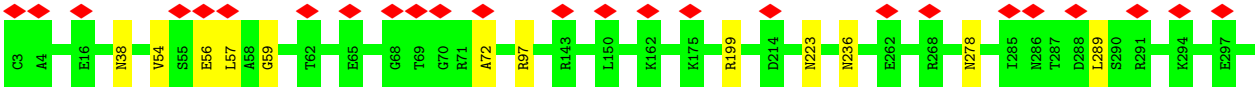
Chain B:

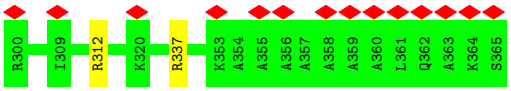




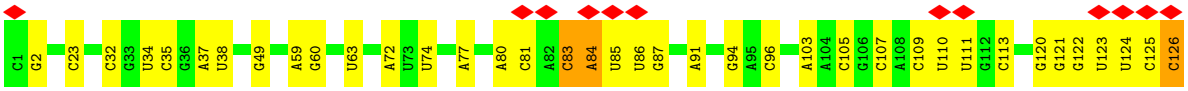


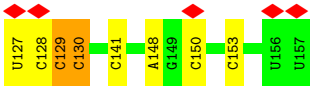
• Molecule 37: 60S ribosomal protein L4



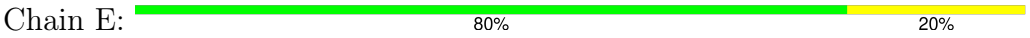


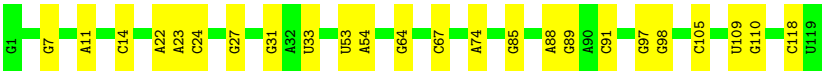
• Molecule 38: 5.8S ribosomal RNA



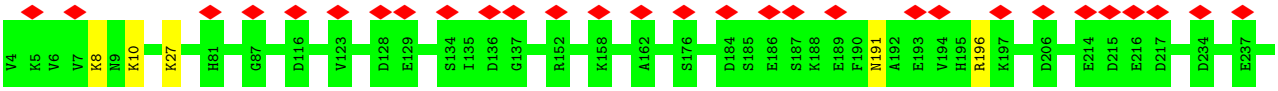


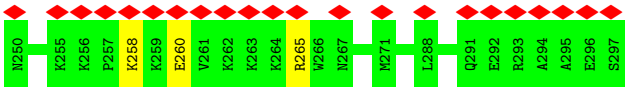
• Molecule 39: 5S ribosomal RNA



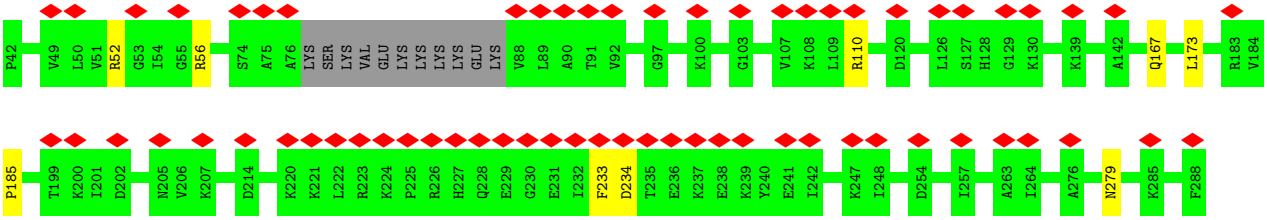


• Molecule 40: 60S ribosomal protein L5





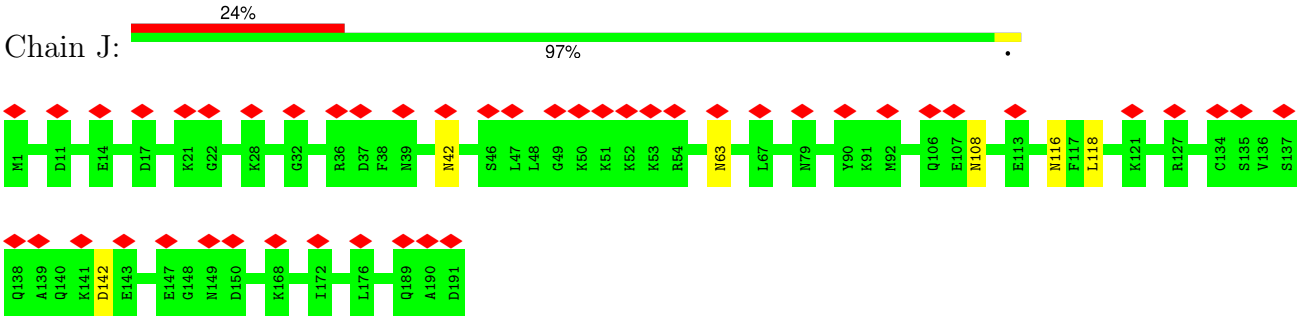
• Molecule 41: 60S ribosomal protein L6



• Molecule 42: 60S ribosomal protein L7

• Molecule 43: 60S ribosomal protein L7a

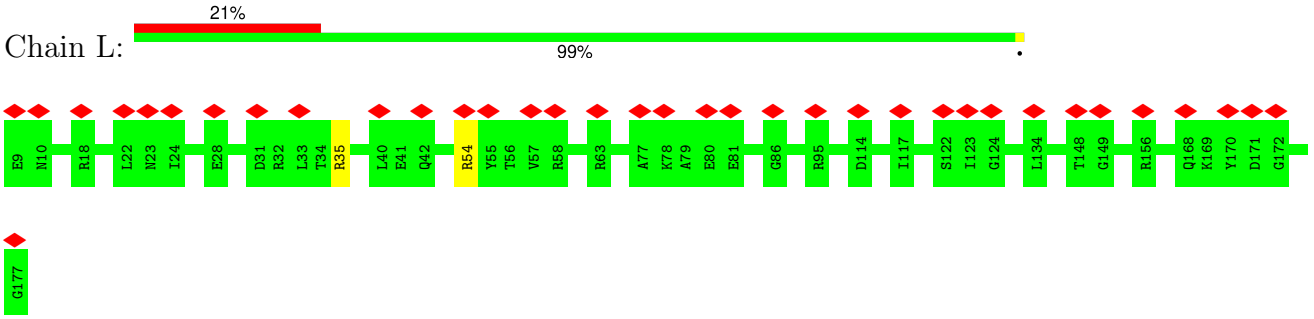
• Molecule 44: 60S ribosomal protein L9



• Molecule 45: 60S ribosomal protein L10

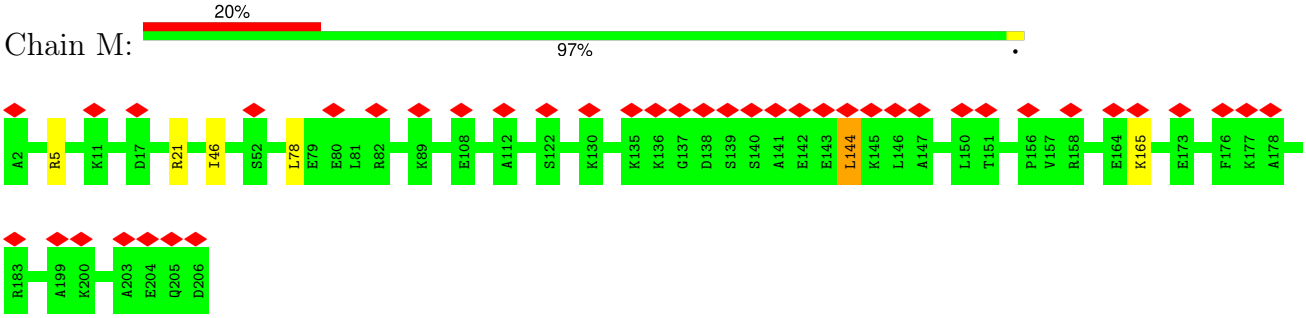
• Molecule 46: 60S ribosomal protein L11

Chain L:



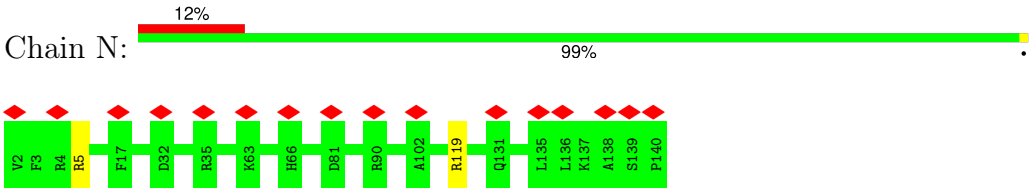
• Molecule 47: 60S ribosomal protein L13

Chain M:



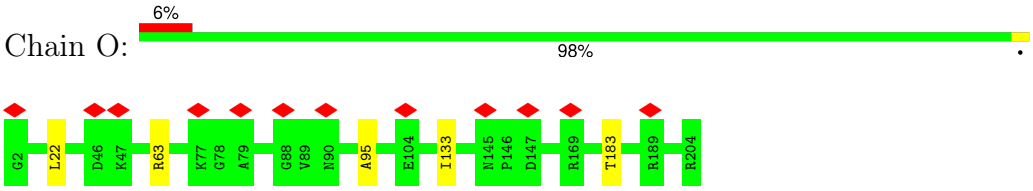
• Molecule 48: 60S ribosomal protein L14

Chain N:



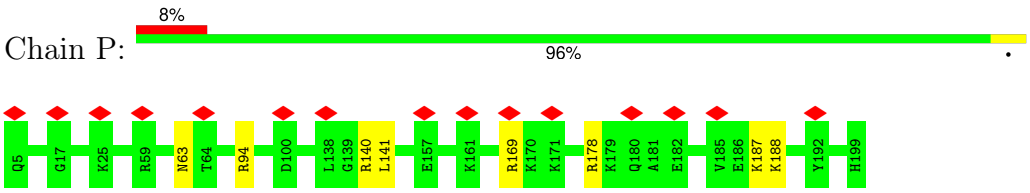
• Molecule 49: 60S ribosomal protein L15

Chain O:



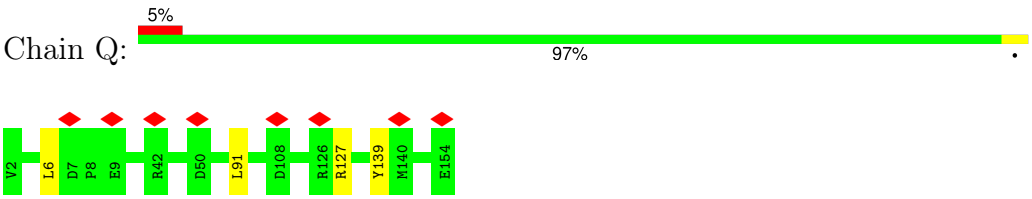
• Molecule 50: 60S ribosomal protein L13a

Chain P:



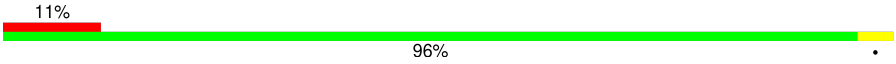
• Molecule 51: 60S ribosomal protein L17

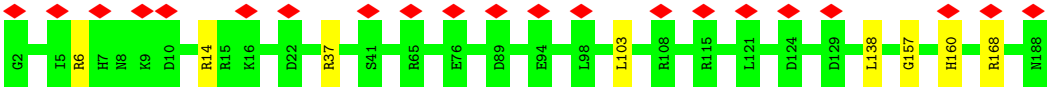
Chain Q:



• Molecule 52: 60S ribosomal protein L18

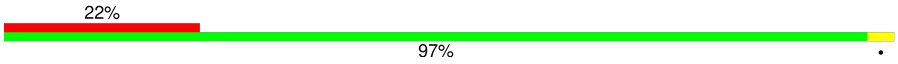
Chain R:

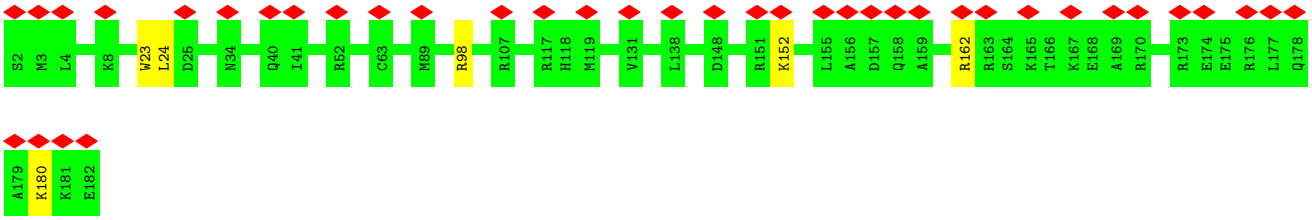




• Molecule 53: 60S ribosomal protein L19

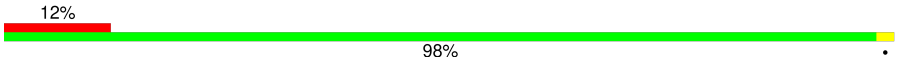
Chain S:

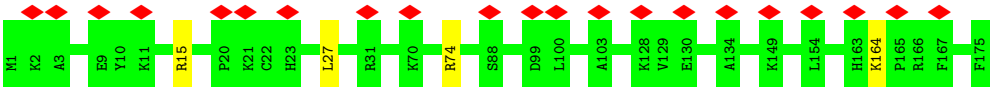




• Molecule 54: 60S ribosomal protein L18a

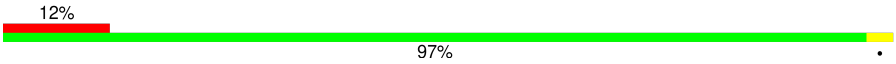
Chain T:





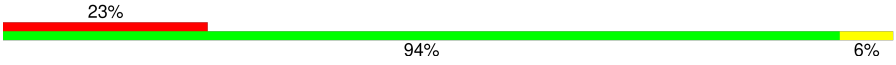
• Molecule 55: 60S ribosomal protein L21

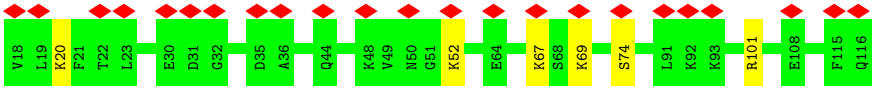
Chain U:



• Molecule 56: 60S ribosomal protein L22

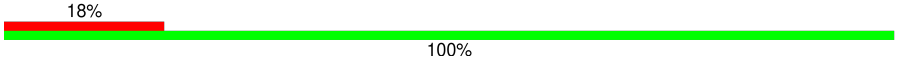
Chain V:

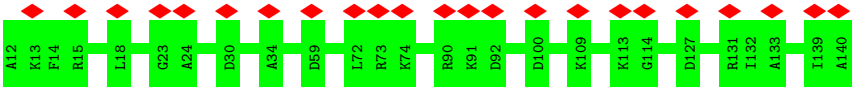




• Molecule 57: 60S ribosomal protein L23

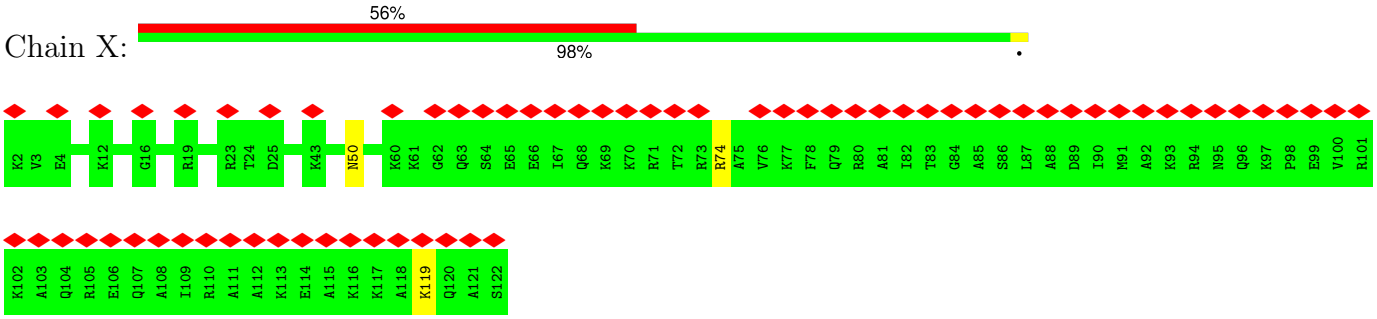
Chain W:





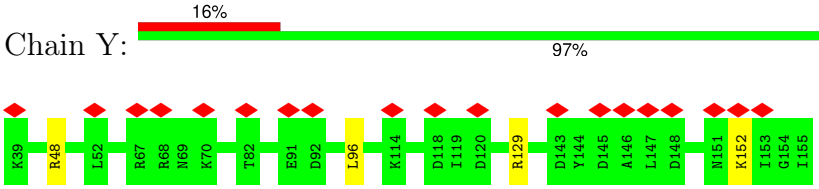
• Molecule 58: 60S ribosomal protein L24

Chain X:



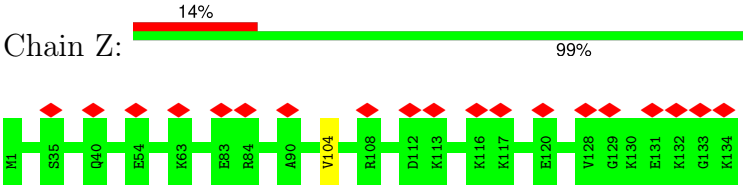
• Molecule 59: 60S ribosomal protein L23a

Chain Y:



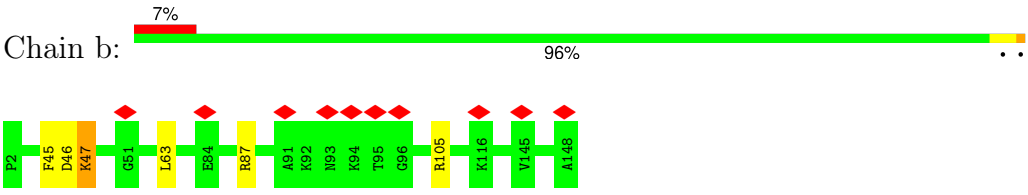
• Molecule 60: 60S ribosomal protein L26

Chain Z:



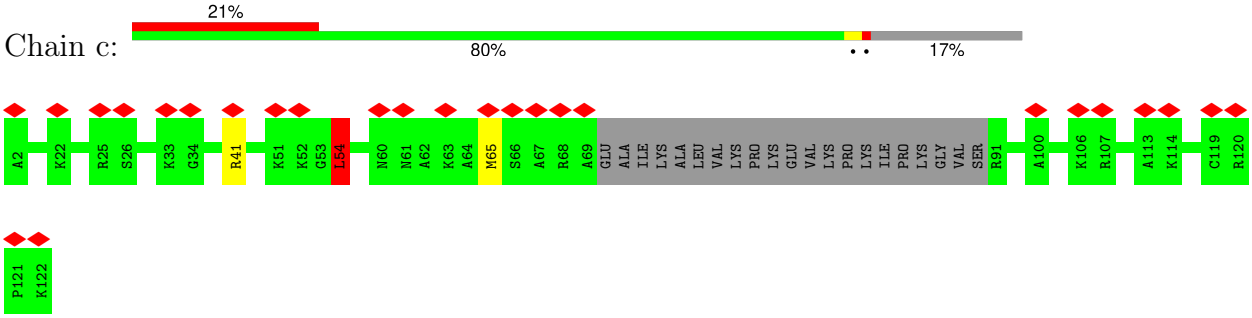
• Molecule 61: 60S ribosomal protein L27a

Chain b:



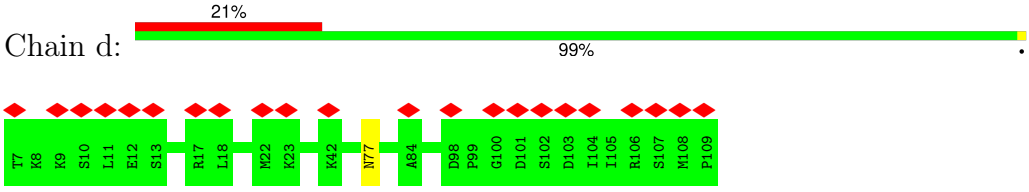
• Molecule 62: 60S ribosomal protein L29

Chain c:



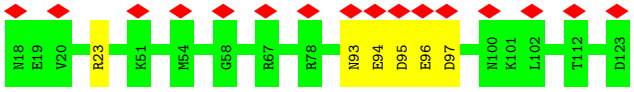
• Molecule 63: 60S ribosomal protein L30

Chain d:



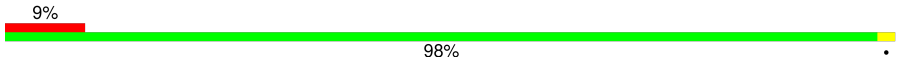
• Molecule 64: 60S ribosomal protein L31

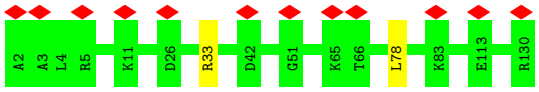
Chain e:



• Molecule 65: 60S ribosomal protein L32

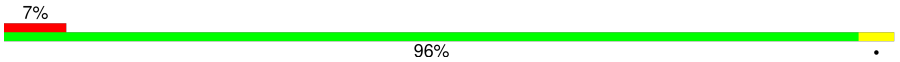
Chain f:

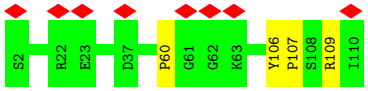




• Molecule 66: 60S ribosomal protein L35a

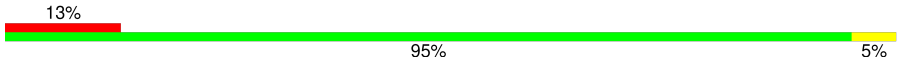
Chain g:

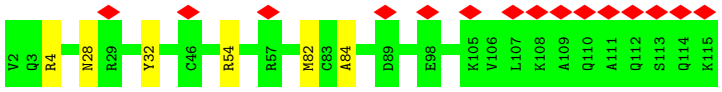




• Molecule 67: 60S ribosomal protein L34

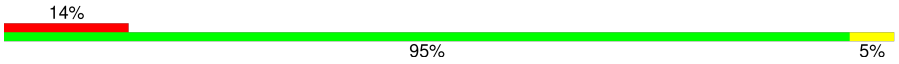
Chain h:

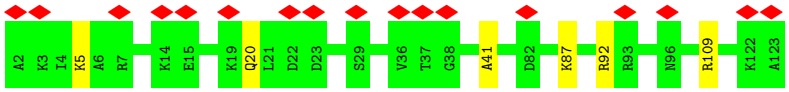




• Molecule 68: 60S ribosomal protein L35

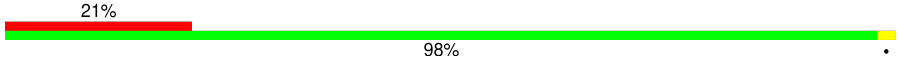
Chain i:

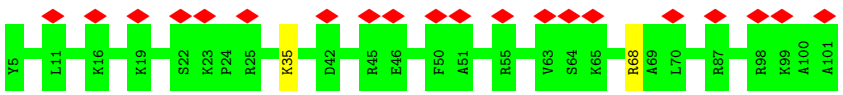




• Molecule 69: 60S ribosomal protein L36

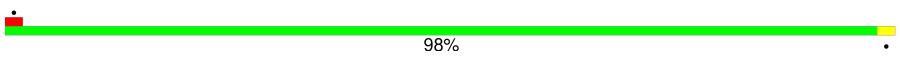
Chain j:

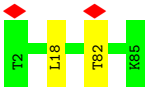




• Molecule 70: 60S ribosomal protein L37

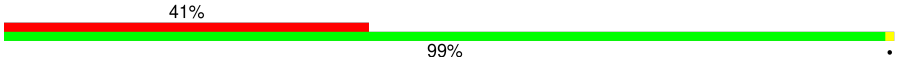
Chain k:

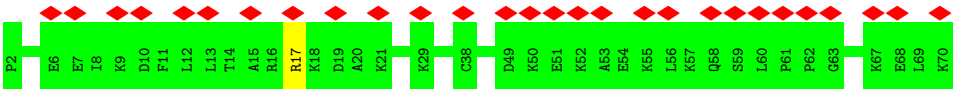




• Molecule 71: 60S ribosomal protein L38

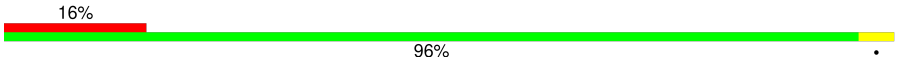
Chain l:

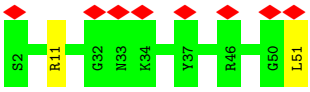




• Molecule 72: 60S ribosomal protein L39

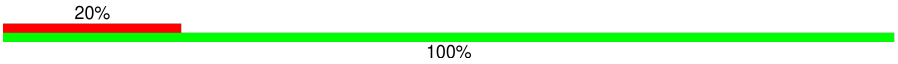
Chain m:

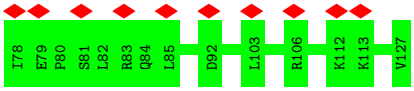




• Molecule 73: 60S ribosomal protein L40

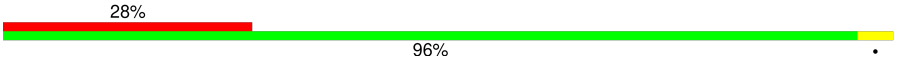
Chain n:

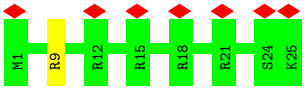




• Molecule 74: 60S ribosomal protein L41

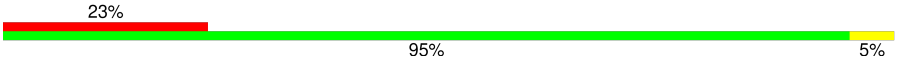
Chain o:

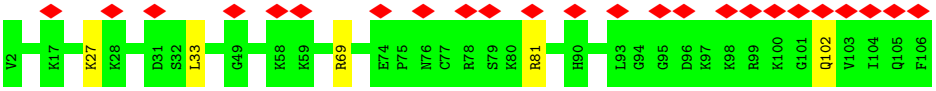




• Molecule 75: 60S ribosomal protein L36a

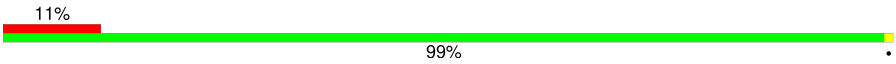
Chain p:

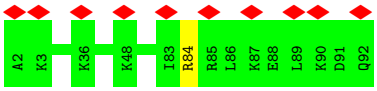




• Molecule 76: 60S ribosomal protein L37a

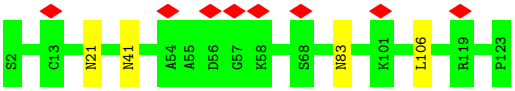
Chain q:





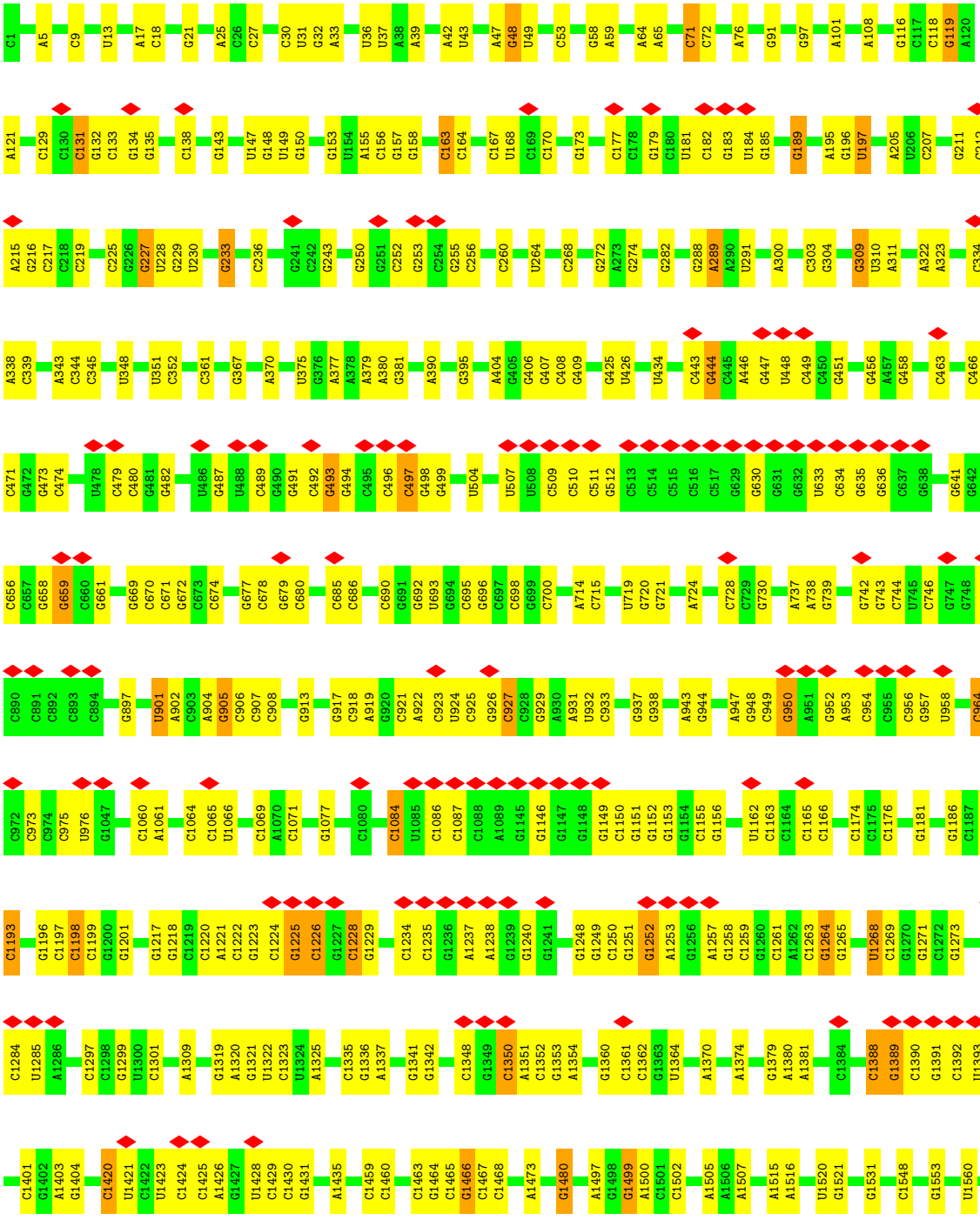
• Molecule 77: 60S ribosomal protein L28

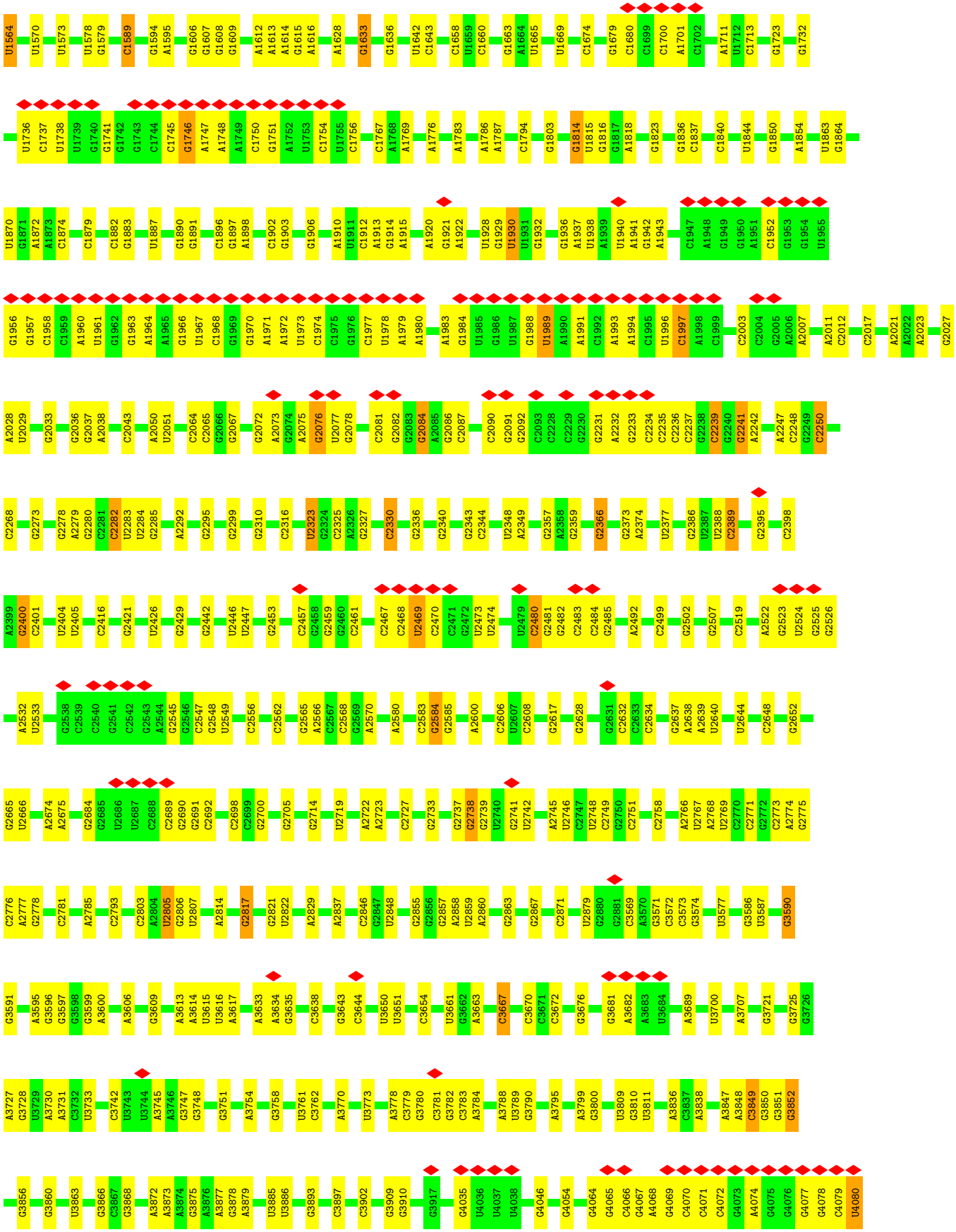
Chain r:

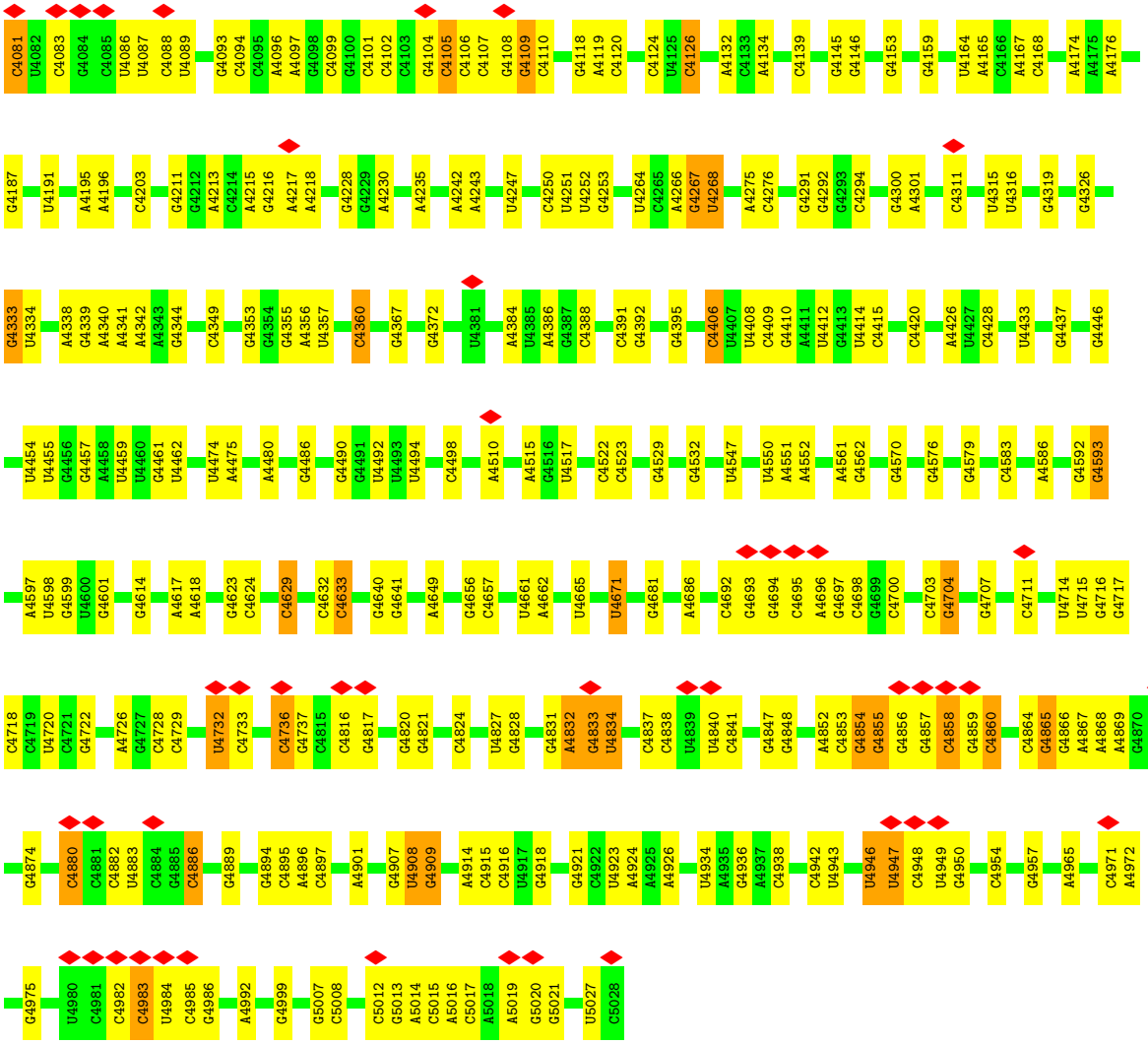


• Molecule 78: 28S ribosomal RNA

Chain t:

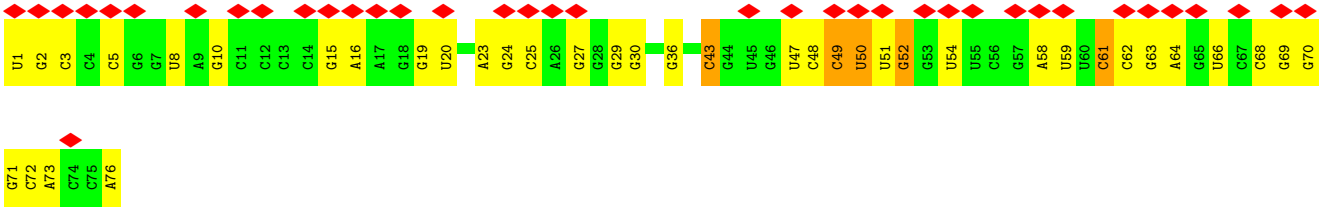






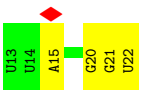
• Molecule 79: PE tRNA

Chain v:



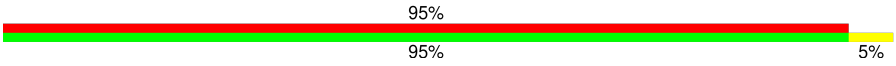
• Molecule 80: mRNA

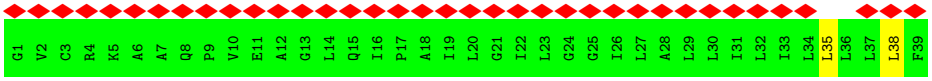
Chain w:



• Molecule 81: Cadherin-1

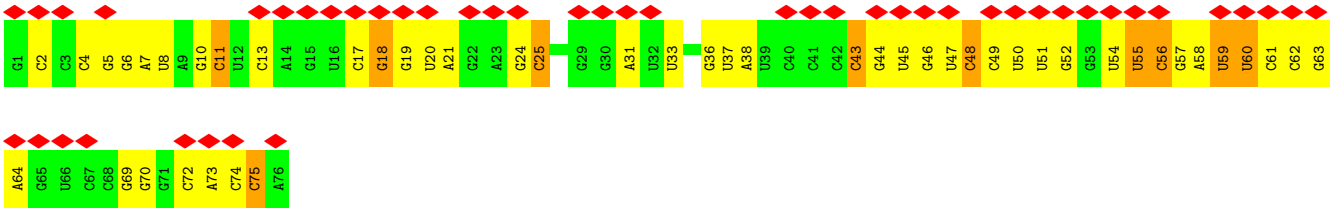
Chain y:





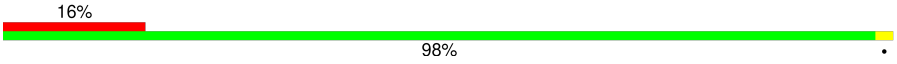
• Molecule 82: AA tRNA

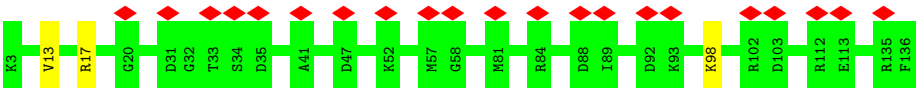
Chain u:



• Molecule 83: 60S ribosomal protein L27

Chain a:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10350	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.096	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	460.0, 460.0, 460.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ, ZN, A2M, B8Q, UR3, MG, OMU, OMG, 5MU, B8N, 4AC, 5MC, E3C, M7A, MA6, PSU, MVM, OMC

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	S2	2.35	14/39959 (0.0%)	1.15	217/62253 (0.3%)
2	SA	0.42	0/1778	0.67	1/2416 (0.0%)
3	SB	0.39	0/1765	0.63	2/2362 (0.1%)
4	SD	0.38	0/1785	0.68	0/2404
5	SE	0.37	0/2101	0.65	0/2828
6	SF	0.36	0/1516	0.64	1/2037 (0.0%)
7	SH	0.40	0/1519	0.69	1/2033 (0.0%)
8	SI	0.38	0/1702	0.69	2/2271 (0.1%)
9	SK	0.42	0/851	0.67	0/1147
10	SL	1.36	1/1268 (0.1%)	0.82	5/1696 (0.3%)
11	SP	0.37	0/1065	0.65	0/1423
12	SQ	0.40	0/1177	0.66	0/1575
13	SR	0.35	0/1097	0.68	0/1474
14	SS	0.36	0/1216	0.66	0/1628
15	ST	0.34	0/1131	0.63	1/1515 (0.1%)
16	SU	0.33	0/831	0.68	1/1115 (0.1%)
17	SV	0.42	0/631	0.73	1/844 (0.1%)
18	SX	0.43	0/1116	0.69	0/1490
19	Sa	0.45	0/836	0.67	0/1121
20	Sc	0.38	0/508	0.68	0/680
21	Sd	0.50	1/470 (0.2%)	0.80	2/623 (0.3%)
22	Sg	0.35	0/2486	0.73	4/3384 (0.1%)
23	SC	0.47	0/1755	0.74	1/2371 (0.0%)
24	SG	0.34	0/1946	0.66	2/2590 (0.1%)
25	SJ	0.38	0/1561	0.73	2/2083 (0.1%)
26	SM	0.32	0/922	0.69	1/1238 (0.1%)
27	SN	0.37	0/1232	0.64	1/1656 (0.1%)
28	SO	0.38	0/1037	0.66	0/1391
29	SW	0.43	0/1051	0.63	0/1406
30	SY	0.35	0/1094	0.60	0/1452
31	SZ	0.36	0/585	0.85	1/785 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Sb	0.37	0/653	0.63	0/876
33	Se	0.34	0/458	0.65	0/604
34	Sf	0.35	0/560	0.72	1/745 (0.1%)
35	A	0.52	0/1968	0.67	0/2639
36	B	0.48	0/3270	0.70	2/4377 (0.0%)
37	C	0.49	0/2942	0.68	1/3951 (0.0%)
38	D	0.91	1/3726 (0.0%)	1.13	20/5804 (0.3%)
39	E	0.86	0/2839	1.07	7/4425 (0.2%)
40	F	0.44	0/2437	0.65	0/3262
41	G	0.43	0/1942	0.74	3/2606 (0.1%)
42	H	0.53	0/1905	0.71	3/2539 (0.1%)
43	I	0.45	0/1913	0.68	0/2576
44	J	0.43	0/1545	0.69	2/2077 (0.1%)
45	K	0.45	0/1730	0.66	1/2311 (0.0%)
46	L	0.42	0/1376	0.68	0/1841
47	M	0.47	0/1688	0.71	1/2260 (0.0%)
48	N	0.45	0/1161	0.62	0/1554
49	O	0.57	0/1746	0.71	0/2338
50	P	0.47	0/1638	0.65	1/2191 (0.0%)
51	Q	0.49	0/1268	0.65	2/1701 (0.1%)
52	R	0.50	0/1537	0.69	2/2052 (0.1%)
53	S	0.46	0/1533	0.71	1/2025 (0.0%)
54	T	0.51	0/1488	0.66	1/1997 (0.1%)
55	U	0.48	0/1312	0.67	0/1753
56	V	0.44	0/822	0.68	0/1103
57	W	0.45	0/983	0.62	0/1319
58	X	4.12	1/1004 (0.1%)	0.74	1/1332 (0.1%)
59	Y	0.45	0/975	0.65	0/1312
60	Z	0.48	0/1132	0.64	0/1504
61	b	0.52	0/1191	0.69	0/1591
62	c	0.39	0/826	0.70	1/1088 (0.1%)
63	d	0.49	0/812	0.72	0/1089
64	e	0.45	0/894	0.67	0/1204
65	f	0.48	0/1082	0.64	1/1443 (0.1%)
66	g	0.53	0/895	0.72	1/1198 (0.1%)
67	h	0.53	1/916 (0.1%)	0.73	0/1220
68	i	0.42	0/1023	0.70	0/1351
69	j	0.38	0/805	0.66	0/1065
70	k	0.51	0/703	0.71	1/929 (0.1%)
71	l	0.37	0/575	0.67	0/761
72	m	0.42	0/454	0.71	1/599 (0.2%)
73	n	0.40	0/417	0.69	0/553
74	o	0.42	0/241	0.72	0/305

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	p	0.46	0/877	0.71	1/1156 (0.1%)
76	q	0.54	0/718	0.74	0/953
77	r	0.53	0/995	0.74	1/1334 (0.1%)
78	t	0.91	4/86502 (0.0%)	1.17	508/134927 (0.4%)
79	v	0.58	0/1802	1.23	14/2797 (0.5%)
80	w	0.70	0/235	1.25	2/365 (0.5%)
81	y	0.35	0/263	1.02	1/359 (0.3%)
82	u	0.56	0/1800	1.39	34/2804 (1.2%)
83	a	0.47	0/1126	0.69	0/1502
All	All	1.21	23/230694 (0.0%)	1.01	861/338958 (0.3%)

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
11	SP	0	1
15	ST	0	1
16	SU	0	1
56	V	0	1
62	c	0	1
All	All	0	5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	291	G	N7-C5	229.25	2.76	1.39
1	S2	291	G	C8-N7	214.07	2.59	1.30
1	S2	291	G	N9-C8	184.78	2.67	1.37
1	S2	291	G	N9-C4	174.09	2.77	1.38
1	S2	291	G	C5-C4	160.98	2.51	1.38
58	X	119	LYS	CD-CE	129.78	4.75	1.51
1	S2	325	C	N1-C6	57.00	1.71	1.37
1	S2	325	C	N3-C4	50.34	1.69	1.33
1	S2	325	C	C2-N3	46.46	1.73	1.35
10	SL	41	GLY	CA-C	45.57	2.24	1.51
1	S2	325	C	N1-C2	35.84	1.75	1.40
1	S2	325	C	C4-C5	35.36	1.71	1.43
1	S2	325	C	C5-C6	33.30	1.60	1.34
38	D	37	A	N9-C4	-7.95	1.33	1.37
78	t	2067	G	N9-C4	-6.71	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	t	4267	G	C2-N3	-6.08	1.27	1.32
1	S2	291	G	N1-C2	5.97	1.42	1.37
67	h	32	TYR	CA-CB	-5.31	1.42	1.53
1	S2	913	A	N9-C4	5.20	1.41	1.37
1	S2	291	G	C5-C6	-5.11	1.37	1.42
21	Sd	42	CYS	CB-SG	-5.07	1.73	1.81
78	t	148	G	N9-C4	-5.07	1.33	1.38
78	t	1628	A	N9-C4	-5.05	1.34	1.37

All (861) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	291	G	C6-N1-C2	25.90	140.64	125.10
1	S2	291	G	N3-C4-C5	-25.47	115.87	128.60
1	S2	291	G	C6-C5-N7	23.18	144.31	130.40
1	S2	115	U	C2-N3-C4	21.35	139.81	127.00
1	S2	291	G	N1-C2-N3	19.64	135.68	123.90
1	S2	291	G	C4-C5-C6	-19.54	107.08	118.80
1	S2	291	G	N3-C4-N9	18.48	137.09	126.00
1	S2	325	C	C6-N1-C2	15.91	126.67	120.30
1	S2	291	G	N7-C8-N9	-15.76	105.22	113.10
10	SL	41	GLY	O-C-N	-14.53	99.45	122.70
79	v	61	C	C2-N1-C1'	14.49	134.74	118.80
78	t	956	C	N1-C2-O2	13.82	127.19	118.90
1	S2	325	C	N1-C2-N3	-13.34	109.86	119.20
78	t	956	C	C2-N1-C1'	11.84	131.82	118.80
1	S2	115	U	N1-C2-N3	11.79	121.97	114.90
78	t	1989	U	N1-C2-O2	11.76	131.03	122.80
78	t	2323	U	N1-C2-O2	11.68	130.97	122.80
78	t	1989	U	N3-C2-O2	-11.64	114.05	122.20
1	S2	291	G	C5-N7-C8	11.37	109.99	104.30
78	t	918	C	N1-C2-O2	11.36	125.72	118.90
79	v	61	C	N1-C2-O2	11.34	125.70	118.90
78	t	2323	U	N3-C2-O2	-11.25	114.32	122.20
78	t	956	C	N3-C2-O2	-11.21	114.06	121.90
79	v	61	C	C6-N1-C1'	-11.17	107.39	120.80
1	S2	1341	C	N1-C2-O2	11.05	125.53	118.90
78	t	1989	U	C2-N1-C1'	10.92	130.81	117.70
78	t	2236	C	N1-C2-O2	10.90	125.44	118.90
78	t	964	C	N1-C2-O2	10.82	125.39	118.90
1	S2	356	C	C2-N1-C1'	10.67	130.53	118.80
78	t	2388	U	C2-N1-C1'	10.60	130.43	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	356	C	N1-C2-O2	10.37	125.12	118.90
78	t	958	U	C2-N1-C1'	10.35	130.12	117.70
78	t	2236	C	N3-C2-O2	-10.35	114.65	121.90
1	S2	1139	C	N1-C2-O2	10.27	125.06	118.90
1	S2	115	U	N3-C4-C5	9.95	120.57	114.60
78	t	2067	G	N3-C4-N9	-9.94	120.04	126.00
1	S2	501	C	N1-C2-O2	9.92	124.85	118.90
78	t	964	C	N3-C2-O2	-9.78	115.05	121.90
78	t	2388	U	N1-C2-O2	9.72	129.61	122.80
78	t	964	C	C2-N1-C1'	9.68	129.45	118.80
1	S2	1816	G	O5'-P-OP1	-9.56	97.09	105.70
78	t	219	C	C6-N1-C2	-9.48	116.51	120.30
1	S2	1341	C	N3-C2-O2	-9.37	115.34	121.90
1	S2	570	C	N1-C2-O2	9.06	124.34	118.90
1	S2	291	G	N3-C2-N2	-9.02	113.59	119.90
78	t	918	C	N3-C2-O2	-9.01	115.59	121.90
78	t	2793	C	N1-C2-O2	8.94	124.26	118.90
78	t	958	U	N1-C2-O2	8.91	129.03	122.80
78	t	918	C	C2-N1-C1'	8.90	128.59	118.80
78	t	2325	C	N3-C2-O2	-8.87	115.69	121.90
54	T	27	LEU	CA-CB-CG	8.86	135.69	115.30
1	S2	1307	U	C2-N1-C1'	8.81	128.28	117.70
82	u	43	C	C6-N1-C2	-8.81	116.78	120.30
1	S2	889	U	N1-C2-O2	8.71	128.90	122.80
78	t	2388	U	N3-C2-O2	-8.70	116.11	122.20
78	t	2236	C	C2-N1-C1'	8.68	128.34	118.80
78	t	2325	C	N1-C2-O2	8.67	124.10	118.90
82	u	43	C	N1-C2-O2	8.66	124.09	118.90
78	t	905	G	C4-N9-C1'	8.65	137.75	126.50
78	t	197	U	C2-N1-C1'	8.61	128.04	117.70
78	t	956	C	C6-N1-C2	-8.57	116.87	120.30
1	S2	1139	C	N3-C2-O2	-8.56	115.91	121.90
66	g	106	TYR	C-N-CD	-8.38	102.17	120.60
1	S2	356	C	N3-C2-O2	-8.32	116.08	121.90
78	t	4267	G	N3-C2-N2	-8.30	114.09	119.90
78	t	471	C	C5-C6-N1	8.23	125.11	121.00
78	t	958	U	N3-C2-O2	-8.23	116.44	122.20
51	Q	6	LEU	CA-CB-CG	8.23	134.22	115.30
78	t	4733	C	C5-C6-N1	8.19	125.10	121.00
82	u	43	C	N3-C2-O2	-8.18	116.17	121.90
78	t	2727	C	C2-N1-C1'	8.17	127.79	118.80
78	t	148	G	N3-C4-N9	-8.17	121.10	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
78	t	217	C	C6-N1-C2	-8.14	117.04	120.30
1	S2	1384	C	N1-C2-O2	8.13	123.78	118.90
82	u	18	G	P-O3'-C3'	8.10	129.42	119.70
1	S2	1139	C	C2-N1-C1'	8.10	127.71	118.80
78	t	659	G	C4-N9-C1'	8.09	137.01	126.50
78	t	4946	U	OP1-P-O3'	8.01	122.81	105.20
1	S2	548	C	N1-C2-O2	8.00	123.70	118.90
78	t	671	C	N1-C2-O2	7.97	123.68	118.90
78	t	2236	C	C6-N1-C2	-7.97	117.11	120.30
1	S2	1341	C	C2-N1-C1'	7.96	127.56	118.80
1	S2	356	C	C6-N1-C1'	-7.96	111.25	120.80
1	S2	913	A	C2-N3-C4	7.96	114.58	110.60
78	t	2067	G	N3-C4-C5	7.95	132.57	128.60
1	S2	1283	C	N1-C2-O2	7.93	123.66	118.90
78	t	956	C	C6-N1-C1'	-7.92	111.29	120.80
79	v	61	C	N3-C2-O2	-7.92	116.35	121.90
78	t	493	G	C4-N9-C1'	7.91	136.78	126.50
1	S2	325	C	N3-C2-O2	7.89	127.42	121.90
1	S2	501	C	C2-N1-C1'	7.87	127.46	118.80
1	S2	325	C	C2-N3-C4	7.85	123.83	119.90
78	t	497	C	C6-N1-C2	-7.85	117.16	120.30
78	t	2805	U	N3-C2-O2	-7.85	116.71	122.20
82	u	59	U	N1-C2-O2	7.84	128.28	122.80
78	t	352	C	N3-C2-O2	-7.81	116.43	121.90
82	u	54	U	C5-C4-O4	-7.81	121.22	125.90
78	t	1564	U	N3-C2-O2	-7.80	116.74	122.20
78	t	964	C	C6-N1-C2	-7.79	117.19	120.30
78	t	905	G	N3-C4-N9	7.77	130.66	126.00
78	t	1459	C	N1-C2-O2	7.77	123.56	118.90
78	t	3616	U	N3-C2-O2	-7.77	116.76	122.20
78	t	1499	G	C4-N9-C1'	7.73	136.55	126.50
78	t	2388	U	C6-N1-C1'	-7.73	110.38	121.20
78	t	4880	C	N1-C2-O2	7.73	123.54	118.90
1	S2	889	U	N3-C2-O2	-7.72	116.79	122.20
38	D	123	U	N1-C2-O2	7.71	128.20	122.80
78	t	4908	U	N1-C2-O2	7.67	128.17	122.80
78	t	1564	U	C2-N1-C1'	7.66	126.89	117.70
78	t	2793	C	N3-C2-O2	-7.65	116.54	121.90
78	t	905	G	C8-N9-C1'	-7.64	117.07	127.00
1	S2	1520	G	C4-N9-C1'	7.59	136.37	126.50
78	t	4908	U	N3-C2-O2	-7.59	116.89	122.20
31	SZ	47	LEU	CA-CB-CG	7.57	132.71	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	548	C	C2-N1-C1'	7.56	127.11	118.80
78	t	163	C	C2-N1-C1'	7.53	127.09	118.80
82	u	43	C	C2-N1-C1'	7.52	127.07	118.80
78	t	671	C	N3-C2-O2	-7.51	116.64	121.90
78	t	4908	U	C2-N1-C1'	7.50	126.70	117.70
77	r	106	LEU	CA-CB-CG	7.50	132.54	115.30
78	t	4736	C	N1-C2-O2	7.48	123.39	118.90
78	t	131	C	C6-N1-C2	-7.47	117.31	120.30
78	t	2805	U	C2-N1-C1'	7.46	126.65	117.70
82	u	18	G	OP1-P-O3'	7.45	121.59	105.20
79	v	61	C	C5-C6-N1	7.43	124.72	121.00
78	t	3595	A	P-O3'-C3'	7.42	128.61	119.70
78	t	1261	C	N1-C2-O2	7.42	123.35	118.90
78	t	219	C	C2-N1-C1'	7.41	126.95	118.80
78	t	1459	C	N3-C2-O2	-7.40	116.72	121.90
78	t	2793	C	C2-N1-C1'	7.39	126.93	118.80
78	t	4728	C	C6-N1-C2	-7.36	117.36	120.30
78	t	150	G	C4-N9-C1'	7.28	135.97	126.50
39	E	14	C	N1-C2-O2	7.27	123.26	118.90
78	t	352	C	N1-C2-O2	7.27	123.26	118.90
78	t	1746	G	C4-N9-C1'	7.27	135.95	126.50
1	S2	291	G	C8-N9-C4	7.26	109.31	106.40
78	t	474	C	N1-C2-O2	7.26	123.26	118.90
78	t	443	C	C6-N1-C2	-7.26	117.40	120.30
78	t	2805	U	N1-C2-O2	7.25	127.88	122.80
78	t	150	G	C8-N9-C1'	-7.24	117.58	127.00
78	t	4946	U	P-O3'-C3'	7.24	128.38	119.70
78	t	2457	C	C6-N1-C2	-7.23	117.41	120.30
78	t	444	G	O4'-C1'-N9	7.22	113.98	108.20
38	D	123	U	N3-C2-O2	-7.22	117.15	122.20
1	S2	1373	C	C6-N1-C2	-7.22	117.41	120.30
78	t	219	C	N3-C2-O2	-7.20	116.86	121.90
1	S2	501	C	C5-C6-N1	7.17	124.59	121.00
78	t	659	G	N3-C4-C5	-7.17	125.02	128.60
78	t	4736	C	C2-N1-C1'	7.17	126.68	118.80
78	t	2241	G	N3-C4-N9	7.14	130.29	126.00
78	t	4498	C	C6-N1-C2	-7.13	117.45	120.30
1	S2	1283	C	N3-C2-O2	-7.12	116.91	121.90
78	t	1564	U	N1-C2-O2	7.12	127.78	122.80
78	t	1633	G	C4-N9-C1'	7.11	135.74	126.50
38	D	83	C	N1-C2-O2	7.09	123.15	118.90
1	S2	1283	C	C2-N1-C1'	7.07	126.58	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
78	t	361	C	N1-C2-O2	7.06	123.14	118.90
78	t	956	C	C5-C6-N1	7.05	124.52	121.00
39	E	14	C	N3-C2-O2	-7.04	116.97	121.90
1	S2	889	U	C5-C6-N1	7.03	126.21	122.70
78	t	4700	C	C5-C6-N1	7.01	124.51	121.00
78	t	4733	C	C6-N1-C2	-7.00	117.50	120.30
82	u	48	C	N1-C2-O2	6.99	123.09	118.90
1	S2	1520	G	C8-N9-C1'	-6.98	117.93	127.00
1	S2	570	C	N3-C2-O2	-6.97	117.02	121.90
1	S2	303	C	N1-C2-O2	6.96	123.08	118.90
78	t	2017	C	C6-N1-C2	-6.95	117.52	120.30
78	t	2241	G	C4-N9-C1'	6.93	135.51	126.50
78	t	148	G	N3-C4-C5	6.92	132.06	128.60
78	t	2400	G	C4-N9-C1'	6.92	135.50	126.50
78	t	2241	G	N3-C4-C5	-6.92	125.14	128.60
78	t	1633	G	C8-N9-C1'	-6.91	118.02	127.00
41	G	234	ASP	CB-CG-OD1	6.89	124.50	118.30
78	t	1261	C	N3-C2-O2	-6.88	117.08	121.90
78	t	268	C	C6-N1-C2	-6.87	117.55	120.30
78	t	659	G	N3-C4-N9	6.87	130.12	126.00
1	S2	1005	G	C4-N9-C1'	6.86	135.41	126.50
78	t	1989	U	C6-N1-C1'	-6.86	111.60	121.20
82	u	25	C	C6-N1-C2	-6.86	117.56	120.30
78	t	670	C	C6-N1-C2	-6.85	117.56	120.30
78	t	3616	U	N1-C2-O2	6.84	127.59	122.80
1	S2	387	C	C6-N1-C2	-6.84	117.56	120.30
78	t	4946	U	C2-N1-C1'	6.84	125.90	117.70
78	t	2323	U	C2-N1-C1'	6.83	125.90	117.70
78	t	700	C	N3-C2-O2	-6.82	117.13	121.90
1	S2	303	C	N3-C2-O2	-6.81	117.13	121.90
78	t	2556	C	C6-N1-C2	-6.81	117.58	120.30
78	t	4406	C	N1-C2-O2	6.81	122.98	118.90
78	t	1466	G	C4-N9-C1'	6.81	135.35	126.50
78	t	4406	C	N3-C2-O2	-6.79	117.14	121.90
38	D	141	C	C6-N1-C2	-6.77	117.59	120.30
78	t	1499	G	C8-N9-C1'	-6.76	118.22	127.00
1	S2	1340	U	N3-C2-O2	-6.75	117.47	122.20
78	t	197	U	N1-C2-O2	6.75	127.53	122.80
78	t	4983	C	C6-N1-C2	-6.75	117.60	120.30
78	t	2398	C	C2-N1-C1'	6.74	126.21	118.80
1	S2	202	G	C4-N9-C1'	6.73	135.25	126.50
1	S2	951	C	C6-N1-C2	-6.72	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	1005	G	C8-N9-C1'	-6.72	118.26	127.00
78	t	4717	G	N3-C4-N9	-6.72	121.97	126.00
78	t	918	C	C6-N1-C1'	-6.72	112.73	120.80
1	S2	291	G	C4-C5-N7	-6.72	108.11	110.80
1	S2	474	G	C4-N9-C1'	6.70	135.21	126.50
78	t	958	U	C6-N1-C1'	-6.70	111.81	121.20
78	t	2325	C	C2-N1-C1'	6.70	126.17	118.80
78	t	2727	C	C6-N1-C1'	-6.70	112.76	120.80
78	t	2234	C	N1-C2-O2	6.70	122.92	118.90
78	t	474	C	N3-C2-O2	-6.67	117.23	121.90
1	S2	202	G	N3-C4-N9	6.66	130.00	126.00
1	S2	1057	C	C6-N1-C2	-6.66	117.64	120.30
1	S2	1340	U	N1-C2-O2	6.65	127.46	122.80
78	t	4886	C	C6-N1-C2	-6.65	117.64	120.30
38	D	129	C	N3-C2-O2	-6.64	117.25	121.90
78	t	207	C	N1-C2-O2	6.64	122.89	118.90
78	t	4946	U	N1-C2-O2	6.64	127.45	122.80
78	t	2519	C	C6-N1-C2	-6.64	117.64	120.30
1	S2	1271	C	N1-C2-O2	6.64	122.88	118.90
1	S2	1139	C	C6-N1-C2	-6.63	117.65	120.30
1	S2	1496	U	N3-C2-O2	-6.63	117.56	122.20
78	t	3638	C	C6-N1-C2	-6.62	117.65	120.30
78	t	670	C	N3-C2-O2	-6.62	117.27	121.90
78	t	463	C	N1-C2-O2	6.62	122.87	118.90
78	t	493	G	N3-C4-N9	6.62	129.97	126.00
82	u	59	U	C2-N1-C1'	6.60	125.62	117.70
78	t	2400	G	C8-N9-C1'	-6.60	118.42	127.00
44	J	142	ASP	CB-CG-OD1	6.60	124.24	118.30
1	S2	202	G	N3-C4-C5	-6.59	125.31	128.60
1	S2	402	C	C6-N1-C2	-6.59	117.67	120.30
1	S2	1520	G	N3-C4-N9	6.58	129.95	126.00
78	t	493	G	C8-N9-C1'	-6.58	118.45	127.00
1	S2	853	C	C5-C6-N1	6.57	124.29	121.00
78	t	189	G	N3-C4-N9	-6.57	122.06	126.00
1	S2	387	C	C5-C6-N1	6.57	124.28	121.00
1	S2	889	U	C2-N1-C1'	6.57	125.58	117.70
45	K	103	LEU	CA-CB-CG	6.56	130.38	115.30
78	t	659	G	C8-N9-C1'	-6.55	118.48	127.00
78	t	219	C	N1-C2-O2	6.55	122.83	118.90
1	S2	1341	C	C6-N1-C2	-6.54	117.68	120.30
78	t	905	G	N3-C4-C5	-6.54	125.33	128.60
78	t	1155	C	C6-N1-C2	-6.54	117.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
78	t	361	C	C6-N1-C2	-6.53	117.69	120.30
78	t	4833	G	C4-N9-C1'	6.52	134.98	126.50
78	t	361	C	N3-C2-O2	-6.52	117.34	121.90
78	t	2250	C	C6-N1-C2	-6.51	117.69	120.30
78	t	4833	G	N3-C4-C5	-6.51	125.34	128.60
78	t	150	G	N3-C4-N9	6.51	129.91	126.00
78	t	4833	G	N3-C4-N9	6.49	129.89	126.00
1	S2	1578	U	N3-C2-O2	-6.48	117.67	122.20
79	v	61	C	C6-N1-C2	-6.48	117.71	120.30
1	S2	1314	U	N1-C2-O2	6.47	127.33	122.80
24	SG	68	LEU	CA-CB-CG	6.46	130.16	115.30
17	SV	79	VAL	N-CA-C	6.46	128.45	111.00
82	u	50	U	N1-C2-O2	6.46	127.32	122.80
82	u	59	U	N3-C2-O2	-6.46	117.68	122.20
78	t	37	U	N3-C2-O2	-6.46	117.68	122.20
78	t	197	U	C6-N1-C1'	-6.46	112.16	121.20
78	t	2373	G	C4-N9-C1'	6.46	134.90	126.50
1	S2	1384	C	C2-N1-C1'	6.44	125.89	118.80
82	u	60	U	N1-C2-O2	6.44	127.31	122.80
78	t	670	C	N1-C2-O2	6.44	122.76	118.90
82	u	54	U	C5-C6-N1	6.44	125.92	122.70
1	S2	1496	U	C5-C6-N1	6.44	125.92	122.70
78	t	4707	G	N3-C2-N2	-6.43	115.40	119.90
78	t	4733	C	N1-C2-O2	6.43	122.76	118.90
78	t	4099	C	C6-N1-C2	-6.42	117.73	120.30
1	S2	1683	C	N3-C2-O2	-6.42	117.41	121.90
78	t	1814	G	N3-C4-N9	-6.42	122.15	126.00
1	S2	1527	C	N1-C2-O2	6.40	122.74	118.90
78	t	905	G	C6-C5-N7	-6.40	126.56	130.40
78	t	1614	A	C2-N3-C4	6.40	113.80	110.60
82	u	60	U	N3-C2-O2	-6.40	117.72	122.20
78	t	43	U	N3-C2-O2	-6.39	117.72	122.20
79	v	50	U	P-O3'-C3'	6.39	127.37	119.70
1	S2	501	C	N3-C2-O2	-6.38	117.43	121.90
1	S2	1307	U	N1-C2-O2	6.38	127.27	122.80
70	k	18	LEU	CA-CB-CG	6.38	129.97	115.30
78	t	4268	U	N3-C2-O2	-6.38	117.73	122.20
1	S2	1815	A	P-O3'-C3'	6.38	127.35	119.70
78	t	964	C	C6-N1-C1'	-6.37	113.16	120.80
1	S2	1565	C	C6-N1-C2	-6.36	117.76	120.30
78	t	71	C	P-O3'-C3'	6.36	127.33	119.70
78	t	4409	C	C6-N1-C2	-6.36	117.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	291	G	N1-C6-O6	6.36	123.71	119.90
82	u	59	U	C5-C6-N1	6.36	125.88	122.70
1	S2	118	C	C2-N1-C1'	6.35	125.79	118.80
1	S2	325	C	N1-C2-O2	6.35	122.71	118.90
1	S2	1676	U	N1-C2-O2	6.34	127.24	122.80
78	t	4704	G	N3-C4-N9	-6.34	122.19	126.00
39	E	14	C	C2-N1-C1'	6.33	125.77	118.80
1	S2	1472	C	C6-N1-C2	-6.33	117.77	120.30
78	t	1594	G	C4-N9-C1'	6.32	134.72	126.50
1	S2	559	G	P-O3'-C3'	6.31	127.27	119.70
78	t	4733	C	C2-N1-C1'	6.31	125.74	118.80
78	t	4886	C	C5-C6-N1	6.31	124.15	121.00
78	t	2398	C	N3-C2-O2	-6.31	117.48	121.90
78	t	37	U	N1-C2-O2	6.30	127.21	122.80
78	t	656	C	C6-N1-C2	-6.30	117.78	120.30
78	t	4360	C	N1-C2-O2	6.30	122.68	118.90
78	t	4728	C	C5-C6-N1	6.29	124.15	121.00
78	t	197	U	N3-C2-O2	-6.29	117.80	122.20
7	SH	148	LEU	CA-CB-CG	6.28	129.74	115.30
1	S2	1556	A	C2-N3-C4	6.28	113.74	110.60
1	S2	1283	C	C6-N1-C2	-6.27	117.79	120.30
78	t	2234	C	C2-N1-C1'	6.27	125.69	118.80
78	t	1997	C	C6-N1-C2	-6.26	117.80	120.30
39	E	14	C	C6-N1-C2	-6.25	117.80	120.30
78	t	4126	C	N1-C2-O2	6.25	122.65	118.90
36	B	360	LEU	CA-CB-CG	6.24	129.66	115.30
1	S2	1807	C	N1-C2-O2	6.23	122.64	118.90
1	S2	321	C	C6-N1-C2	-6.21	117.81	120.30
78	t	901	U	P-O3'-C3'	6.21	127.15	119.70
78	t	1401	C	N1-C2-O2	6.21	122.63	118.90
1	S2	853	C	C6-N1-C2	-6.20	117.82	120.30
78	t	2749	C	N1-C2-O2	6.20	122.62	118.90
78	t	1060	C	C5-C6-N1	6.19	124.09	121.00
1	S2	106	C	C6-N1-C2	-6.19	117.82	120.30
78	t	1189	C	N1-C2-O2	6.19	122.61	118.90
78	t	3638	C	C5-C6-N1	6.19	124.09	121.00
1	S2	1661	A	P-O3'-C3'	6.19	127.12	119.70
78	t	4717	G	C8-N9-C1'	6.19	135.04	127.00
78	t	2239	C	N1-C2-O2	6.17	122.60	118.90
1	S2	1496	U	C2-N1-C1'	6.17	125.10	117.70
78	t	2817	G	C4-N9-C1'	6.17	134.52	126.50
78	t	1989	U	C5-C6-N1	6.16	125.78	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	D	130	C	N1-C2-O2	6.15	122.59	118.90
78	t	1163	C	N1-C2-O2	6.15	122.59	118.90
78	t	1977	C	C6-N1-C2	-6.14	117.84	120.30
1	S2	1578	U	N1-C2-O2	6.13	127.09	122.80
78	t	268	C	C5-C6-N1	6.13	124.06	121.00
78	t	2727	C	N1-C2-O2	6.13	122.58	118.90
78	t	715	C	N3-C2-O2	-6.12	117.61	121.90
1	S2	563	G	P-O3'-C3'	6.12	127.05	119.70
1	S2	1371	U	C2-N1-C1'	6.12	125.04	117.70
82	u	55	U	C2-N1-C1'	6.12	125.04	117.70
78	t	2499	C	C2-N1-C1'	6.12	125.53	118.80
78	t	4983	C	C5-C6-N1	6.11	124.06	121.00
1	S2	118	C	N1-C2-O2	6.11	122.57	118.90
1	S2	1816	G	O5'-P-OP2	6.11	118.03	110.70
78	t	3780	G	C4-C5-N7	6.11	113.24	110.80
78	t	1084	C	C6-N1-C2	-6.10	117.86	120.30
78	t	3681	G	N3-C4-C5	-6.09	125.55	128.60
38	D	129	C	N1-C2-O2	6.09	122.56	118.90
78	t	4391	C	C6-N1-C2	-6.09	117.86	120.30
78	t	1335	C	N1-C2-O2	6.09	122.55	118.90
78	t	1460	C	C6-N1-C2	-6.09	117.86	120.30
78	t	4947	U	OP1-P-OP2	-6.09	110.47	119.60
1	S2	1303	C	N1-C2-O2	6.08	122.55	118.90
78	t	1737	C	C6-N1-C2	-6.08	117.87	120.30
82	u	48	C	N3-C2-O2	-6.08	117.64	121.90
1	S2	291	G	N1-C2-N2	-6.08	110.73	116.20
39	E	67	C	C6-N1-C2	-6.08	117.87	120.30
78	t	2556	C	N1-C2-O2	6.07	122.54	118.90
82	u	56	C	C6-N1-C2	-6.07	117.87	120.30
42	H	179	LEU	CA-CB-CG	6.07	129.25	115.30
1	S2	1314	U	N3-C2-O2	-6.06	117.96	122.20
1	S2	1440	C	C6-N1-C2	-6.06	117.88	120.30
78	t	1155	C	C5-C6-N1	6.05	124.03	121.00
78	t	443	C	C5-C6-N1	6.05	124.03	121.00
1	S2	474	G	N3-C4-N9	6.05	129.63	126.00
82	u	75	C	C6-N1-C2	-6.05	117.88	120.30
1	S2	548	C	N3-C2-O2	-6.04	117.67	121.90
78	t	4360	C	N3-C2-O2	-6.04	117.67	121.90
78	t	2692	C	N3-C2-O2	-6.03	117.68	121.90
78	t	4946	U	N3-C2-O2	-6.02	117.98	122.20
78	t	2480	C	C2-N1-C1'	6.01	125.42	118.80
81	y	38	LEU	CA-CB-CG	6.01	129.13	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
78	t	2330	C	N1-C2-O2	6.00	122.50	118.90
78	t	950	G	N3-C4-C5	-6.00	125.60	128.60
78	t	2065	C	N3-C2-O2	-6.00	117.70	121.90
78	t	1930	U	C2-N1-C1'	5.99	124.89	117.70
78	t	3780	G	C6-C5-N7	-5.99	126.81	130.40
82	u	25	C	C5-C6-N1	5.99	123.99	121.00
78	t	950	G	C4-N9-C1'	5.98	134.28	126.50
10	SL	41	GLY	CA-C-O	5.97	131.35	120.60
78	t	2250	C	C2-N1-C1'	5.97	125.37	118.80
78	t	4717	G	C4-N9-C1'	-5.97	118.74	126.50
78	t	1874	C	N1-C2-O2	5.96	122.48	118.90
78	t	1930	U	N3-C2-O2	-5.96	118.03	122.20
78	t	2507	G	C8-N9-C4	-5.96	104.02	106.40
78	t	3783	C	C2-N1-C1'	5.95	125.34	118.80
1	S2	872	A	P-O3'-C3'	5.94	126.83	119.70
1	S2	1307	U	C6-N1-C1'	-5.94	112.88	121.20
78	t	2758	C	C5-C6-N1	5.94	123.97	121.00
78	t	3783	C	N1-C2-O2	5.94	122.46	118.90
1	S2	1496	U	C6-N1-C2	-5.93	117.44	121.00
78	t	1746	G	C8-N9-C1'	-5.93	119.29	127.00
8	SI	130	THR	N-CA-C	5.92	126.99	111.00
78	t	700	C	N1-C2-O2	5.92	122.45	118.90
78	t	361	C	C2-N1-C1'	5.91	125.30	118.80
1	S2	913	A	N3-C4-N9	5.90	132.12	127.40
78	t	2241	G	C8-N9-C1'	-5.90	119.33	127.00
41	G	233	PHE	C-N-CA	5.89	136.44	121.70
78	t	163	C	N1-C2-O2	5.88	122.43	118.90
78	t	2499	C	N1-C2-O2	5.88	122.43	118.90
1	S2	1277	C	C5-C6-N1	5.88	123.94	121.00
78	t	2234	C	N3-C2-O2	-5.88	117.78	121.90
78	t	43	U	N1-C2-O2	5.88	126.92	122.80
1	S2	303	C	C2-N1-C1'	5.88	125.26	118.80
37	C	289	LEU	CA-CB-CG	5.87	128.79	115.30
78	t	27	C	C6-N1-C2	-5.86	117.96	120.30
22	Sg	7	LEU	CA-CB-CG	5.85	128.76	115.30
1	S2	1116	C	C6-N1-C2	-5.85	117.96	120.30
78	t	36	U	N3-C2-O2	-5.84	118.11	122.20
78	t	1966	G	C4-N9-C1'	5.84	134.09	126.50
1	S2	1384	C	N3-C2-O2	-5.83	117.82	121.90
78	t	686	C	N1-C2-O2	5.83	122.40	118.90
1	S2	1472	C	C5-C6-N1	5.83	123.91	121.00
78	t	1466	G	N3-C4-N9	5.83	129.50	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	SL	24	LEU	CA-CB-CG	5.82	128.69	115.30
78	t	1420	C	N1-C2-O2	5.82	122.39	118.90
78	t	4704	G	N3-C2-N2	-5.82	115.83	119.90
1	S2	1005	G	N3-C4-N9	5.82	129.49	126.00
1	S2	1527	C	C5-C6-N1	5.82	123.91	121.00
1	S2	1307	U	C5-C6-N1	5.81	125.61	122.70
1	S2	1314	U	C2-N1-C1'	5.81	124.67	117.70
78	t	217	C	N3-C2-O2	-5.80	117.84	121.90
78	t	264	U	C5-C6-N1	5.80	125.60	122.70
78	t	4736	C	N3-C2-O2	-5.80	117.84	121.90
1	S2	839	C	N1-C2-O2	5.79	122.38	118.90
1	S2	570	C	C2-N1-C1'	5.79	125.17	118.80
42	H	169	LEU	CA-CB-CG	5.79	128.62	115.30
78	t	1989	U	C6-N1-C2	-5.79	117.53	121.00
78	t	3681	G	N3-C4-N9	5.78	129.47	126.00
82	u	50	U	N3-C2-O2	-5.78	118.15	122.20
78	t	4820	G	C4-C5-N7	5.78	113.11	110.80
23	SC	83	LEU	CA-CB-CG	5.78	128.59	115.30
78	t	749	G	N7-C8-N9	5.78	115.99	113.10
78	t	4080	U	C5-C6-N1	5.78	125.59	122.70
82	u	25	C	N1-C2-O2	5.77	122.36	118.90
78	t	288	G	C4-N9-C1'	5.76	133.99	126.50
78	t	1594	G	C6-C5-N7	-5.76	126.94	130.40
38	D	83	C	C6-N1-C2	-5.76	118.00	120.30
78	t	2064	C	C6-N1-C2	-5.76	118.00	120.30
1	S2	1865	C	C2-N1-C1'	5.75	125.12	118.80
78	t	471	C	C4-C5-C6	-5.75	114.53	117.40
1	S2	474	G	C8-N9-C1'	-5.74	119.53	127.00
78	t	2499	C	N3-C2-O2	-5.74	117.88	121.90
34	Sf	103	LEU	CA-CB-CG	5.74	128.51	115.30
38	D	126	C	C6-N1-C2	-5.74	118.00	120.30
78	t	1268	U	C5-C6-N1	-5.73	119.83	122.70
78	t	964	C	C5-C6-N1	5.73	123.86	121.00
1	S2	1813	A	P-O3'-C3'	5.72	126.57	119.70
78	t	1193	C	C5-C4-N4	-5.72	116.19	120.20
78	t	4729	C	N3-C2-O2	-5.72	117.90	121.90
1	S2	291	G	C5-C6-O6	-5.72	125.17	128.60
78	t	227	G	C6-C5-N7	-5.72	126.97	130.40
78	t	2316	C	C6-N1-C2	-5.71	118.01	120.30
78	t	3902	C	C5-C6-N1	5.71	123.86	121.00
1	S2	1090	C	C6-N1-C2	-5.71	118.02	120.30
78	t	493	G	N3-C4-C5	-5.71	125.75	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	S	24	LEU	CA-CB-CG	5.70	128.42	115.30
78	t	471	C	C6-N1-C2	-5.70	118.02	120.30
78	t	2330	C	N3-C2-O2	-5.70	117.91	121.90
78	t	4633	C	N1-C2-O2	5.70	122.32	118.90
78	t	4624	C	C6-N1-C2	-5.70	118.02	120.30
78	t	2738	G	C4-N9-C1'	5.69	133.90	126.50
79	v	59	U	N3-C2-O2	-5.69	118.22	122.20
1	S2	1811	C	N1-C2-O2	5.69	122.31	118.90
22	Sg	261	LEU	CA-CB-CG	5.69	128.38	115.30
78	t	958	U	C5-C6-N1	5.69	125.54	122.70
1	S2	1574	C	C6-N1-C2	-5.68	118.03	120.30
78	t	1970	G	N3-C4-C5	-5.68	125.76	128.60
1	S2	1265	A	C2-N3-C4	5.68	113.44	110.60
1	S2	1022	U	C2-N1-C1'	5.67	124.51	117.70
78	t	1614	A	C4-N9-C1'	5.67	136.51	126.30
78	t	1669	U	N3-C2-O2	-5.67	118.23	122.20
78	t	2282	C	C6-N1-C2	-5.67	118.03	120.30
78	t	2584	G	C4-N9-C1'	5.67	133.88	126.50
1	S2	913	A	N3-C4-C5	-5.67	122.83	126.80
78	t	4717	G	N3-C4-C5	5.67	131.43	128.60
82	u	45	U	C2-N1-C1'	5.67	124.50	117.70
1	S2	474	G	N3-C4-C5	-5.67	125.77	128.60
1	S2	1363	C	N1-C2-O2	5.67	122.30	118.90
1	S2	501	C	C6-N1-C2	-5.66	118.04	120.30
8	SI	172	LEU	CA-CB-CG	5.66	128.32	115.30
47	M	144	LEU	CA-CB-CG	5.66	128.31	115.30
78	t	4880	C	C2-N1-C1'	5.66	125.02	118.80
78	t	2065	C	N1-C2-O2	5.65	122.29	118.90
82	u	43	C	C5-C6-N1	5.65	123.83	121.00
78	t	1388	C	C6-N1-C2	-5.65	118.04	120.30
78	t	1746	G	N3-C4-N9	5.65	129.39	126.00
1	S2	1749	G	P-O3'-C3'	5.64	126.47	119.70
82	u	50	U	C5-C6-N1	5.64	125.52	122.70
50	P	141	LEU	CA-CB-CG	5.64	128.27	115.30
78	t	669	G	C2-N3-C4	-5.64	109.08	111.90
78	t	975	C	N1-C2-O2	5.64	122.28	118.90
78	t	4267	G	N1-C2-N2	5.64	121.27	116.20
10	SL	41	GLY	N-CA-C	5.63	127.18	113.10
78	t	4629	C	C6-N1-C2	-5.62	118.05	120.30
22	Sg	104	HIS	C-N-CA	5.62	135.75	121.70
52	R	138	LEU	CA-CB-CG	5.62	128.22	115.30
1	S2	638	C	N3-C2-O2	-5.62	117.97	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
75	p	33	LEU	CA-CB-CG	5.61	128.20	115.30
39	E	118	C	N1-C2-O2	5.61	122.27	118.90
78	t	216	G	N3-C2-N2	-5.60	115.98	119.90
78	t	1228	C	N1-C2-O2	5.60	122.26	118.90
1	S2	638	C	C6-N1-C2	-5.60	118.06	120.30
1	S2	1277	C	C6-N1-C2	-5.60	118.06	120.30
1	S2	1371	U	N1-C2-O2	5.60	126.72	122.80
78	t	4671	U	C5-C6-N1	5.60	125.50	122.70
78	t	1460	C	N1-C2-O2	5.59	122.26	118.90
1	S2	1812	U	N3-C2-O2	-5.59	118.29	122.20
78	t	214	C	N1-C2-O2	5.59	122.25	118.90
78	t	211	G	N3-C4-C5	-5.58	125.81	128.60
65	f	78	LEU	CA-CB-CG	5.58	128.14	115.30
78	t	2803	C	C6-N1-C2	-5.57	118.07	120.30
82	u	50	U	C2-N1-C1'	5.57	124.39	117.70
78	t	4858	C	N1-C2-O2	5.57	122.24	118.90
1	S2	1116	C	C5-C6-N1	5.57	123.78	121.00
78	t	207	C	N3-C2-O2	-5.57	118.00	121.90
78	t	217	C	C5-C6-N1	5.57	123.78	121.00
78	t	48	G	O4'-C1'-N9	5.56	112.65	108.20
1	S2	844	U	C5-C6-N1	5.56	125.48	122.70
78	t	3682	A	C2-N3-C4	5.56	113.38	110.60
78	t	2556	C	N3-C2-O2	-5.56	118.01	121.90
78	t	2727	C	N3-C2-O2	-5.56	118.01	121.90
1	S2	1813	A	OP2-P-O3'	5.55	117.42	105.20
78	t	2829	A	N7-C8-N9	5.55	116.58	113.80
78	t	2373	G	C6-C5-N7	-5.55	127.07	130.40
1	S2	1375	G	P-O3'-C3'	5.54	126.35	119.70
78	t	4360	C	C6-N1-C2	-5.54	118.08	120.30
78	t	4268	U	N1-C2-O2	5.54	126.68	122.80
38	D	83	C	N3-C2-O2	-5.53	118.03	121.90
78	t	1189	C	N3-C2-O2	-5.53	118.03	121.90
1	S2	1807	C	N3-C2-O2	-5.53	118.03	121.90
78	t	1628	A	C4-C5-C6	-5.53	114.23	117.00
78	t	1218	G	N3-C4-N9	-5.53	122.68	126.00
78	t	3902	C	C6-N1-C2	-5.53	118.09	120.30
78	t	1350	C	N1-C2-O2	5.53	122.22	118.90
1	S2	457	C	C6-N1-C2	-5.52	118.09	120.30
78	t	973	C	C5-C6-N1	5.52	123.76	121.00
78	t	2076	G	C4-N9-C1'	5.52	133.68	126.50
78	t	4671	U	N1-C2-O2	5.52	126.66	122.80
78	t	4218	A	O4'-C1'-N9	5.52	112.61	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
78	t	2017	C	N1-C2-O2	5.52	122.21	118.90
72	m	51	LEU	CA-CB-CG	5.51	127.98	115.30
78	t	1166	C	C6-N1-C2	-5.51	118.09	120.30
78	t	1335	C	N3-C2-O2	-5.51	118.04	121.90
78	t	1502	C	C5-C6-N1	5.51	123.76	121.00
1	S2	379	C	C6-N1-C2	-5.51	118.10	120.30
26	SM	76	LEU	CA-CB-CG	5.51	127.98	115.30
78	t	669	G	N3-C4-N9	-5.51	122.69	126.00
78	t	4624	C	N3-C2-O2	-5.51	118.04	121.90
1	S2	1681	U	P-O3'-C3'	5.51	126.31	119.70
78	t	163	C	C6-N1-C1'	-5.51	114.19	120.80
78	t	1466	G	N3-C4-C5	-5.50	125.85	128.60
78	t	148	G	N3-C2-N2	-5.50	116.05	119.90
78	t	3569	C	N1-C2-O2	5.50	122.20	118.90
80	w	20	G	P-O3'-C3'	5.50	126.30	119.70
1	S2	1660	C	C2-N1-C1'	5.50	124.85	118.80
1	S2	1022	U	N1-C2-O2	5.50	126.65	122.80
78	t	2469	U	N1-C2-O2	5.49	126.65	122.80
78	t	1225	G	N3-C4-C5	-5.49	125.86	128.60
78	t	3856	G	C6-C5-N7	-5.49	127.11	130.40
38	D	113	C	C6-N1-C2	-5.48	118.11	120.30
78	t	2692	C	C6-N1-C2	-5.48	118.11	120.30
78	t	4698	C	C5-C6-N1	5.48	123.74	121.00
1	S2	1542	C	C6-N1-C2	-5.48	118.11	120.30
22	Sg	79	LEU	CA-CB-CG	5.48	127.90	115.30
78	t	669	G	N1-C2-N3	5.48	127.19	123.90
78	t	3875	G	N3-C4-N9	-5.47	122.72	126.00
38	D	123	U	C5-C6-N1	5.47	125.43	122.70
78	t	150	G	C6-C5-N7	-5.47	127.12	130.40
2	SA	159	ILE	CG1-CB-CG2	-5.46	99.38	111.40
38	D	84	A	C2-N3-C4	5.46	113.33	110.60
58	X	50	ASN	N-CA-C	5.46	125.75	111.00
78	t	1268	U	O4'-C1'-N1	5.46	112.57	108.20
78	t	1069	C	C5-C4-N4	-5.46	116.38	120.20
78	t	1952	C	N1-C2-O2	5.46	122.18	118.90
78	t	749	G	C6-C5-N7	-5.46	127.13	130.40
78	t	746	C	O4'-C1'-N1	5.45	112.56	108.20
78	t	4992	A	O4'-C1'-N9	5.45	112.56	108.20
78	t	1466	G	C8-N9-C1'	-5.45	119.91	127.00
78	t	1997	C	C5-C6-N1	5.45	123.72	121.00
1	S2	1802	C	C6-N1-C2	-5.45	118.12	120.30
1	S2	1363	C	C2-N1-C1'	5.45	124.79	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	1805	G	N3-C4-C5	-5.45	125.88	128.60
78	t	2817	G	C8-N9-C1'	-5.45	119.92	127.00
24	SG	109	LEU	CA-CB-CG	5.44	127.82	115.30
78	t	36	U	N1-C2-O2	5.44	126.61	122.80
10	SL	41	GLY	CA-C-N	5.44	129.17	117.20
1	S2	1527	C	C2-N1-C1'	5.44	124.78	118.80
82	u	54	U	N3-C4-O4	5.44	123.21	119.40
78	t	685	C	C6-N1-C2	-5.43	118.13	120.30
78	t	2584	G	C8-N9-C1'	-5.43	119.94	127.00
78	t	4515	A	N7-C8-N9	5.43	116.52	113.80
42	H	190	LEU	CA-CB-CG	5.43	127.79	115.30
78	t	2829	A	C8-N9-C4	-5.43	103.63	105.80
78	t	211	G	C2-N3-C4	5.43	114.61	111.90
78	t	1322	U	C5-C6-N1	5.42	125.41	122.70
78	t	4736	C	C6-N1-C1'	-5.42	114.29	120.80
1	S2	1022	U	N3-C2-O2	-5.42	118.41	122.20
79	v	52	G	N3-C4-N9	5.42	129.25	126.00
38	D	83	C	C5-C6-N1	5.42	123.71	121.00
25	SJ	81	LEU	CA-CB-CG	5.41	127.75	115.30
78	t	1257	A	C8-N9-C4	-5.41	103.64	105.80
78	t	4109	G	N3-C4-N9	5.41	129.25	126.00
78	t	2400	G	N3-C4-N9	5.41	129.25	126.00
78	t	3849	C	C2-N1-C1'	5.41	124.75	118.80
78	t	219	C	C5-C6-N1	5.41	123.70	121.00
1	S2	548	C	C6-N1-C1'	-5.40	114.32	120.80
52	R	103	LEU	CA-CB-CG	5.40	127.73	115.30
78	t	1389	G	C4-N9-C1'	5.40	133.52	126.50
21	Sd	6	LEU	CA-CB-CG	5.40	127.72	115.30
78	t	2480	C	N1-C2-O2	5.40	122.14	118.90
78	t	4035	G	N3-C4-C5	-5.40	125.90	128.60
78	t	119	G	C4-N9-C1'	5.40	133.51	126.50
1	S2	202	G	C8-N9-C1'	-5.39	119.99	127.00
78	t	4833	G	C8-N9-C1'	-5.39	119.99	127.00
78	t	4593	G	C4-N9-C1'	5.39	133.51	126.50
78	t	211	G	N1-C6-O6	-5.39	116.67	119.90
1	S2	1272	C	C6-N1-C2	-5.39	118.14	120.30
1	S2	1315	U	N1-C2-O2	5.39	126.57	122.80
78	t	973	C	C6-N1-C2	-5.39	118.15	120.30
78	t	164	C	N1-C2-O2	5.38	122.13	118.90
78	t	3681	G	C4-N9-C1'	5.38	133.49	126.50
82	u	75	C	C5-C6-N1	5.38	123.69	121.00
78	t	968	C	C2-N1-C1'	5.37	124.71	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
78	t	2398	C	N1-C2-O2	5.37	122.12	118.90
79	v	43	C	C2-N1-C1'	5.37	124.71	118.80
78	t	150	G	N3-C4-C5	-5.37	125.92	128.60
1	S2	1520	G	N3-C4-C5	-5.37	125.92	128.60
78	t	3590	G	C4-C5-N7	5.36	112.94	110.80
78	t	2017	C	C5-C6-N1	5.36	123.68	121.00
38	D	83	C	C2-N1-C1'	5.36	124.69	118.80
78	t	2043	C	C5-C6-N1	5.36	123.68	121.00
1	S2	1683	C	N1-C2-O2	5.35	122.11	118.90
78	t	1235	C	C6-N1-C2	-5.35	118.16	120.30
78	t	4523	C	C6-N1-C2	-5.35	118.16	120.30
78	t	4865	G	P-O3'-C3'	5.35	126.12	119.70
38	D	153	C	O4'-C1'-N1	5.35	112.48	108.20
1	S2	1174	U	C5-C6-N1	5.35	125.37	122.70
38	D	150	C	N1-C2-O2	5.35	122.11	118.90
78	t	4315	U	N1-C2-O2	5.34	126.54	122.80
1	S2	570	C	C6-N1-C2	-5.34	118.16	120.30
78	t	2388	U	C5-C6-N1	5.34	125.37	122.70
79	v	1	U	N1-C2-O2	5.34	126.54	122.80
78	t	4099	C	C5-C6-N1	5.34	123.67	121.00
1	S2	1565	C	C5-C6-N1	5.33	123.67	121.00
1	S2	1738	C	C6-N1-C2	-5.33	118.17	120.30
78	t	1844	U	N3-C2-O2	-5.33	118.47	122.20
1	S2	1676	U	N3-C2-O2	-5.33	118.47	122.20
1	S2	183	G	N3-C4-C5	-5.33	125.94	128.60
78	t	742	G	C8-N9-C4	-5.33	104.27	106.40
78	t	4909	G	C4-C5-N7	5.33	112.93	110.80
1	S2	115	U	N3-C2-O2	-5.33	118.47	122.20
78	t	656	C	C5-C6-N1	5.33	123.66	121.00
82	u	56	C	N1-C2-O2	5.33	122.09	118.90
1	S2	1805	G	N3-C4-N9	5.32	129.19	126.00
78	t	4203	C	C5-C6-N1	5.32	123.66	121.00
78	t	4855	G	O5'-P-OP2	-5.32	100.91	105.70
78	t	1466	G	C6-C5-N7	-5.32	127.21	130.40
78	t	2608	C	N1-C2-O2	5.32	122.09	118.90
78	t	2727	C	O4'-C1'-N1	5.32	112.45	108.20
78	t	4834	U	C5-C6-N1	5.32	125.36	122.70
1	S2	1716	C	C6-N1-C2	-5.31	118.17	120.30
78	t	497	C	N1-C2-O2	5.31	122.09	118.90
51	Q	91	LEU	CA-CB-CG	5.30	127.50	115.30
79	v	49	C	O5'-P-OP2	-5.30	100.92	105.70
15	ST	123	LEU	CA-CB-CG	5.30	127.50	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
78	t	1814	G	C8-N9-C4	-5.30	104.28	106.40
78	t	4909	G	C6-C5-N7	-5.30	127.22	130.40
78	t	4109	G	N3-C4-C5	-5.30	125.95	128.60
1	S2	1496	U	N1-C2-O2	5.30	126.51	122.80
78	t	4942	C	C6-N1-C2	-5.30	118.18	120.30
78	t	4102	C	N1-C2-O2	5.29	122.08	118.90
1	S2	78	C	C6-N1-C2	-5.29	118.18	120.30
78	t	3893	G	C4-N9-C1'	5.29	133.38	126.50
78	t	3762	C	C2-N1-C1'	5.29	124.62	118.80
1	S2	216	C	C6-N1-C2	-5.29	118.19	120.30
62	c	54	LEU	CB-CG-CD2	-5.28	102.02	111.00
1	S2	501	C	C6-N1-C1'	-5.28	114.47	120.80
78	t	698	C	N3-C2-O2	-5.27	118.21	121.90
78	t	1163	C	N3-C2-O2	-5.27	118.21	121.90
78	t	698	C	C2-N1-C1'	5.27	124.59	118.80
78	t	1264	G	C4-N9-C1'	5.27	133.35	126.50
1	S2	1865	C	N3-C2-O2	-5.26	118.21	121.90
78	t	4562	G	O4'-C1'-N9	5.26	112.41	108.20
1	S2	356	C	C6-N1-C2	-5.26	118.20	120.30
78	t	463	C	N3-C2-O2	-5.26	118.22	121.90
78	t	2323	U	C6-N1-C2	-5.26	117.84	121.00
78	t	3780	G	N9-C4-C5	-5.26	103.30	105.40
78	t	497	C	N3-C2-O2	-5.26	118.22	121.90
78	t	3897	C	C6-N1-C2	-5.26	118.20	120.30
1	S2	375	U	C5-C6-N1	5.26	125.33	122.70
78	t	2017	C	N3-C2-O2	-5.26	118.22	121.90
78	t	1335	C	C6-N1-C2	-5.25	118.20	120.30
1	S2	183	G	C2-N3-C4	5.25	114.53	111.90
1	S2	496	C	N1-C2-O2	5.25	122.05	118.90
78	t	1225	G	C2-N3-C4	5.25	114.53	111.90
1	S2	638	C	N1-C2-O2	5.25	122.05	118.90
78	t	901	U	OP1-P-O3'	5.25	116.74	105.20
78	t	4858	C	N3-C2-O2	-5.24	118.23	121.90
78	t	1665	U	C5-C6-N1	5.24	125.32	122.70
78	t	1319	G	C4-C5-N7	5.23	112.89	110.80
78	t	1198	C	N1-C2-O2	5.23	122.04	118.90
78	t	4909	G	N9-C4-C5	-5.23	103.31	105.40
78	t	1594	G	C8-N9-C1'	-5.22	120.21	127.00
78	t	2234	C	C6-N1-C2	-5.22	118.21	120.30
3	SB	74	LEU	CA-CB-CG	5.22	127.31	115.30
78	t	1480	G	C4-N9-C1'	5.22	133.29	126.50
78	t	473	G	N3-C2-N2	-5.22	116.25	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
78	t	1146	G	C5-C6-O6	-5.22	125.47	128.60
78	t	4267	G	C4-N9-C1'	5.22	133.28	126.50
78	t	2236	C	C6-N1-C1'	-5.22	114.54	120.80
78	t	4105	C	C6-N1-C2	-5.22	118.21	120.30
78	t	167	C	N1-C2-O2	5.21	122.03	118.90
78	t	233	G	N3-C2-N2	-5.21	116.25	119.90
1	S2	321	C	N1-C2-O2	5.21	122.02	118.90
78	t	163	C	C5-C6-N1	5.20	123.60	121.00
82	u	69	G	C4-N9-C1'	5.20	133.26	126.50
78	t	493	G	C6-C5-N7	-5.20	127.28	130.40
36	B	3	HIS	N-CA-C	-5.20	96.97	111.00
3	SB	188	LEU	CA-CB-CG	5.20	127.25	115.30
78	t	1665	U	C6-N1-C2	-5.20	117.88	121.00
78	t	4409	C	C5-C6-N1	5.20	123.60	121.00
78	t	4880	C	C5-C6-N1	5.20	123.60	121.00
78	t	2386	G	N3-C4-N9	5.19	129.12	126.00
78	t	1966	G	C8-N9-C1'	-5.19	120.25	127.00
78	t	309	G	O4'-C1'-N9	-5.19	104.05	108.20
78	t	1746	G	N3-C4-C5	-5.19	126.00	128.60
1	S2	1303	C	N3-C2-O2	-5.19	118.27	121.90
78	t	2067	G	C8-N9-C1'	5.19	133.74	127.00
78	t	4700	C	C6-N1-C2	-5.19	118.22	120.30
39	E	105	C	N1-C2-O2	5.18	122.01	118.90
78	t	1502	C	C6-N1-C2	-5.18	118.23	120.30
78	t	214	C	C2-N1-C1'	5.18	124.50	118.80
1	S2	23	G	C4-N9-C1'	5.18	133.23	126.50
78	t	4729	C	N1-C2-O2	5.18	122.01	118.90
1	S2	427	U	C2-N1-C1'	5.18	123.91	117.70
78	t	1323	C	C6-N1-C2	-5.18	118.23	120.30
1	S2	176	U	C2-N1-C1'	5.17	123.91	117.70
1	S2	496	C	N3-C2-O2	-5.17	118.28	121.90
44	J	118	LEU	CA-CB-CG	5.17	127.20	115.30
1	S2	303	C	C6-N1-C2	-5.17	118.23	120.30
1	S2	857	U	C2-N1-C1'	5.17	123.91	117.70
78	t	975	C	N3-C2-O2	-5.17	118.28	121.90
78	t	3783	C	C6-N1-C2	-5.17	118.23	120.30
78	t	669	G	N3-C2-N2	-5.17	116.28	119.90
78	t	698	C	N1-C2-O2	5.16	122.00	118.90
78	t	950	G	N3-C4-N9	5.16	129.09	126.00
78	t	1069	C	C5-C6-N1	5.16	123.58	121.00
82	u	11	C	N1-C2-O2	5.16	121.99	118.90
1	S2	1470	C	C6-N1-C2	-5.16	118.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
78	t	744	C	C6-N1-C2	-5.16	118.24	120.30
1	S2	967	C	C6-N1-C2	-5.15	118.24	120.30
78	t	4834	U	N1-C2-O2	5.15	126.41	122.80
1	S2	645	C	N1-C2-O2	5.15	121.99	118.90
1	S2	1139	C	C6-N1-C1'	-5.15	114.62	120.80
38	D	123	U	C6-N1-C2	-5.15	117.91	121.00
1	S2	292	A	P-O3'-C3'	5.15	125.88	119.70
78	t	289	A	N3-C4-N9	5.15	131.52	127.40
78	t	1226	C	C6-N1-C2	-5.14	118.24	120.30
78	t	2480	C	C6-N1-C2	-5.14	118.24	120.30
79	v	1	U	N3-C2-O2	-5.14	118.60	122.20
78	t	225	C	C6-N1-C2	-5.14	118.24	120.30
78	t	4333	G	P-O3'-C3'	5.14	125.87	119.70
78	t	2065	C	C2-N1-C1'	5.14	124.45	118.80
1	S2	118	C	C6-N1-C1'	-5.13	114.64	120.80
78	t	2805	U	C6-N1-C1'	-5.13	114.01	121.20
78	t	4120	C	N3-C2-O2	-5.13	118.31	121.90
78	t	1460	C	N3-C2-O2	-5.13	118.31	121.90
78	t	2389	C	N1-C2-O2	5.13	121.98	118.90
1	S2	196	C	C5-C6-N1	5.13	123.56	121.00
1	S2	1003	U	N1-C2-O2	5.13	126.39	122.80
78	t	53	C	N1-C2-O2	5.13	121.98	118.90
38	D	113	C	C5-C6-N1	5.12	123.56	121.00
78	t	243	G	N3-C4-N9	-5.12	122.93	126.00
78	t	927	C	N3-C2-O2	-5.12	118.31	121.90
1	S2	192	C	C6-N1-C2	-5.12	118.25	120.30
78	t	219	C	O4'-C1'-N1	5.12	112.30	108.20
78	t	4909	G	C8-N9-C1'	-5.12	120.34	127.00
78	t	4936	G	O4'-C1'-N9	5.12	112.30	108.20
78	t	2562	C	N1-C2-O2	5.12	121.97	118.90
78	t	2758	C	C6-N1-C2	-5.12	118.25	120.30
80	w	20	G	N3-C4-C5	-5.12	126.04	128.60
78	t	1460	C	C5-C6-N1	5.12	123.56	121.00
78	t	1669	U	N1-C2-O2	5.12	126.38	122.80
78	t	2634	C	C6-N1-C2	-5.11	118.25	120.30
78	t	4081	C	C6-N1-C2	-5.11	118.25	120.30
21	Sd	55	LEU	CA-CB-CG	5.11	127.05	115.30
78	t	31	U	P-O3'-C3'	5.11	125.83	119.70
78	t	2084	G	C4-N9-C1'	5.11	133.14	126.50
78	t	217	C	N1-C2-O2	5.11	121.97	118.90
78	t	4523	C	N1-C2-O2	5.11	121.96	118.90
78	t	493	G	N7-C8-N9	5.10	115.65	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
78	t	4523	C	N3-C2-O2	-5.10	118.33	121.90
78	t	288	G	C8-N9-C1'	-5.10	120.37	127.00
79	v	59	U	N1-C2-O2	5.09	126.37	122.80
78	t	288	G	N3-C4-N9	5.09	129.06	126.00
78	t	4832	A	O4'-C1'-N9	5.09	112.27	108.20
78	t	2793	C	C6-N1-C1'	-5.09	114.69	120.80
41	G	173	LEU	CA-CB-CG	5.09	127.00	115.30
1	S2	1341	C	C6-N1-C1'	-5.08	114.70	120.80
1	S2	1574	C	C5-C6-N1	5.08	123.54	121.00
78	t	2282	C	C6-N1-C1'	5.08	126.90	120.80
78	t	4109	G	C4-N9-C1'	5.08	133.11	126.50
1	S2	65	C	N1-C2-O2	5.08	121.95	118.90
1	S2	663	C	C6-N1-C2	-5.08	118.27	120.30
1	S2	291	G	C4-N9-C1'	-5.08	119.90	126.50
1	S2	1340	U	C2-N1-C1'	5.08	123.80	117.70
78	t	1589	C	C6-N1-C2	-5.08	118.27	120.30
1	S2	795	A	O4'-C1'-N9	5.08	112.26	108.20
1	S2	65	C	C2-N1-C1'	5.07	124.38	118.80
1	S2	445	A	P-O3'-C3'	5.07	125.79	119.70
1	S2	494	C	N1-C2-O2	5.07	121.94	118.90
1	S2	559	G	OP2-P-O3'	5.07	116.36	105.20
78	t	289	A	C4-N9-C1'	5.07	135.43	126.30
78	t	2373	G	C8-N9-C1'	-5.07	120.41	127.00
78	t	37	U	C5-C6-N1	5.07	125.24	122.70
38	D	129	C	C6-N1-C2	-5.07	118.27	120.30
82	u	37	U	N3-C2-O2	-5.07	118.65	122.20
78	t	2400	G	C6-C5-N7	-5.07	127.36	130.40
1	S2	117	C	C6-N1-C2	-5.07	118.27	120.30
1	S2	1307	U	N3-C2-O2	-5.07	118.65	122.20
78	t	4880	C	N3-C2-O2	-5.06	118.36	121.90
78	t	4732	U	N1-C2-O2	5.06	126.34	122.80
1	S2	1447	G	C8-N9-C4	-5.06	104.38	106.40
78	t	926	G	N3-C4-C5	-5.06	126.07	128.60
78	t	2507	G	N7-C8-N9	5.06	115.63	113.10
78	t	2067	G	C2-N3-C4	-5.05	109.37	111.90
78	t	1153	G	N9-C4-C5	5.05	107.42	105.40
78	t	1977	C	C5-C6-N1	5.05	123.53	121.00
27	SN	40	LEU	CA-CB-CG	5.05	126.92	115.30
78	t	1914	G	N7-C8-N9	5.05	115.62	113.10
78	t	4661	U	OP1-P-O3'	5.05	116.31	105.20
78	t	2084	G	N3-C4-C5	-5.05	126.08	128.60
78	t	4661	U	P-O3'-C3'	5.05	125.76	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	402	C	C5-C6-N1	5.04	123.52	121.00
78	t	3852	G	N7-C8-N9	5.04	115.62	113.10
78	t	4860	C	C6-N1-C2	-5.04	118.28	120.30
78	t	3681	G	C2-N3-C4	5.03	114.42	111.90
78	t	4315	U	N3-C2-O2	-5.03	118.68	122.20
1	S2	1856	C	C5-C6-N1	5.03	123.52	121.00
78	t	1252	G	N3-C4-N9	5.03	129.02	126.00
78	t	2283	U	N1-C2-O2	5.03	126.32	122.80
78	t	2547	C	C6-N1-C2	-5.03	118.29	120.30
1	S2	951	C	N3-C2-O2	-5.03	118.38	121.90
78	t	255	G	N3-C4-N9	5.03	129.02	126.00
78	t	3667	C	C6-N1-C2	-5.03	118.29	120.30
78	t	4583	C	C6-N1-C2	-5.03	118.29	120.30
6	SF	19	LEU	CA-CB-CG	5.03	126.87	115.30
78	t	4854	G	OP2-P-O3'	5.03	116.26	105.20
78	t	1480	G	C8-N9-C1'	-5.03	120.47	127.00
1	S2	1472	C	N1-C2-O2	5.02	121.92	118.90
1	S2	1589	A	C8-N9-C4	-5.02	103.79	105.80
78	t	153	G	C8-N9-C4	-5.02	104.39	106.40
78	t	1814	G	C2-N3-C4	-5.02	109.39	111.90
78	t	1745	C	C6-N1-C2	-5.02	118.29	120.30
78	t	3856	G	C4-C5-N7	5.02	112.81	110.80
78	t	1225	G	C4-N9-C1'	5.02	133.02	126.50
78	t	4392	G	C4-N9-C1'	5.02	133.02	126.50
25	SJ	50	LEU	CA-CB-CG	5.01	126.83	115.30
78	t	510	C	C6-N1-C2	-5.01	118.30	120.30
78	t	2366	G	N3-C4-C5	-5.01	126.09	128.60
78	t	4856	G	C8-N9-C4	-5.01	104.39	106.40
78	t	4420	C	C6-N1-C2	-5.01	118.30	120.30
1	S2	1557	C	C2-N1-C1'	5.01	124.31	118.80
16	SU	32	LEU	CA-CB-CG	5.00	126.81	115.30
78	t	233	G	N1-C2-N2	5.00	120.70	116.20
78	t	1217	G	N3-C4-N9	-5.00	123.00	126.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	SP	14	LYS	Peptide
15	ST	98	SER	Peptide
16	SU	95	SER	Peptide
56	V	74	SER	Mainchain

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Mol	Chain	Res	Type	Group
62	c	54	LEU	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	SA	219/221 (99%)	185 (84%)	33 (15%)	1 (0%)	25 60
3	SB	212/214 (99%)	183 (86%)	28 (13%)	1 (0%)	25 60
4	SD	224/226 (99%)	191 (85%)	33 (15%)	0	100 100
5	SE	257/259 (99%)	223 (87%)	34 (13%)	0	100 100
6	SF	187/189 (99%)	161 (86%)	26 (14%)	0	100 100
7	SH	182/189 (96%)	159 (87%)	23 (13%)	0	100 100
8	SI	202/204 (99%)	171 (85%)	31 (15%)	0	100 100
9	SK	96/98 (98%)	83 (86%)	13 (14%)	0	100 100
10	SL	151/153 (99%)	134 (89%)	17 (11%)	0	100 100
11	SP	125/127 (98%)	109 (87%)	16 (13%)	0	100 100
12	SQ	144/146 (99%)	123 (85%)	19 (13%)	2 (1%)	9 39
13	SR	132/134 (98%)	107 (81%)	25 (19%)	0	100 100
14	SS	143/145 (99%)	126 (88%)	17 (12%)	0	100 100
15	ST	141/143 (99%)	127 (90%)	13 (9%)	1 (1%)	19 54
16	SU	102/104 (98%)	91 (89%)	11 (11%)	0	100 100
17	SV	80/82 (98%)	68 (85%)	11 (14%)	1 (1%)	10 41
18	SX	139/141 (99%)	120 (86%)	19 (14%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	Sa	100/102 (98%)	84 (84%)	15 (15%)	1 (1%)	13 46
20	Sc	62/64 (97%)	48 (77%)	14 (23%)	0	100 100
21	Sd	53/55 (96%)	39 (74%)	13 (24%)	1 (2%)	6 34
22	Sg	310/312 (99%)	245 (79%)	65 (21%)	0	100 100
23	SC	219/220 (100%)	191 (87%)	27 (12%)	1 (0%)	25 60
24	SG	235/237 (99%)	207 (88%)	28 (12%)	0	100 100
25	SJ	184/185 (100%)	163 (89%)	20 (11%)	1 (0%)	25 60
26	SM	116/118 (98%)	97 (84%)	19 (16%)	0	100 100
27	SN	148/150 (99%)	142 (96%)	6 (4%)	0	100 100
28	SO	135/137 (98%)	116 (86%)	19 (14%)	0	100 100
29	SW	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	16 51
30	SY	130/131 (99%)	118 (91%)	12 (9%)	0	100 100
31	SZ	71/73 (97%)	58 (82%)	12 (17%)	1 (1%)	9 39
32	Sb	80/82 (98%)	68 (85%)	12 (15%)	0	100 100
33	Se	55/57 (96%)	45 (82%)	10 (18%)	0	100 100
34	Sf	65/67 (97%)	51 (78%)	14 (22%)	0	100 100
35	A	250/252 (99%)	219 (88%)	30 (12%)	1 (0%)	30 65
36	B	395/397 (100%)	342 (87%)	52 (13%)	1 (0%)	37 70
37	C	361/363 (99%)	326 (90%)	32 (9%)	3 (1%)	16 51
40	F	292/294 (99%)	253 (87%)	38 (13%)	1 (0%)	37 70
41	G	232/247 (94%)	188 (81%)	43 (18%)	1 (0%)	30 65
42	H	223/225 (99%)	202 (91%)	21 (9%)	0	100 100
43	I	232/234 (99%)	213 (92%)	18 (8%)	1 (0%)	30 65
44	J	189/191 (99%)	162 (86%)	27 (14%)	0	100 100
45	K	204/211 (97%)	183 (90%)	19 (9%)	2 (1%)	13 46
46	L	167/169 (99%)	143 (86%)	24 (14%)	0	100 100
47	M	203/205 (99%)	166 (82%)	36 (18%)	1 (0%)	25 60
48	N	137/139 (99%)	122 (89%)	15 (11%)	0	100 100
49	O	201/203 (99%)	174 (87%)	26 (13%)	1 (0%)	25 60
50	P	193/195 (99%)	183 (95%)	10 (5%)	0	100 100
51	Q	151/153 (99%)	142 (94%)	9 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
52	R	185/187 (99%)	163 (88%)	21 (11%)	1 (0%)	25 60
53	S	179/181 (99%)	164 (92%)	15 (8%)	0	100 100
54	T	173/175 (99%)	153 (88%)	19 (11%)	1 (1%)	22 57
55	U	155/157 (99%)	130 (84%)	23 (15%)	2 (1%)	10 41
56	V	97/99 (98%)	89 (92%)	8 (8%)	0	100 100
57	W	127/129 (98%)	119 (94%)	8 (6%)	0	100 100
58	X	119/121 (98%)	101 (85%)	17 (14%)	1 (1%)	16 51
59	Y	115/117 (98%)	106 (92%)	9 (8%)	0	100 100
60	Z	132/134 (98%)	118 (89%)	14 (11%)	0	100 100
61	b	145/147 (99%)	124 (86%)	20 (14%)	1 (1%)	19 54
62	c	94/121 (78%)	82 (87%)	12 (13%)	0	100 100
63	d	101/103 (98%)	87 (86%)	14 (14%)	0	100 100
64	e	104/106 (98%)	94 (90%)	8 (8%)	2 (2%)	6 34
65	f	127/129 (98%)	111 (87%)	16 (13%)	0	100 100
66	g	107/109 (98%)	93 (87%)	12 (11%)	2 (2%)	6 34
67	h	112/114 (98%)	98 (88%)	12 (11%)	2 (2%)	7 35
68	i	120/122 (98%)	110 (92%)	8 (7%)	2 (2%)	7 36
69	j	95/97 (98%)	88 (93%)	6 (6%)	1 (1%)	12 45
70	k	82/84 (98%)	72 (88%)	10 (12%)	0	100 100
71	l	67/69 (97%)	62 (92%)	5 (8%)	0	100 100
72	m	48/50 (96%)	44 (92%)	4 (8%)	0	100 100
73	n	48/50 (96%)	39 (81%)	9 (19%)	0	100 100
74	o	23/25 (92%)	22 (96%)	1 (4%)	0	100 100
75	p	103/105 (98%)	89 (86%)	14 (14%)	0	100 100
76	q	89/91 (98%)	85 (96%)	4 (4%)	0	100 100
77	r	120/122 (98%)	104 (87%)	15 (12%)	1 (1%)	16 51
81	y	37/39 (95%)	18 (49%)	19 (51%)	0	100 100
83	a	132/134 (98%)	113 (86%)	19 (14%)	0	100 100
All	All	11292/11489 (98%)	9844 (87%)	1408 (12%)	40 (0%)	32 65

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	SB	86	LEU
12	SQ	117	ARG
17	SV	79	VAL
23	SC	78	LEU
37	C	59	GLY
37	C	72	ALA
55	U	20	ARG
58	X	74	ARG
64	e	97	ASP
66	g	107	PRO
68	i	87	LYS
15	ST	41	LYS
21	Sd	4	GLN
40	F	260	GLU
47	M	78	LEU
61	b	47	LYS
67	h	84	ALA
68	i	41	ALA
2	SA	12	GLU
19	Sa	47	ALA
35	A	251	THR
37	C	57	LEU
49	O	95	ALA
52	R	157	GLY
64	e	95	ASP
36	B	3	HIS
45	K	11	TYR
54	T	164	LYS
55	U	53	PRO
77	r	21	ASN
12	SQ	45	ARG
31	SZ	50	PHE
45	K	10	ARG
66	g	60	PRO
67	h	28	ASN
69	j	35	LYS
29	SW	95	PRO
41	G	185	PRO
25	SJ	123	ILE
43	I	30	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	SA	183/183 (100%)	176 (96%)	7 (4%)	28 52
3	SB	195/195 (100%)	191 (98%)	4 (2%)	48 67
4	SD	189/189 (100%)	187 (99%)	2 (1%)	70 79
5	SE	222/222 (100%)	216 (97%)	6 (3%)	40 60
6	SF	159/159 (100%)	157 (99%)	2 (1%)	65 76
7	SH	166/169 (98%)	165 (99%)	1 (1%)	84 88
8	SI	177/177 (100%)	174 (98%)	3 (2%)	56 72
9	SK	89/89 (100%)	86 (97%)	3 (3%)	32 55
10	SL	137/137 (100%)	132 (96%)	5 (4%)	30 54
11	SP	113/113 (100%)	112 (99%)	1 (1%)	75 83
12	SQ	121/121 (100%)	118 (98%)	3 (2%)	42 62
13	SR	121/121 (100%)	119 (98%)	2 (2%)	56 72
14	SS	126/126 (100%)	125 (99%)	1 (1%)	79 84
15	ST	113/113 (100%)	110 (97%)	3 (3%)	40 60
16	SU	94/94 (100%)	90 (96%)	4 (4%)	25 49
17	SV	66/66 (100%)	63 (96%)	3 (4%)	23 48
18	SX	113/113 (100%)	110 (97%)	3 (3%)	40 60
19	Sa	89/89 (100%)	87 (98%)	2 (2%)	47 65
20	Sc	57/57 (100%)	57 (100%)	0	100 100
21	Sd	48/48 (100%)	46 (96%)	2 (4%)	25 49
22	Sg	271/271 (100%)	268 (99%)	3 (1%)	70 79
23	SC	187/186 (100%)	184 (98%)	3 (2%)	58 73
24	SG	207/207 (100%)	202 (98%)	5 (2%)	44 63
25	SJ	162/161 (101%)	155 (96%)	7 (4%)	25 49
26	SM	98/100 (98%)	95 (97%)	3 (3%)	35 56
27	SN	130/130 (100%)	129 (99%)	1 (1%)	79 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	SO	107/107 (100%)	107 (100%)	0	100	100
29	SW	112/112 (100%)	110 (98%)	2 (2%)	54	71
30	SY	114/113 (101%)	110 (96%)	4 (4%)	31	54
31	SZ	64/64 (100%)	62 (97%)	2 (3%)	35	56
32	Sb	74/74 (100%)	74 (100%)	0	100	100
33	Se	46/46 (100%)	45 (98%)	1 (2%)	47	65
34	Sf	60/60 (100%)	58 (97%)	2 (3%)	33	56
35	A	194/194 (100%)	190 (98%)	4 (2%)	48	67
36	B	345/345 (100%)	338 (98%)	7 (2%)	50	68
37	C	302/302 (100%)	292 (97%)	10 (3%)	33	56
40	F	248/248 (100%)	241 (97%)	7 (3%)	38	59
41	G	209/220 (95%)	204 (98%)	5 (2%)	44	63
42	H	194/194 (100%)	190 (98%)	4 (2%)	48	67
43	I	199/199 (100%)	199 (100%)	0	100	100
44	J	170/170 (100%)	166 (98%)	4 (2%)	44	63
45	K	178/179 (99%)	175 (98%)	3 (2%)	56	72
46	L	142/142 (100%)	140 (99%)	2 (1%)	62	75
47	M	171/171 (100%)	166 (97%)	5 (3%)	37	59
48	N	118/118 (100%)	116 (98%)	2 (2%)	56	72
49	O	171/171 (100%)	167 (98%)	4 (2%)	45	64
50	P	168/168 (100%)	161 (96%)	7 (4%)	25	49
51	Q	134/134 (100%)	132 (98%)	2 (2%)	60	74
52	R	164/164 (100%)	159 (97%)	5 (3%)	36	58
53	S	160/160 (100%)	155 (97%)	5 (3%)	35	56
54	T	156/156 (100%)	154 (99%)	2 (1%)	65	76
55	U	138/138 (100%)	135 (98%)	3 (2%)	47	65
56	V	89/89 (100%)	84 (94%)	5 (6%)	17	43
57	W	100/100 (100%)	100 (100%)	0	100	100
58	X	100/100 (100%)	100 (100%)	0	100	100
59	Y	105/105 (100%)	101 (96%)	4 (4%)	28	52
60	Z	124/124 (100%)	123 (99%)	1 (1%)	79	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
61	b	120/120 (100%)	114 (95%)	6 (5%)	20 45
62	c	82/101 (81%)	79 (96%)	3 (4%)	29 53
63	d	88/88 (100%)	87 (99%)	1 (1%)	70 79
64	e	97/97 (100%)	93 (96%)	4 (4%)	26 50
65	f	115/115 (100%)	114 (99%)	1 (1%)	75 83
66	g	88/88 (100%)	87 (99%)	1 (1%)	70 79
67	h	98/98 (100%)	95 (97%)	3 (3%)	35 56
68	i	109/109 (100%)	105 (96%)	4 (4%)	29 53
69	j	83/83 (100%)	82 (99%)	1 (1%)	67 78
70	k	71/71 (100%)	70 (99%)	1 (1%)	62 75
71	l	64/64 (100%)	63 (98%)	1 (2%)	58 73
72	m	47/47 (100%)	46 (98%)	1 (2%)	48 67
73	n	46/46 (100%)	46 (100%)	0	100 100
74	o	24/24 (100%)	23 (96%)	1 (4%)	25 49
75	p	93/93 (100%)	89 (96%)	4 (4%)	25 49
76	q	74/74 (100%)	73 (99%)	1 (1%)	62 75
77	r	106/106 (100%)	104 (98%)	2 (2%)	52 70
81	y	23/29 (79%)	22 (96%)	1 (4%)	25 49
83	a	117/117 (100%)	114 (97%)	3 (3%)	41 61
All	All	9834/9873 (100%)	9614 (98%)	220 (2%)	47 65

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SA	48	ILE
2	SA	50	ASN
2	SA	121	LEU
2	SA	122	LEU
2	SA	123	VAL
2	SA	186	ARG
2	SA	220	LYS
3	SB	86	LEU
3	SB	87	ILE
3	SB	186	ASN
3	SB	224	GLU

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Mol	Chain	Res	Type
4	SD	40	ARG
4	SD	76	ARG
5	SE	3	ARG
5	SE	49	ARG
5	SE	90	ILE
5	SE	198	ARG
5	SE	238	LEU
5	SE	254	LYS
6	SF	77	MET
6	SF	83	ASN
7	SH	57	ARG
8	SI	47	ARG
8	SI	124	LYS
8	SI	128	LYS
9	SK	42	ASN
9	SK	43	LEU
9	SK	55	ARG
10	SL	32	LYS
10	SL	40	ILE
10	SL	65	ASN
10	SL	69	ARG
10	SL	147	LYS
11	SP	89	MET
12	SQ	115	TYR
12	SQ	117	ARG
12	SQ	125	ARG
13	SR	3	ARG
13	SR	83	ASN
14	SS	108	ARG
15	ST	41	LYS
15	ST	82	ARG
15	ST	131	LEU
16	SU	49	LYS
16	SU	51	LYS
16	SU	56	MET
16	SU	66	ARG
17	SV	21	ASN
17	SV	27	LYS
17	SV	79	VAL
18	SX	8	ARG
18	SX	18	ARG
18	SX	107	ARG

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Mol	Chain	Res	Type
19	Sa	28	ARG
19	Sa	51	ARG
21	Sd	19	ARG
21	Sd	26	ASN
22	Sg	30	MET
22	Sg	162	ASN
22	Sg	280	LYS
23	SC	103	LYS
23	SC	200[A]	ARG
23	SC	200[B]	ARG
24	SG	98	ARG
24	SG	119	LYS
24	SG	132	ARG
24	SG	163	ASN
24	SG	224	ARG
25	SJ	5	ARG
25	SJ	66	LYS
25	SJ	79	ARG
25	SJ	92	MET
25	SJ	121	LYS
25	SJ	138[A]	ARG
25	SJ	138[B]	ARG
26	SM	55	ASN
26	SM	93	LYS
26	SM	116	LYS
27	SN	133	ARG
29	SW	57	ARG
29	SW	103	VAL
30	SY	2	ASN
30	SY	10	ARG
30	SY	113[A]	ARG
30	SY	113[B]	ARG
31	SZ	62	VAL
31	SZ	66	LYS
33	Se	6	LEU
34	Sf	89	LYS
34	Sf	96	LYS
35	A	64	ARG
35	A	140	ASN
35	A	193	ARG
35	A	250	LYS
36	B	121	ASN

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Mol	Chain	Res	Type
36	B	144	LYS
36	B	213	GLN
36	B	271	GLN
36	B	301	ASN
36	B	378	ARG
36	B	396	ARG
37	C	38	ASN
37	C	54	VAL
37	C	56	GLU
37	C	97	ARG
37	C	199	ARG
37	C	223	ASN
37	C	236	ASN
37	C	278	ASN
37	C	312	ARG
37	C	337	ARG
40	F	8	LYS
40	F	10	LYS
40	F	27	LYS
40	F	191	ASN
40	F	196	ARG
40	F	258	LYS
40	F	265	ARG
41	G	52	ARG
41	G	56	ARG
41	G	110	ARG
41	G	167	GLN
41	G	279	ASN
42	H	24	ASN
42	H	41	MET
42	H	106	ARG
42	H	245	ARG
44	J	42	ASN
44	J	63	ASN
44	J	108	ASN
44	J	116	ASN
45	K	3	ARG
45	K	69	ARG
45	K	169	LYS
46	L	35	ARG
46	L	54	ARG
47	M	5	ARG

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Mol	Chain	Res	Type
47	M	21	ARG
47	M	46	ILE
47	M	144	LEU
47	M	165	LYS
48	N	5	ARG
48	N	119	ARG
49	O	22	LEU
49	O	63	ARG
49	O	133	ILE
49	O	183	THR
50	P	63	ASN
50	P	94	ARG
50	P	140	ARG
50	P	169	ARG
50	P	178	ARG
50	P	187	LYS
50	P	188	LYS
51	Q	127	ARG
51	Q	139	TYR
52	R	6	ARG
52	R	14	ARG
52	R	37	ARG
52	R	160	HIS
52	R	168	ARG
53	S	23	TRP
53	S	98	ARG
53	S	152	LYS
53	S	162	ARG
53	S	180	LYS
54	T	15	ARG
54	T	74	ARG
55	U	9	ARG
55	U	107	LYS
55	U	117	LYS
56	V	20	LYS
56	V	52	LYS
56	V	67	LYS
56	V	69	LYS
56	V	101	ARG
59	Y	48	ARG
59	Y	96	LEU
59	Y	129	ARG

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Mol	Chain	Res	Type
59	Y	152	LYS
60	Z	104	VAL
61	b	45	PHE
61	b	46	ASP
61	b	47	LYS
61	b	63	LEU
61	b	87	ARG
61	b	105	ARG
62	c	41	ARG
62	c	54	LEU
62	c	65	MET
63	d	77	ASN
64	e	23	ARG
64	e	93	ASN
64	e	94	GLU
64	e	96	GLU
65	f	33	ARG
66	g	109	ARG
67	h	4	ARG
67	h	54	ARG
67	h	82	MET
68	i	5	LYS
68	i	20	GLN
68	i	92	ARG
68	i	109	ARG
69	j	68	ARG
70	k	82	THR
71	l	17	ARG
72	m	11	ARG
74	o	9	ARG
75	p	27	LYS
75	p	69	ARG
75	p	81	ARG
75	p	102	GLN
76	q	84	ARG
77	r	41	ASN
77	r	83	ASN
81	y	35	LEU
83	a	13	VAL
83	a	17	ARG
83	a	98	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134)

such sidechains are listed below:

Mol	Chain	Res	Type
2	SA	50	ASN
3	SB	177	GLN
3	SB	186	ASN
3	SB	202	GLN
4	SD	159	HIS
5	SE	112	HIS
5	SE	138	HIS
6	SF	179	ASN
7	SH	114	GLN
7	SH	168	HIS
8	SI	168	GLN
9	SK	28	HIS
9	SK	42	ASN
9	SK	44	HIS
10	SL	18	GLN
10	SL	65	ASN
10	SL	83	GLN
10	SL	106	HIS
11	SP	104	GLN
12	SQ	48	GLN
12	SQ	80	GLN
13	SR	83	ASN
13	SR	93	GLN
14	SS	11	HIS
14	SS	17	ASN
14	SS	72	GLN
14	SS	101	ASN
14	SS	120	HIS
15	ST	51	ASN
15	ST	128	GLN
16	SU	100	GLN
17	SV	21	ASN
17	SV	29	HIS
17	SV	35	ASN
18	SX	87	ASN
19	Sa	72	HIS
20	Sc	7	GLN
20	Sc	29	GLN
21	Sd	5	GLN
21	Sd	26	ASN
22	Sg	4	GLN
22	Sg	117	ASN

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Mol	Chain	Res	Type
22	Sg	162	ASN
23	SC	267	GLN
24	SG	59	GLN
24	SG	163	ASN
24	SG	197	GLN
25	SJ	111	GLN
25	SJ	140	GLN
27	SN	5	HIS
28	SO	103	ASN
30	SY	2	ASN
30	SY	124	ASN
31	SZ	106	GLN
32	Sb	19	HIS
35	A	132	ASN
35	A	140	ASN
35	A	218	HIS
36	B	121	ASN
36	B	167	GLN
36	B	213	GLN
36	B	301	ASN
36	B	322	HIS
36	B	380	GLN
37	C	38	ASN
37	C	61	GLN
37	C	85	HIS
37	C	223	ASN
37	C	236	ASN
37	C	278	ASN
37	C	346	ASN
40	F	57	ASN
40	F	191	ASN
40	F	198	HIS
41	G	182	ASN
41	G	190	HIS
41	G	250	GLN
41	G	279	ASN
42	H	24	ASN
42	H	80	ASN
42	H	119	ASN
42	H	226	HIS
43	I	64	GLN
43	I	149	ASN

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Mol	Chain	Res	Type
43	I	225	ASN
44	J	42	ASN
44	J	63	ASN
44	J	108	ASN
44	J	116	ASN
46	L	110	GLN
46	L	112	HIS
48	N	44	GLN
48	N	56	GLN
49	O	87	HIS
49	O	109	HIS
49	O	145	ASN
49	O	201	HIS
50	P	14	HIS
50	P	63	ASN
51	Q	80	GLN
52	R	160	HIS
53	S	58	HIS
53	S	130	ASN
54	T	50	GLN
55	U	49	GLN
55	U	95	HIS
57	W	77	HIS
57	W	101	ASN
58	X	63	GLN
59	Y	111	GLN
60	Z	61	HIS
61	b	25	HIS
61	b	44	ASN
61	b	60	HIS
61	b	89	ASN
63	d	77	ASN
64	e	79	ASN
64	e	93	ASN
65	f	43	ASN
66	g	55	ASN
66	g	99	HIS
68	i	20	GLN
69	j	26	HIS
70	k	66	HIS
72	m	43	HIS
73	n	90	ASN

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Mol	Chain	Res	Type
75	p	102	GLN
76	q	34	HIS
76	q	56	HIS
76	q	92	GLN
77	r	12	ASN
77	r	41	ASN
77	r	45	HIS
77	r	83	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1690/1714 (98%)	617 (36%)	26 (1%)
38	D	156/157 (99%)	40 (25%)	0
39	E	118/119 (99%)	20 (16%)	0
78	t	3590/3607 (99%)	1000 (27%)	0
79	v	71/76 (93%)	37 (52%)	0
80	w	9/10 (90%)	3 (33%)	0
82	u	75/76 (98%)	43 (57%)	0
All	All	5709/5759 (99%)	1760 (30%)	26 (0%)

All (1760) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	2	A
1	S2	4	C
1	S2	5	U
1	S2	9	U
1	S2	10	G
1	S2	11	A
1	S2	23	G
1	S2	24	C
1	S2	25	A
1	S2	33	G
1	S2	37	C
1	S2	38	A
1	S2	39	A
1	S2	41	G
1	S2	43	U
1	S2	44	U
1	S2	46	A

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Mol	Chain	Res	Type
1	S2	49	C
1	S2	54	A
1	S2	55	U
1	S2	56	G
1	S2	58	C
1	S2	59	U
1	S2	60	A
1	S2	61	A
1	S2	62	G
1	S2	64	A
1	S2	65	C
1	S2	66	G
1	S2	67	C
1	S2	68	A
1	S2	70	G
1	S2	71	G
1	S2	72	C
1	S2	73	C
1	S2	74	G
1	S2	75	G
1	S2	76	U
1	S2	79	A
1	S2	80	G
1	S2	93	U
1	S2	94	G
1	S2	99	A
1	S2	102	A
1	S2	103	A
1	S2	108	G
1	S2	113	G
1	S2	115	U
1	S2	116	OMU
1	S2	121	OMU
1	S2	125	C
1	S2	126	G
1	S2	129	C
1	S2	139	C
1	S2	140	C
1	S2	142	C
1	S2	143	U
1	S2	155	G
1	S2	157	U

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Mol	Chain	Res	Type
1	S2	159	A2M
1	S2	160	U
1	S2	161	U
1	S2	163	U
1	S2	168	C
1	S2	170	A
1	S2	173	A
1	S2	176	U
1	S2	178	C
1	S2	187	G
1	S2	191	A
1	S2	192	C
1	S2	193	C
1	S2	194	C
1	S2	195	C
1	S2	196	C
1	S2	197	U
1	S2	198	U
1	S2	199	C
1	S2	200	G
1	S2	203	G
1	S2	204	G
1	S2	206	G
1	S2	208	G
1	S2	209	A
1	S2	214	U
1	S2	215	G
1	S2	289	G
1	S2	291	G
1	S2	292	A
1	S2	293	C
1	S2	294	U
1	S2	295	C
1	S2	305	U
1	S2	306	C
1	S2	308	G
1	S2	311	C
1	S2	312	G
1	S2	313	A
1	S2	316	G
1	S2	318	A
1	S2	319	C

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Mol	Chain	Res	Type
1	S2	323	C
1	S2	324	C
1	S2	325	C
1	S2	326	C
1	S2	327	G
1	S2	328	U
1	S2	329	G
1	S2	331	C
1	S2	335	G
1	S2	337	C
1	S2	340	C
1	S2	347	G
1	S2	351	G
1	S2	360	A
1	S2	364	A
1	S2	368	U
1	S2	369	C
1	S2	375	U
1	S2	376	A
1	S2	377	G
1	S2	379	C
1	S2	380	G
1	S2	382	C
1	S2	384	U
1	S2	385	G
1	S2	386	C
1	S2	387	C
1	S2	395	G
1	S2	400	C
1	S2	407	G
1	S2	408	A
1	S2	409	C
1	S2	413	G
1	S2	419	G
1	S2	426	A
1	S2	428	U
1	S2	429	C
1	S2	435	A
1	S2	446	G
1	S2	447	A
1	S2	448	A
1	S2	449	A

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Mol	Chain	Res	Type
1	S2	450	C
1	S2	451	G
1	S2	452	G
1	S2	464	A
1	S2	465	A
1	S2	466	G
1	S2	467	G
1	S2	470	G
1	S2	471	G
1	S2	472	C
1	S2	473	A
1	S2	474	G
1	S2	482	G
1	S2	485	A
1	S2	487	U
1	S2	488	U
1	S2	492	C
1	S2	493	A
1	S2	495	U
1	S2	496	C
1	S2	500	A
1	S2	502	C
1	S2	503	C
1	S2	507	G
1	S2	517	OMC
1	S2	518	G
1	S2	525	A
1	S2	526	A
1	S2	528	A
1	S2	529	A
1	S2	531	A
1	S2	532	C
1	S2	533	A
1	S2	537	C
1	S2	538	U
1	S2	539	C
1	S2	540	U
1	S2	541	U
1	S2	542	U
1	S2	543	C
1	S2	544	G
1	S2	545	A

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Mol	Chain	Res	Type
1	S2	546	G
1	S2	547	G
1	S2	548	C
1	S2	549	C
1	S2	554	A
1	S2	555	A
1	S2	556	U
1	S2	557	U
1	S2	558	G
1	S2	559	G
1	S2	560	A
1	S2	561	A
1	S2	564	A
1	S2	574	A
1	S2	578	C
1	S2	579	C
1	S2	583	C
1	S2	585	C
1	S2	588	G
1	S2	589	G
1	S2	590	A
1	S2	593	C
1	S2	594	A
1	S2	597	G
1	S2	600	G
1	S2	603	C
1	S2	607	U
1	S2	608	C
1	S2	614	C
1	S2	617	G
1	S2	621	C
1	S2	625	G
1	S2	626	G
1	S2	627	U
1	S2	628	A
1	S2	629	A
1	S2	631	U
1	S2	643	A
1	S2	645	C
1	S2	647	U
1	S2	650	A
1	S2	654	A

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Mol	Chain	Res	Type
1	S2	655	A
1	S2	657	U
1	S2	664	A
1	S2	668	A2M
1	S2	669	A
1	S2	671	A
1	S2	672	A
1	S2	673	G
1	S2	675	U
1	S2	681	U
1	S2	683	OMG
1	S2	684	G
1	S2	689	U
1	S2	690	G
1	S2	692	G
1	S2	693	A
1	S2	695	C
1	S2	696	G
1	S2	697	G
1	S2	698	G
1	S2	731	G
1	S2	732	U
1	S2	733	C
1	S2	734	C
1	S2	735	C
1	S2	736	C
1	S2	737	G
1	S2	738	C
1	S2	739	C
1	S2	748	C
1	S2	749	U
1	S2	751	G
1	S2	752	G
1	S2	753	C
1	S2	787	G
1	S2	788	G
1	S2	790	C
1	S2	791	C
1	S2	792	C
1	S2	795	A
1	S2	797	C
1	S2	799	U

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Mol	Chain	Res	Type
1	S2	811	A
1	S2	815	U
1	S2	817	G
1	S2	821	G
1	S2	822	PSU
1	S2	823	PSU
1	S2	824	C
1	S2	827	A
1	S2	830	A
1	S2	831	G
1	S2	835	C
1	S2	836	G
1	S2	837	A
1	S2	838	G
1	S2	839	C
1	S2	840	C
1	S2	841	G
1	S2	842	C
1	S2	847	A
1	S2	849	A
1	S2	851	C
1	S2	857	U
1	S2	858	A
1	S2	859	G
1	S2	865	A
1	S2	866	U
1	S2	867	G
1	S2	868	G
1	S2	869	A
1	S2	870	A
1	S2	871	U
1	S2	872	A
1	S2	873	G
1	S2	878	G
1	S2	879	C
1	S2	881	G
1	S2	886	A
1	S2	887	U
1	S2	888	U
1	S2	889	U
1	S2	890	U
1	S2	891	G

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Mol	Chain	Res	Type
1	S2	892	U
1	S2	894	G
1	S2	895	G
1	S2	896	U
1	S2	897	U
1	S2	898	U
1	S2	899	U
1	S2	900	C
1	S2	901	G
1	S2	903	A
1	S2	904	A
1	S2	905	C
1	S2	907	G
1	S2	908	A
1	S2	910	G
1	S2	913	A
1	S2	914	U
1	S2	917	U
1	S2	920	A
1	S2	921	G
1	S2	924	G
1	S2	933	G
1	S2	938	A
1	S2	949	G
1	S2	951	C
1	S2	954	U
1	S2	968	U
1	S2	969	U
1	S2	970	G
1	S2	971	G
1	S2	972	A
1	S2	973	C
1	S2	978	G
1	S2	983	A
1	S2	986	G
1	S2	990	A
1	S2	991	G
1	S2	992	A
1	S2	998	A
1	S2	999	G
1	S2	1001	A
1	S2	1002	U

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Mol	Chain	Res	Type
1	S2	1005	G
1	S2	1006	C
1	S2	1007	C
1	S2	1016	U
1	S2	1017	U
1	S2	1021	U
1	S2	1023	A
1	S2	1026	C
1	S2	1027	A
1	S2	1028	A
1	S2	1029	G
1	S2	1031	A2M
1	S2	1038	U
1	S2	1045	U
1	S2	1049	A
1	S2	1058	A
1	S2	1061	U
1	S2	1062	A
1	S2	1064	C
1	S2	1082	A
1	S2	1083	A
1	S2	1085	C
1	S2	1087	A
1	S2	1088	U
1	S2	1089	G
1	S2	1109	C
1	S2	1114	U
1	S2	1115	U
1	S2	1117	C
1	S2	1119	A
1	S2	1120	U
1	S2	1133	A
1	S2	1138	C
1	S2	1149	A
1	S2	1150	A
1	S2	1154	U
1	S2	1155	U
1	S2	1158	G
1	S2	1166	G
1	S2	1168	G
1	S2	1170	A
1	S2	1181	A

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Mol	Chain	Res	Type
1	S2	1183	A
1	S2	1190	A
1	S2	1195	A
1	S2	1200	A
1	S2	1207	G
1	S2	1208	A
1	S2	1209	A
1	S2	1215	C
1	S2	1217	A
1	S2	1222	G
1	S2	1224	G
1	S2	1231	C
1	S2	1240	A
1	S2	1242	U
1	S2	1245	G
1	S2	1246	A
1	S2	1249	C
1	S2	1250	A
1	S2	1251	A
1	S2	1253	A
1	S2	1254	C
1	S2	1255	G
1	S2	1256	G
1	S2	1257	G
1	S2	1259	A
1	S2	1260	A
1	S2	1262	C
1	S2	1263	U
1	S2	1265	A
1	S2	1266	C
1	S2	1274	G
1	S2	1275	G
1	S2	1277	C
1	S2	1283	C
1	S2	1284	A
1	S2	1285	G
1	S2	1286	G
1	S2	1287	A
1	S2	1294	G
1	S2	1295	A
1	S2	1296	U
1	S2	1298	G

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Mol	Chain	Res	Type
1	S2	1300	U
1	S2	1301	A
1	S2	1303	C
1	S2	1312	G
1	S2	1313	A
1	S2	1315	U
1	S2	1322	G
1	S2	1323	U
1	S2	1330	G
1	S2	1331	C
1	S2	1333	U
1	S2	1340	U
1	S2	1341	C
1	S2	1342	U
1	S2	1345	G
1	S2	1348	G
1	S2	1351	G
1	S2	1354	G
1	S2	1355	C
1	S2	1371	U
1	S2	1372	U
1	S2	1376	A
1	S2	1378	A
1	S2	1384	C
1	S2	1393	G
1	S2	1396	A
1	S2	1397	U
1	S2	1398	G
1	S2	1402	A
1	S2	1403	C
1	S2	1411	G
1	S2	1418	C
1	S2	1420	G
1	S2	1421	A
1	S2	1424	G
1	S2	1433	C
1	S2	1435	C
1	S2	1436	C
1	S2	1438	A
1	S2	1442	U
1	S2	1446	A
1	S2	1447	G

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Mol	Chain	Res	Type
1	S2	1452	A
1	S2	1453	C
1	S2	1454	A
1	S2	1455	A
1	S2	1462	U
1	S2	1463	U
1	S2	1464	C
1	S2	1466	G
1	S2	1469	A
1	S2	1477	U
1	S2	1478	U
1	S2	1480	A
1	S2	1481	G
1	S2	1482	C
1	S2	1483	A
1	S2	1484	A
1	S2	1489	A
1	S2	1490	G
1	S2	1493	C
1	S2	1494	U
1	S2	1495	G
1	S2	1496	U
1	S2	1497	G
1	S2	1498	A
1	S2	1505	U
1	S2	1507	G
1	S2	1508	A
1	S2	1509	U
1	S2	1518	C
1	S2	1519	U
1	S2	1520	G
1	S2	1521	C
1	S2	1522	A
1	S2	1531	A
1	S2	1533	A
1	S2	1534	C
1	S2	1543	U
1	S2	1544	C
1	S2	1545	A
1	S2	1550	G
1	S2	1552	G
1	S2	1553	C

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Mol	Chain	Res	Type
1	S2	1556	A
1	S2	1557	C
1	S2	1558	C
1	S2	1560	U
1	S2	1566	G
1	S2	1568	C
1	S2	1570	G
1	S2	1572	C
1	S2	1573	G
1	S2	1575	G
1	S2	1578	U
1	S2	1580	A
1	S2	1581	C
1	S2	1585	U
1	S2	1586	U
1	S2	1587	G
1	S2	1588	A
1	S2	1591	C
1	S2	1598	G
1	S2	1599	U
1	S2	1601	A
1	S2	1606	G
1	S2	1619	A
1	S2	1621	U
1	S2	1623	A
1	S2	1634	A
1	S2	1637	A
1	S2	1646	C
1	S2	1647	A
1	S2	1648	G
1	S2	1649	U
1	S2	1654	G
1	S2	1657	G
1	S2	1662	U
1	S2	1663	A
1	S2	1665	G
1	S2	1675	A
1	S2	1676	U
1	S2	1680	G
1	S2	1682	C
1	S2	1686	G
1	S2	1692	U

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Mol	Chain	Res	Type
1	S2	1695	A
1	S2	1698	C
1	S2	1699	A
1	S2	1704	C
1	S2	1707	U
1	S2	1721	U
1	S2	1722	G
1	S2	1726	G
1	S2	1728	U
1	S2	1729	U
1	S2	1744	G
1	S2	1750	C
1	S2	1751	C
1	S2	1752	C
1	S2	1780	G
1	S2	1781	A
1	S2	1782	G
1	S2	1783	C
1	S2	1784	G
1	S2	1785	C
1	S2	1786	U
1	S2	1787	G
1	S2	1793	A
1	S2	1803	U
1	S2	1804	U
1	S2	1805	G
1	S2	1811	C
1	S2	1813	A
1	S2	1814	G
1	S2	1815	A
1	S2	1816	G
1	S2	1817	G
1	S2	1823	A
1	S2	1824	A
1	S2	1826	G
1	S2	1829	G
1	S2	1830	UR3
1	S2	1831	A
1	S2	1835	A
1	S2	1836	G
1	S2	1838	U
1	S2	1839	U

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Mol	Chain	Res	Type
1	S2	1841	C
1	S2	1849	G
1	S2	1852	C
1	S2	1855	G
1	S2	1861	G
1	S2	1862	G
1	S2	1863	A
1	S2	1864	U
1	S2	1865	C
1	S2	1867	U
1	S2	1868	U
1	S2	1869	A
38	D	2	G
38	D	23	C
38	D	32	C
38	D	34	U
38	D	35	C
38	D	38	U
38	D	49	G
38	D	59	A
38	D	60	G
38	D	63	U
38	D	72	A
38	D	74	U
38	D	77	A
38	D	80	A
38	D	81	C
38	D	83	C
38	D	84	A
38	D	85	U
38	D	86	U
38	D	87	G
38	D	91	A
38	D	94	G
38	D	96	C
38	D	103	A
38	D	105	C
38	D	107	C
38	D	109	C
38	D	110	U
38	D	111	U
38	D	120	G

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Mol	Chain	Res	Type
38	D	121	G
38	D	122	G
38	D	124	U
38	D	125	C
38	D	126	C
38	D	127	U
38	D	128	C
38	D	129	C
38	D	130	C
38	D	148	A
39	E	7	G
39	E	11	A
39	E	22	A
39	E	23	A
39	E	24	C
39	E	27	G
39	E	31	G
39	E	33	U
39	E	53	U
39	E	54	A
39	E	64	G
39	E	74	A
39	E	85	G
39	E	88	A
39	E	89	G
39	E	91	C
39	E	97	G
39	E	98	G
39	E	109	U
39	E	110	G
78	t	5	A
78	t	9	C
78	t	13	U
78	t	17	A
78	t	18	C
78	t	21	G
78	t	25	A
78	t	30	C
78	t	32	G
78	t	33	A
78	t	39	A
78	t	42	A

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Mol	Chain	Res	Type
78	t	47	A
78	t	48	G
78	t	49	U
78	t	58	G
78	t	59	A
78	t	64	A
78	t	65	A
78	t	71	C
78	t	72	C
78	t	76	A
78	t	91	G
78	t	97	G
78	t	101	A
78	t	108	A
78	t	116	G
78	t	118	C
78	t	119	G
78	t	121	A
78	t	129	C
78	t	131	C
78	t	132	G
78	t	133	C
78	t	134	G
78	t	135	G
78	t	138	C
78	t	143	G
78	t	147	U
78	t	149	U
78	t	155	A
78	t	156	C
78	t	157	G
78	t	158	G
78	t	163	C
78	t	168	U
78	t	170	C
78	t	173	G
78	t	177	C
78	t	179	G
78	t	181	U
78	t	182	C
78	t	183	G
78	t	184	U

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Mol	Chain	Res	Type
78	t	185	G
78	t	189	G
78	t	195	A
78	t	196	G
78	t	197	U
78	t	205	A
78	t	212	C
78	t	213	C
78	t	214	C
78	t	215	A
78	t	227	G
78	t	228	U
78	t	229	G
78	t	230	U
78	t	233	G
78	t	236	C
78	t	250	G
78	t	252	C
78	t	253	G
78	t	256	C
78	t	260	C
78	t	272	G
78	t	274	G
78	t	282	G
78	t	289	A
78	t	291	U
78	t	300	A
78	t	303	C
78	t	304	G
78	t	309	G
78	t	310	U
78	t	311	A
78	t	322	A
78	t	323	A
78	t	334	C
78	t	338	A
78	t	339	C
78	t	343	A
78	t	344	C
78	t	345	C
78	t	348	U
78	t	351	U

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Mol	Chain	Res	Type
78	t	367	G
78	t	370	A
78	t	375	U
78	t	377	A
78	t	379	A
78	t	380	A
78	t	381	G
78	t	390	A
78	t	395	G
78	t	404	A
78	t	406	G
78	t	407	G
78	t	408	C
78	t	409	G
78	t	425	G
78	t	426	U
78	t	434	U
78	t	444	G
78	t	446	A
78	t	447	G
78	t	448	U
78	t	449	C
78	t	451	G
78	t	456	G
78	t	458	G
78	t	466	C
78	t	479	C
78	t	480	C
78	t	482	G
78	t	487	G
78	t	489	C
78	t	491	G
78	t	492	C
78	t	493	G
78	t	494	G
78	t	496	C
78	t	497	C
78	t	498	G
78	t	499	G
78	t	504	U
78	t	507	U
78	t	509	C

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Mol	Chain	Res	Type
78	t	511	C
78	t	512	G
78	t	630	G
78	t	633	U
78	t	634	C
78	t	635	G
78	t	636	G
78	t	641	G
78	t	643	A
78	t	647	U
78	t	649	C
78	t	654	G
78	t	658	G
78	t	659	G
78	t	661	G
78	t	672	G
78	t	674	C
78	t	677	G
78	t	678	C
78	t	679	G
78	t	680	C
78	t	690	C
78	t	692	G
78	t	693	U
78	t	695	C
78	t	696	G
78	t	714	A
78	t	719	U
78	t	720	G
78	t	721	G
78	t	724	A
78	t	728	C
78	t	730	G
78	t	737	A
78	t	738	A
78	t	739	G
78	t	743	G
78	t	897	G
78	t	901	U
78	t	902	A
78	t	904	A
78	t	905	G

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Mol	Chain	Res	Type
78	t	906	C
78	t	907	C
78	t	908	C
78	t	913	G
78	t	917	G
78	t	919	A
78	t	921	C
78	t	922	A
78	t	923	C
78	t	924	U
78	t	925	C
78	t	927	C
78	t	929	G
78	t	931	A
78	t	932	U
78	t	933	C
78	t	937	G
78	t	938	G
78	t	943	A
78	t	944	G
78	t	947	A
78	t	948	G
78	t	949	C
78	t	950	G
78	t	952	G
78	t	953	A
78	t	954	C
78	t	957	G
78	t	964	C
78	t	976	U
78	t	1061	A
78	t	1064	C
78	t	1065	C
78	t	1066	U
78	t	1071	C
78	t	1077	G
78	t	1084	C
78	t	1086	C
78	t	1087	C
78	t	1149	G
78	t	1150	C
78	t	1151	G

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Mol	Chain	Res	Type
78	t	1152	G
78	t	1156	G
78	t	1162	U
78	t	1165	C
78	t	1174	C
78	t	1176	C
78	t	1181	G
78	t	1186	G
78	t	1188	G
78	t	1191	G
78	t	1192	U
78	t	1193	C
78	t	1196	G
78	t	1197	C
78	t	1198	C
78	t	1199	C
78	t	1201	G
78	t	1220	C
78	t	1221	A
78	t	1222	C
78	t	1223	G
78	t	1224	C
78	t	1225	G
78	t	1226	C
78	t	1228	C
78	t	1229	G
78	t	1234	C
78	t	1237	A
78	t	1238	A
78	t	1240	G
78	t	1248	G
78	t	1249	G
78	t	1250	C
78	t	1251	G
78	t	1252	G
78	t	1253	A
78	t	1258	G
78	t	1259	C
78	t	1263	C
78	t	1264	G
78	t	1265	G
78	t	1268	U

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Mol	Chain	Res	Type
78	t	1269	C
78	t	1271	G
78	t	1273	G
78	t	1277	A
78	t	1278	C
78	t	1279	G
78	t	1284	C
78	t	1285	U
78	t	1297	C
78	t	1299	G
78	t	1301	C
78	t	1309	A
78	t	1320	A
78	t	1321	G
78	t	1325	A
78	t	1336	G
78	t	1337	A
78	t	1341	G
78	t	1342	G
78	t	1348	C
78	t	1350	C
78	t	1351	A
78	t	1352	C
78	t	1353	G
78	t	1354	A
78	t	1360	G
78	t	1361	C
78	t	1362	C
78	t	1364	U
78	t	1370	A
78	t	1374	A
78	t	1379	G
78	t	1380	A
78	t	1381	A
78	t	1388	C
78	t	1389	G
78	t	1390	C
78	t	1391	G
78	t	1392	C
78	t	1393	U
78	t	1394	C
78	t	1395	G

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Mol	Chain	Res	Type
78	t	1396	C
78	t	1403	A
78	t	1404	G
78	t	1420	C
78	t	1421	U
78	t	1423	U
78	t	1424	C
78	t	1425	C
78	t	1426	A
78	t	1428	U
78	t	1429	C
78	t	1430	C
78	t	1431	G
78	t	1435	A
78	t	1463	C
78	t	1464	G
78	t	1465	C
78	t	1466	G
78	t	1467	C
78	t	1468	C
78	t	1473	A
78	t	1480	G
78	t	1497	A
78	t	1499	G
78	t	1500	A
78	t	1505	A
78	t	1507	A
78	t	1515	A
78	t	1516	A
78	t	1520	U
78	t	1521	G
78	t	1531	G
78	t	1548	C
78	t	1553	G
78	t	1560	U
78	t	1564	U
78	t	1570	U
78	t	1573	U
78	t	1578	U
78	t	1579	G
78	t	1589	C
78	t	1595	A

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Mol	Chain	Res	Type
78	t	1606	G
78	t	1607	G
78	t	1608	G
78	t	1609	G
78	t	1612	A
78	t	1613	A
78	t	1615	G
78	t	1616	A
78	t	1633	G
78	t	1636	G
78	t	1642	U
78	t	1643	C
78	t	1658	C
78	t	1660	C
78	t	1663	G
78	t	1674	C
78	t	1679	G
78	t	1680	C
78	t	1700	C
78	t	1701	A
78	t	1711	A
78	t	1713	C
78	t	1723	G
78	t	1732	G
78	t	1736	U
78	t	1738	U
78	t	1741	G
78	t	1746	G
78	t	1747	A
78	t	1748	A
78	t	1750	C
78	t	1751	G
78	t	1754	C
78	t	1756	C
78	t	1767	C
78	t	1769	A
78	t	1776	A
78	t	1783	A
78	t	1786	A
78	t	1787	A
78	t	1794	C
78	t	1803	G

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Mol	Chain	Res	Type
78	t	1814	G
78	t	1815	U
78	t	1816	G
78	t	1818	A
78	t	1823	G
78	t	1836	G
78	t	1837	C
78	t	1840	C
78	t	1850	G
78	t	1854	A
78	t	1863	U
78	t	1864	G
78	t	1870	U
78	t	1872	A
78	t	1879	C
78	t	1882	C
78	t	1883	G
78	t	1887	U
78	t	1890	G
78	t	1891	G
78	t	1896	C
78	t	1897	G
78	t	1898	A
78	t	1902	C
78	t	1903	G
78	t	1906	G
78	t	1910	A
78	t	1912	C
78	t	1913	A
78	t	1915	A
78	t	1920	A
78	t	1921	G
78	t	1922	A
78	t	1928	U
78	t	1929	G
78	t	1930	U
78	t	1932	G
78	t	1936	G
78	t	1937	A
78	t	1938	U
78	t	1940	U
78	t	1941	A

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Mol	Chain	Res	Type
78	t	1942	G
78	t	1943	A
78	t	1956	G
78	t	1957	G
78	t	1958	C
78	t	1960	A
78	t	1961	U
78	t	1963	G
78	t	1964	A
78	t	1967	U
78	t	1968	C
78	t	1971	A
78	t	1972	A
78	t	1973	U
78	t	1974	C
78	t	1978	U
78	t	1979	A
78	t	1980	A
78	t	1983	A
78	t	1984	G
78	t	1988	G
78	t	1989	U
78	t	1991	A
78	t	1993	A
78	t	1994	A
78	t	1996	U
78	t	1997	C
78	t	2003	C
78	t	2007	A
78	t	2011	A
78	t	2012	C
78	t	2021	A
78	t	2023	A
78	t	2027	G
78	t	2028	A
78	t	2029	U
78	t	2033	G
78	t	2036	G
78	t	2037	G
78	t	2038	A
78	t	2050	A
78	t	2051	U

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Mol	Chain	Res	Type
78	t	2072	G
78	t	2073	A
78	t	2075	A
78	t	2076	G
78	t	2077	U
78	t	2078	G
78	t	2081	C
78	t	2082	G
78	t	2084	G
78	t	2086	G
78	t	2087	C
78	t	2090	C
78	t	2091	G
78	t	2092	G
78	t	2231	G
78	t	2232	A
78	t	2233	G
78	t	2235	C
78	t	2237	C
78	t	2239	C
78	t	2241	G
78	t	2242	A
78	t	2247	A
78	t	2248	C
78	t	2250	C
78	t	2268	C
78	t	2273	G
78	t	2278	G
78	t	2279	A
78	t	2280	G
78	t	2282	C
78	t	2284	U
78	t	2285	G
78	t	2292	A
78	t	2295	G
78	t	2299	G
78	t	2310	G
78	t	2323	U
78	t	2327	G
78	t	2330	C
78	t	2336	G
78	t	2340	G

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Mol	Chain	Res	Type
78	t	2343	G
78	t	2344	C
78	t	2348	U
78	t	2349	A
78	t	2357	G
78	t	2359	G
78	t	2366	G
78	t	2374	A
78	t	2377	U
78	t	2389	C
78	t	2395	G
78	t	2400	G
78	t	2401	C
78	t	2404	U
78	t	2405	U
78	t	2416	C
78	t	2421	G
78	t	2426	U
78	t	2429	G
78	t	2442	G
78	t	2446	U
78	t	2447	U
78	t	2453	G
78	t	2459	G
78	t	2461	C
78	t	2467	C
78	t	2468	C
78	t	2469	U
78	t	2470	C
78	t	2473	U
78	t	2474	U
78	t	2480	C
78	t	2481	G
78	t	2482	G
78	t	2483	C
78	t	2484	C
78	t	2485	G
78	t	2492	A
78	t	2502	G
78	t	2522	A
78	t	2523	G
78	t	2524	U

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Mol	Chain	Res	Type
78	t	2525	G
78	t	2526	G
78	t	2532	A
78	t	2533	U
78	t	2545	G
78	t	2548	G
78	t	2549	U
78	t	2565	G
78	t	2566	A
78	t	2568	C
78	t	2570	A
78	t	2580	A
78	t	2583	C
78	t	2584	G
78	t	2585	G
78	t	2600	A
78	t	2606	C
78	t	2617	G
78	t	2628	G
78	t	2632	C
78	t	2637	G
78	t	2638	A
78	t	2639	A
78	t	2640	U
78	t	2644	U
78	t	2648	C
78	t	2652	G
78	t	2665	G
78	t	2666	U
78	t	2674	A
78	t	2675	A
78	t	2684	G
78	t	2689	C
78	t	2690	G
78	t	2691	G
78	t	2698	C
78	t	2700	G
78	t	2705	G
78	t	2714	G
78	t	2719	U
78	t	2722	A
78	t	2723	A

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Mol	Chain	Res	Type
78	t	2733	G
78	t	2737	G
78	t	2738	G
78	t	2739	G
78	t	2741	G
78	t	2742	U
78	t	2745	A
78	t	2746	U
78	t	2748	U
78	t	2751	C
78	t	2766	A
78	t	2767	U
78	t	2768	A
78	t	2769	U
78	t	2771	C
78	t	2773	C
78	t	2774	A
78	t	2775	G
78	t	2776	C
78	t	2777	A
78	t	2778	G
78	t	2781	C
78	t	2785	A
78	t	2805	U
78	t	2806	G
78	t	2807	U
78	t	2814	A
78	t	2817	G
78	t	2821	G
78	t	2822	U
78	t	2837	A
78	t	2846	C
78	t	2848	U
78	t	2855	G
78	t	2857	G
78	t	2858	A
78	t	2859	U
78	t	2860	A
78	t	2863	G
78	t	2867	G
78	t	2871	C
78	t	2879	U

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Mol	Chain	Res	Type
78	t	3571	G
78	t	3572	C
78	t	3573	C
78	t	3574	G
78	t	3577	U
78	t	3586	G
78	t	3587	U
78	t	3590	G
78	t	3591	G
78	t	3596	G
78	t	3597	G
78	t	3599	G
78	t	3600	A
78	t	3606	A
78	t	3609	G
78	t	3613	A
78	t	3614	A
78	t	3615	U
78	t	3617	A
78	t	3633	A
78	t	3634	A
78	t	3635	G
78	t	3643	G
78	t	3644	C
78	t	3650	U
78	t	3651	U
78	t	3654	C
78	t	3661	U
78	t	3663	A
78	t	3667	C
78	t	3670	C
78	t	3672	C
78	t	3676	G
78	t	3689	A
78	t	3700	U
78	t	3707	A
78	t	3721	G
78	t	3725	G
78	t	3727	A
78	t	3728	G
78	t	3730	A
78	t	3731	A

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Mol	Chain	Res	Type
78	t	3733	U
78	t	3742	C
78	t	3745	A
78	t	3747	G
78	t	3748	G
78	t	3751	G
78	t	3754	A
78	t	3758	G
78	t	3761	U
78	t	3770	A
78	t	3773	U
78	t	3778	A
78	t	3779	C
78	t	3781	C
78	t	3782	G
78	t	3784	A
78	t	3788	A
78	t	3789	U
78	t	3790	G
78	t	3795	A
78	t	3799	A
78	t	3800	G
78	t	3809	U
78	t	3810	G
78	t	3811	U
78	t	3836	A
78	t	3838	A
78	t	3847	A
78	t	3848	A
78	t	3849	C
78	t	3850	G
78	t	3851	G
78	t	3852	G
78	t	3860	G
78	t	3863	U
78	t	3866	G
78	t	3868	G
78	t	3872	A
78	t	3873	A
78	t	3877	A
78	t	3878	G
78	t	3879	A

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Mol	Chain	Res	Type
78	t	3885	U
78	t	3886	U
78	t	3909	G
78	t	3910	G
78	t	4046	G
78	t	4054	G
78	t	4064	G
78	t	4065	G
78	t	4066	C
78	t	4067	G
78	t	4068	A
78	t	4069	G
78	t	4070	C
78	t	4071	C
78	t	4072	C
78	t	4074	A
78	t	4077	G
78	t	4078	G
78	t	4079	C
78	t	4080	U
78	t	4081	C
78	t	4083	C
78	t	4086	U
78	t	4087	U
78	t	4088	C
78	t	4089	U
78	t	4093	G
78	t	4094	C
78	t	4096	A
78	t	4097	A
78	t	4101	C
78	t	4104	G
78	t	4105	C
78	t	4106	C
78	t	4107	C
78	t	4108	G
78	t	4109	G
78	t	4110	C
78	t	4118	G
78	t	4119	A
78	t	4124	C
78	t	4126	C

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Mol	Chain	Res	Type
78	t	4132	A
78	t	4134	A
78	t	4139	C
78	t	4145	G
78	t	4146	G
78	t	4153	G
78	t	4159	G
78	t	4164	U
78	t	4165	A
78	t	4167	A
78	t	4168	C
78	t	4174	A
78	t	4176	A
78	t	4187	G
78	t	4191	U
78	t	4195	A
78	t	4196	A
78	t	4211	G
78	t	4213	A
78	t	4215	A
78	t	4216	G
78	t	4217	A
78	t	4228	G
78	t	4230	A
78	t	4235	A
78	t	4242	A
78	t	4243	A
78	t	4247	U
78	t	4250	C
78	t	4251	U
78	t	4252	U
78	t	4253	G
78	t	4264	U
78	t	4266	A
78	t	4267	G
78	t	4268	U
78	t	4275	A
78	t	4276	C
78	t	4291	G
78	t	4292	G
78	t	4294	C
78	t	4300	G

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Mol	Chain	Res	Type
78	t	4301	A
78	t	4311	C
78	t	4316	U
78	t	4319	G
78	t	4326	G
78	t	4333	G
78	t	4334	U
78	t	4338	A
78	t	4339	G
78	t	4340	A
78	t	4341	A
78	t	4342	A
78	t	4344	G
78	t	4349	C
78	t	4353	G
78	t	4355	G
78	t	4356	A
78	t	4357	U
78	t	4360	C
78	t	4367	G
78	t	4372	G
78	t	4384	A
78	t	4386	A
78	t	4388	C
78	t	4395	G
78	t	4406	C
78	t	4408	U
78	t	4410	G
78	t	4412	U
78	t	4414	U
78	t	4415	C
78	t	4426	A
78	t	4428	C
78	t	4433	U
78	t	4437	G
78	t	4446	G
78	t	4454	U
78	t	4455	U
78	t	4457	G
78	t	4459	U
78	t	4461	G
78	t	4462	U

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Mol	Chain	Res	Type
78	t	4474	U
78	t	4475	A
78	t	4480	A
78	t	4486	G
78	t	4490	G
78	t	4492	U
78	t	4494	U
78	t	4510	A
78	t	4517	U
78	t	4522	C
78	t	4529	G
78	t	4532	G
78	t	4547	U
78	t	4550	U
78	t	4551	A
78	t	4552	A
78	t	4561	A
78	t	4570	G
78	t	4576	G
78	t	4579	G
78	t	4586	A
78	t	4592	G
78	t	4593	G
78	t	4597	A
78	t	4598	U
78	t	4599	G
78	t	4601	G
78	t	4614	G
78	t	4617	A
78	t	4618	A
78	t	4623	G
78	t	4629	C
78	t	4632	C
78	t	4633	C
78	t	4640	G
78	t	4641	G
78	t	4649	A
78	t	4656	G
78	t	4657	C
78	t	4662	A
78	t	4665	U
78	t	4671	U

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Mol	Chain	Res	Type
78	t	4681	G
78	t	4686	A
78	t	4692	C
78	t	4693	G
78	t	4694	G
78	t	4695	C
78	t	4696	A
78	t	4697	G
78	t	4703	C
78	t	4704	G
78	t	4711	C
78	t	4714	U
78	t	4715	U
78	t	4716	G
78	t	4718	C
78	t	4720	U
78	t	4722	G
78	t	4726	A
78	t	4732	U
78	t	4736	C
78	t	4737	G
78	t	4816	C
78	t	4817	G
78	t	4821	G
78	t	4824	C
78	t	4827	U
78	t	4828	G
78	t	4831	G
78	t	4832	A
78	t	4833	G
78	t	4834	U
78	t	4837	C
78	t	4838	C
78	t	4840	U
78	t	4841	C
78	t	4847	G
78	t	4848	G
78	t	4852	A
78	t	4853	C
78	t	4854	G
78	t	4855	G
78	t	4857	G

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Mol	Chain	Res	Type
78	t	4858	C
78	t	4859	G
78	t	4860	C
78	t	4864	C
78	t	4865	G
78	t	4866	G
78	t	4867	A
78	t	4868	A
78	t	4869	A
78	t	4871	G
78	t	4874	G
78	t	4880	C
78	t	4882	C
78	t	4883	U
78	t	4886	C
78	t	4889	G
78	t	4894	G
78	t	4895	C
78	t	4896	A
78	t	4897	C
78	t	4901	A
78	t	4907	G
78	t	4908	U
78	t	4909	G
78	t	4914	A
78	t	4915	C
78	t	4916	C
78	t	4918	G
78	t	4921	G
78	t	4923	U
78	t	4924	A
78	t	4926	A
78	t	4934	U
78	t	4938	C
78	t	4943	U
78	t	4946	U
78	t	4947	U
78	t	4948	C
78	t	4949	U
78	t	4950	G
78	t	4954	C
78	t	4957	G

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Mol	Chain	Res	Type
78	t	4965	A
78	t	4971	C
78	t	4972	A
78	t	4975	G
78	t	4982	C
78	t	4983	C
78	t	4984	U
78	t	4985	C
78	t	4986	G
78	t	4999	G
78	t	5007	G
78	t	5008	C
78	t	5012	C
78	t	5013	G
78	t	5014	A
78	t	5015	C
78	t	5016	A
78	t	5017	C
78	t	5019	A
78	t	5020	G
78	t	5021	G
78	t	5027	U
79	v	2	G
79	v	3	C
79	v	5	C
79	v	8	U
79	v	10	G
79	v	15	G
79	v	16	A
79	v	19	G
79	v	20	U
79	v	23	A
79	v	24	G
79	v	25	C
79	v	27	G
79	v	29	G
79	v	30	G
79	v	36	G
79	v	43	C
79	v	47	U
79	v	48	C
79	v	49	C

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Mol	Chain	Res	Type
79	v	50	U
79	v	51	U
79	v	52	G
79	v	54	U
79	v	58	A
79	v	61	C
79	v	62	C
79	v	63	G
79	v	64	A
79	v	66	U
79	v	68	C
79	v	69	G
79	v	70	G
79	v	71	G
79	v	72	C
79	v	73	A
79	v	76	A
80	w	15	A
80	w	21	G
80	w	22	U
82	u	2	C
82	u	4	C
82	u	5	G
82	u	6	G
82	u	7	A
82	u	8	U
82	u	10	G
82	u	11	C
82	u	13	C
82	u	17	C
82	u	18	G
82	u	19	G
82	u	20	U
82	u	21	A
82	u	24	G
82	u	25	C
82	u	31	A
82	u	33	U
82	u	36	G
82	u	38	A
82	u	43	C
82	u	44	G

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Mol	Chain	Res	Type
82	u	46	G
82	u	47	U
82	u	48	C
82	u	49	C
82	u	51	U
82	u	52	G
82	u	55	U
82	u	56	C
82	u	57	G
82	u	58	A
82	u	59	U
82	u	60	U
82	u	61	C
82	u	62	C
82	u	63	G
82	u	64	A
82	u	70	G
82	u	72	C
82	u	73	A
82	u	74	C
82	u	75	C

All (26) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	53	C
1	S2	79	A
1	S2	196	C
1	S2	205	G
1	S2	292	A
1	S2	304	C
1	S2	317	C
1	S2	445	A
1	S2	536	A
1	S2	559	G
1	S2	563	G
1	S2	814	5MU
1	S2	823	PSU
1	S2	872	A
1	S2	1375	G
1	S2	1556	A
1	S2	1567	G

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Mol	Chain	Res	Type
1	S2	1572	C
1	S2	1600	G
1	S2	1661	A
1	S2	1681	U
1	S2	1749	G
1	S2	1802	C
1	S2	1813	A
1	S2	1815	A
1	S2	1828	C

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

34 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	$\#\|Z\| > 2$
1	4AC	S2	1337	1	21,24,25	3.36	9 (42%)	28,34,37	1.28	4 (14%)
1	PSU	S2	119	1	18,21,22	4.54	7 (38%)	21,30,33	1.94	4 (19%)
1	MA6	S2	1850	1	19,26,27	1.63	2 (10%)	18,38,41	3.79	4 (22%)
1	E3C	S2	568	1	19,23,24	3.56	7 (36%)	21,33,36	2.73	6 (28%)
1	OMC	S2	1703	1	19,22,23	3.49	8 (42%)	25,31,34	0.80	1 (4%)
1	4AC	S2	1842	85,1	21,24,25	3.32	9 (42%)	28,34,37	1.26	5 (17%)
1	B8Q	S2	1219	1	18,22,23	4.80	7 (38%)	21,32,35	1.76	5 (23%)
1	A2M	S2	1678	1	18,25,26	4.27	6 (33%)	20,36,39	3.26	6 (30%)
1	5MC	S2	1374	1	19,22,23	3.70	8 (42%)	26,32,35	1.11	4 (15%)
1	PSU	S2	612	1	18,21,22	4.42	8 (44%)	21,30,33	2.12	6 (28%)
1	A2M	S2	484	1	18,25,26	4.22	5 (27%)	20,36,39	3.76	5 (25%)
1	PSU	S2	822	1	18,21,22	4.44	8 (44%)	21,30,33	1.96	4 (19%)
1	OMC	S2	174	1	19,22,23	3.59	8 (42%)	25,31,34	0.80	0
1	A2M	S2	27	1	18,25,26	4.21	5 (27%)	20,36,39	3.51	5 (25%)
1	UR3	S2	1830	1	19,22,23	2.61	6 (31%)	26,32,35	2.82	8 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMG	S2	683	1	19,26,27	2.42	8 (42%)	21,38,41	1.41	4 (19%)
1	A2M	S2	159	1	18,25,26	4.23	6 (33%)	20,36,39	3.72	9 (45%)
1	PSU	S2	823	1	18,21,22	4.43	8 (44%)	21,30,33	2.14	5 (23%)
1	5MU	S2	814	1	19,22,23	7.62	8 (42%)	27,32,35	3.52	11 (40%)
1	PSU	S2	1243	1	18,21,22	4.40	8 (44%)	21,30,33	1.76	4 (19%)
1	M7A	S2	1806	1	19,25,26	1.66	2 (10%)	25,37,40	3.69	8 (32%)
1	6MZ	S2	1832	1	17,25,26	1.42	3 (17%)	15,36,39	1.99	3 (20%)
1	A2M	S2	668	1	18,25,26	4.06	5 (27%)	20,36,39	4.20	8 (40%)
1	OMU	S2	116	1	19,22,23	3.16	6 (31%)	25,31,34	1.88	5 (20%)
1	OMG	S2	509	1	19,26,27	2.47	7 (36%)	21,38,41	1.41	4 (19%)
1	PSU	S2	1081	1	18,21,22	4.37	8 (44%)	21,30,33	1.99	5 (23%)
1	OMU	S2	121	1	19,22,23	3.10	7 (36%)	25,31,34	1.99	5 (20%)
1	OMC	S2	517	1	19,22,23	3.54	8 (42%)	25,31,34	0.85	1 (4%)
1	B8N	S2	1248	1	25,29,30	3.11	6 (24%)	28,42,45	2.17	9 (32%)
1	MA6	S2	1851	1	19,26,27	1.77	2 (10%)	18,38,41	3.76	4 (22%)
1	A2M	S2	166	1	18,25,26	4.28	6 (33%)	20,36,39	3.55	6 (30%)
1	OMG	S2	644	1	19,26,27	2.50	8 (42%)	21,38,41	1.43	4 (19%)
1	A2M	S2	1031	1	18,25,26	4.10	5 (27%)	20,36,39	3.68	6 (30%)
1	OMC	S2	1710	1	19,22,23	3.57	8 (42%)	25,31,34	0.73	0

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
1	4AC	S2	1337	1	-	0/11/29/30	0/2/2/2
1	PSU	S2	119	1	-	1/7/25/26	0/2/2/2
1	MA6	S2	1850	1	-	4/7/29/30	0/3/3/3
1	E3C	S2	568	1	-	4/9/44/45	0/2/2/2
1	OMC	S2	1703	1	-	1/9/27/28	0/2/2/2
1	4AC	S2	1842	85,1	-	0/11/29/30	0/2/2/2
1	B8Q	S2	1219	1	-	0/7/42/43	0/2/2/2
1	A2M	S2	1678	1	-	0/5/27/28	0/3/3/3
1	5MC	S2	1374	1	-	1/7/25/26	0/2/2/2
1	PSU	S2	612	1	-	1/7/25/26	0/2/2/2
1	A2M	S2	484	1	-	1/5/27/28	0/3/3/3
1	PSU	S2	822	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	S2	174	1	-	0/9/27/28	0/2/2/2
1	A2M	S2	27	1	-	1/5/27/28	0/3/3/3
1	UR3	S2	1830	1	-	7/7/25/26	0/2/2/2
1	OMG	S2	683	1	-	2/5/27/28	0/3/3/3
1	A2M	S2	159	1	-	4/5/27/28	0/3/3/3
1	PSU	S2	823	1	-	3/7/25/26	0/2/2/2
1	5MU	S2	814	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1243	1	-	2/7/25/26	0/2/2/2
1	M7A	S2	1806	1	-	3/7/37/38	0/3/3/3
1	6MZ	S2	1832	1	-	2/5/27/28	0/3/3/3
1	A2M	S2	668	1	-	2/5/27/28	0/3/3/3
1	OMU	S2	116	1	-	2/9/27/28	0/2/2/2
1	OMG	S2	509	1	-	1/5/27/28	0/3/3/3
1	PSU	S2	1081	1	-	2/7/25/26	0/2/2/2
1	OMU	S2	121	1	-	3/9/27/28	0/2/2/2
1	OMC	S2	517	1	-	2/9/27/28	0/2/2/2
1	B8N	S2	1248	1	-	0/16/34/35	0/2/2/2
1	MA6	S2	1851	1	-	4/7/29/30	0/3/3/3
1	A2M	S2	166	1	-	0/5/27/28	0/3/3/3
1	OMG	S2	644	1	-	2/5/27/28	0/3/3/3
1	A2M	S2	1031	1	-	3/5/27/28	0/3/3/3
1	OMC	S2	1710	1	-	0/9/27/28	0/2/2/2

All (222) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	814	5MU	C4-C5	22.51	1.81	1.44
1	S2	814	5MU	C6-N1	16.74	1.66	1.38
1	S2	119	PSU	C6-C5	11.92	1.48	1.35
1	S2	814	5MU	C6-C5	-11.87	1.15	1.34
1	S2	166	A2M	O4'-C1'	11.84	1.56	1.40
1	S2	1243	PSU	C6-C5	11.69	1.48	1.35
1	S2	1219	B8Q	C4-N3	11.60	1.66	1.48
1	S2	823	PSU	C6-C5	11.52	1.48	1.35
1	S2	159	A2M	O4'-C1'	11.42	1.55	1.40
1	S2	822	PSU	C6-C5	11.32	1.47	1.35
1	S2	484	A2M	O4'-C1'	11.26	1.55	1.40
1	S2	27	A2M	O4'-C1'	11.22	1.55	1.40
1	S2	1678	A2M	O4'-C1'	11.19	1.55	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1219	B8Q	C6-C5	11.10	1.56	1.33
1	S2	814	5MU	C4-N3	-11.09	1.18	1.38
1	S2	1081	PSU	C6-C5	11.07	1.47	1.35
1	S2	612	PSU	C6-C5	11.03	1.47	1.35
1	S2	1031	A2M	O4'-C1'	10.88	1.55	1.40
1	S2	668	A2M	O4'-C1'	10.44	1.54	1.40
1	S2	668	A2M	C3'-C4'	-10.38	1.26	1.53
1	S2	27	A2M	C3'-C4'	-10.29	1.26	1.53
1	S2	166	A2M	C3'-C4'	-10.19	1.27	1.53
1	S2	1678	A2M	C3'-C4'	-10.10	1.27	1.53
1	S2	484	A2M	C3'-C4'	-10.03	1.27	1.53
1	S2	1031	A2M	C3'-C4'	-10.01	1.27	1.53
1	S2	159	A2M	C3'-C4'	-9.85	1.28	1.53
1	S2	1219	B8Q	C2-N1	9.71	1.51	1.38
1	S2	119	PSU	C2-N1	9.67	1.49	1.36
1	S2	612	PSU	C2-N1	9.48	1.49	1.36
1	S2	822	PSU	C2-N1	9.42	1.48	1.36
1	S2	1081	PSU	C2-N1	9.35	1.48	1.36
1	S2	823	PSU	C2-N1	9.16	1.48	1.36
1	S2	1243	PSU	C2-N1	9.09	1.48	1.36
1	S2	1374	5MC	C6-C5	9.04	1.49	1.34
1	S2	1703	OMC	C4-N4	8.54	1.54	1.33
1	S2	174	OMC	C4-N4	8.38	1.54	1.33
1	S2	1710	OMC	C4-N4	8.37	1.54	1.33
1	S2	517	OMC	C4-N4	8.32	1.54	1.33
1	S2	116	OMU	C2-N1	8.28	1.51	1.38
1	S2	1842	4AC	C4-N3	8.11	1.46	1.32
1	S2	1248	B8N	C4-N3	-8.09	1.26	1.40
1	S2	568	E3C	C6-C5	7.96	1.49	1.33
1	S2	568	E3C	C2-N3	7.95	1.47	1.37
1	S2	568	E3C	C2-N1	7.89	1.49	1.38
1	S2	1337	4AC	C4-N3	7.81	1.45	1.32
1	S2	1830	UR3	C2-N1	7.80	1.49	1.38
1	S2	612	PSU	C2-N3	7.60	1.50	1.37
1	S2	121	OMU	C2-N1	7.57	1.50	1.38
1	S2	823	PSU	C2-N3	7.52	1.49	1.37
1	S2	1248	B8N	C6-N1	7.35	1.54	1.36
1	S2	119	PSU	C2-N3	7.25	1.49	1.37
1	S2	174	OMC	C2-N3	6.98	1.50	1.36
1	S2	1081	PSU	C2-N3	6.94	1.48	1.37
1	S2	1243	PSU	C2-N3	6.89	1.48	1.37
1	S2	517	OMC	C6-C5	6.84	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	822	PSU	C2-N3	6.81	1.48	1.37
1	S2	1248	B8N	C4-C5	6.81	1.63	1.47
1	S2	1710	OMC	C2-N3	6.77	1.49	1.36
1	S2	174	OMC	C6-C5	6.77	1.50	1.35
1	S2	121	OMU	C2-N3	6.73	1.49	1.38
1	S2	1710	OMC	C6-C5	6.66	1.50	1.35
1	S2	517	OMC	C2-N3	6.65	1.49	1.36
1	S2	116	OMU	C2-N3	6.53	1.49	1.38
1	S2	1703	OMC	C6-C5	6.52	1.50	1.35
1	S2	1703	OMC	C2-N3	6.51	1.49	1.36
1	S2	1374	5MC	C5-C4	6.46	1.49	1.44
1	S2	1842	4AC	C2-N3	6.37	1.49	1.36
1	S2	1374	5MC	C4-N3	6.28	1.44	1.34
1	S2	1337	4AC	C2-N3	6.26	1.48	1.36
1	S2	1710	OMC	C4-N3	6.25	1.46	1.34
1	S2	174	OMC	C4-N3	6.11	1.46	1.34
1	S2	116	OMU	C6-C5	6.05	1.49	1.35
1	S2	1678	A2M	C3'-C2'	6.02	1.66	1.53
1	S2	121	OMU	C6-C5	5.99	1.49	1.35
1	S2	484	A2M	C3'-C2'	5.98	1.66	1.53
1	S2	159	A2M	C3'-C2'	5.95	1.66	1.53
1	S2	1374	5MC	C2-N3	5.92	1.48	1.36
1	S2	1703	OMC	C4-N3	5.89	1.46	1.34
1	S2	1851	MA6	C6-C5	-5.87	1.35	1.44
1	S2	517	OMC	C4-N3	5.82	1.46	1.34
1	S2	1337	4AC	C6-C5	5.79	1.48	1.35
1	S2	1248	B8N	C2-N1	5.75	1.56	1.39
1	S2	668	A2M	C3'-C2'	5.73	1.65	1.53
1	S2	27	A2M	C3'-C2'	5.55	1.65	1.53
1	S2	644	OMG	C2-N3	5.51	1.46	1.33
1	S2	1842	4AC	C6-C5	5.48	1.47	1.35
1	S2	509	OMG	C2-N3	5.44	1.46	1.33
1	S2	683	OMG	C2-N3	5.38	1.46	1.33
1	S2	166	A2M	C3'-C2'	5.32	1.64	1.53
1	S2	1031	A2M	C3'-C2'	5.29	1.64	1.53
1	S2	814	5MU	C2-N3	5.26	1.47	1.38
1	S2	823	PSU	O2-C2	-5.17	1.12	1.23
1	S2	1850	MA6	C6-C5	-5.17	1.36	1.44
1	S2	822	PSU	O2-C2	-5.16	1.12	1.23
1	S2	568	E3C	C4-N3	5.10	1.56	1.48
1	S2	1081	PSU	O2-C2	-5.06	1.12	1.23
1	S2	509	OMG	C4-N3	5.06	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1243	PSU	O2-C2	-5.02	1.12	1.23
1	S2	644	OMG	C4-N3	4.99	1.49	1.37
1	S2	121	OMU	C4-N3	4.97	1.47	1.38
1	S2	1219	B8Q	C2-N3	-4.94	1.26	1.35
1	S2	1081	PSU	O4-C4	-4.91	1.14	1.23
1	S2	612	PSU	O4-C4	-4.87	1.14	1.23
1	S2	166	A2M	O4'-C4'	4.86	1.55	1.45
1	S2	1337	4AC	C2-N1	4.86	1.50	1.40
1	S2	1678	A2M	O4'-C4'	4.85	1.55	1.45
1	S2	822	PSU	O4-C4	-4.84	1.14	1.23
1	S2	1806	M7A	C6-N6	4.82	1.46	1.34
1	S2	119	PSU	O2-C2	-4.81	1.13	1.23
1	S2	683	OMG	C2-N2	4.81	1.45	1.34
1	S2	683	OMG	C4-N3	4.79	1.48	1.37
1	S2	612	PSU	O2-C2	-4.77	1.13	1.23
1	S2	116	OMU	C4-N3	4.77	1.46	1.38
1	S2	1243	PSU	O4-C4	-4.76	1.14	1.23
1	S2	1842	4AC	C7-N4	4.76	1.46	1.37
1	S2	27	A2M	O4'-C4'	4.74	1.55	1.45
1	S2	119	PSU	O4-C4	-4.73	1.14	1.23
1	S2	159	A2M	O4'-C4'	4.73	1.55	1.45
1	S2	1337	4AC	C7-N4	4.71	1.46	1.37
1	S2	1031	A2M	O4'-C4'	4.69	1.55	1.45
1	S2	1248	B8N	C6-C5	4.65	1.41	1.35
1	S2	484	A2M	O4'-C4'	4.62	1.55	1.45
1	S2	644	OMG	C2-N2	4.60	1.44	1.34
1	S2	509	OMG	C2-N2	4.57	1.44	1.34
1	S2	1842	4AC	C2-N1	4.53	1.49	1.40
1	S2	1219	B8Q	C4-C5	-4.46	1.39	1.49
1	S2	1830	UR3	C6-C5	4.43	1.45	1.35
1	S2	1337	4AC	C4-N4	4.41	1.46	1.39
1	S2	1830	UR3	C2-N3	4.33	1.47	1.39
1	S2	1374	5MC	C4-N4	4.30	1.45	1.34
1	S2	1678	A2M	C6-N6	4.27	1.49	1.34
1	S2	119	PSU	C6-N1	4.25	1.43	1.36
1	S2	822	PSU	C6-N1	4.24	1.43	1.36
1	S2	174	OMC	C2-N1	4.24	1.49	1.40
1	S2	1081	PSU	C6-N1	4.17	1.43	1.36
1	S2	1374	5MC	C6-N1	4.14	1.45	1.38
1	S2	668	A2M	O4'-C4'	4.08	1.54	1.45
1	S2	1374	5MC	C2-N1	4.08	1.48	1.40
1	S2	1710	OMC	C2-N1	4.07	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	612	PSU	C6-N1	4.02	1.42	1.36
1	S2	517	OMC	C2-N1	4.02	1.48	1.40
1	S2	1842	4AC	C4-N4	4.01	1.45	1.39
1	S2	166	A2M	C6-N6	3.97	1.48	1.34
1	S2	1031	A2M	C6-N6	3.95	1.48	1.34
1	S2	159	A2M	C6-N6	3.95	1.48	1.34
1	S2	27	A2M	C6-N6	3.92	1.48	1.34
1	S2	1243	PSU	C6-N1	3.88	1.42	1.36
1	S2	1337	4AC	C6-N1	3.84	1.47	1.38
1	S2	668	A2M	C6-N6	3.83	1.47	1.34
1	S2	517	OMC	C6-N1	3.83	1.47	1.38
1	S2	1337	4AC	C5-C4	3.82	1.49	1.41
1	S2	823	PSU	C6-N1	3.81	1.42	1.36
1	S2	1806	M7A	C5-N7	3.77	1.48	1.39
1	S2	484	A2M	C6-N6	3.77	1.47	1.34
1	S2	1703	OMC	C6-N1	3.75	1.47	1.38
1	S2	174	OMC	C6-N1	3.73	1.47	1.38
1	S2	1842	4AC	C5-C4	3.72	1.49	1.41
1	S2	1710	OMC	C6-N1	3.71	1.46	1.38
1	S2	1851	MA6	C6-N6	3.58	1.45	1.37
1	S2	1842	4AC	C6-N1	3.56	1.46	1.38
1	S2	644	OMG	C6-N1	3.48	1.43	1.37
1	S2	823	PSU	O4-C4	-3.48	1.17	1.23
1	S2	814	5MU	C2-N1	3.45	1.43	1.38
1	S2	823	PSU	C4-N3	3.44	1.45	1.38
1	S2	509	OMG	C6-N1	3.33	1.42	1.37
1	S2	1850	MA6	C6-N6	3.31	1.45	1.37
1	S2	1703	OMC	C2-N1	3.31	1.47	1.40
1	S2	644	OMG	C5-C6	3.20	1.53	1.47
1	S2	119	PSU	C4-N3	3.12	1.44	1.38
1	S2	509	OMG	C5-C6	3.11	1.53	1.47
1	S2	683	OMG	C6-N1	3.10	1.42	1.37
1	S2	612	PSU	C4-N3	3.05	1.44	1.38
1	S2	683	OMG	C5-C4	-3.05	1.35	1.43
1	S2	1830	UR3	O2-C2	-3.04	1.16	1.22
1	S2	1832	6MZ	C6-C5	-3.03	1.40	1.44
1	S2	1219	B8Q	C31-N3	3.00	1.52	1.46
1	S2	1832	6MZ	C2-N3	3.00	1.36	1.32
1	S2	568	E3C	C6-N1	2.96	1.45	1.38
1	S2	823	PSU	O4'-C1'	-2.90	1.39	1.43
1	S2	568	E3C	C31-N3	2.90	1.55	1.47
1	S2	822	PSU	C4-N3	2.89	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1081	PSU	C4-N3	2.85	1.44	1.38
1	S2	1243	PSU	C4-N3	2.83	1.44	1.38
1	S2	612	PSU	O4'-C1'	-2.79	1.40	1.43
1	S2	644	OMG	C2-N1	2.74	1.44	1.37
1	S2	822	PSU	O4'-C1'	-2.74	1.40	1.43
1	S2	116	OMU	C6-N1	2.71	1.44	1.38
1	S2	509	OMG	C5-C4	-2.71	1.36	1.43
1	S2	1374	5MC	O2-C2	-2.70	1.18	1.23
1	S2	1703	OMC	O2-C2	-2.64	1.18	1.23
1	S2	1830	UR3	C6-N1	2.59	1.44	1.38
1	S2	568	E3C	C4-C5	-2.58	1.44	1.49
1	S2	644	OMG	C5-C4	-2.55	1.36	1.43
1	S2	121	OMU	C6-N1	2.53	1.44	1.38
1	S2	509	OMG	C2-N1	2.52	1.43	1.37
1	S2	1678	A2M	C2-N3	2.51	1.36	1.32
1	S2	1219	B8Q	C6-N1	-2.44	1.32	1.38
1	S2	517	OMC	O2-C2	-2.43	1.19	1.23
1	S2	1248	B8N	O4-C4	-2.41	1.18	1.23
1	S2	814	5MU	O2-C2	-2.36	1.18	1.23
1	S2	814	5MU	O4-C4	-2.35	1.19	1.23
1	S2	683	OMG	C2-N1	2.32	1.43	1.37
1	S2	1832	6MZ	C9-N6	2.31	1.48	1.45
1	S2	517	OMC	C5-C4	2.30	1.48	1.42
1	S2	1337	4AC	O2-C2	-2.28	1.19	1.23
1	S2	1830	UR3	C4-N3	2.24	1.45	1.40
1	S2	683	OMG	C5-C6	2.24	1.51	1.47
1	S2	116	OMU	O4-C4	-2.23	1.20	1.24
1	S2	174	OMC	O2-C2	-2.23	1.19	1.23
1	S2	1710	OMC	C5-C4	2.19	1.48	1.42
1	S2	1710	OMC	O2-C2	-2.19	1.19	1.23
1	S2	1842	4AC	O2-C2	-2.18	1.19	1.23
1	S2	1703	OMC	C5-C4	2.18	1.48	1.42
1	S2	1081	PSU	O4'-C1'	-2.17	1.40	1.43
1	S2	174	OMC	C5-C4	2.13	1.47	1.42
1	S2	683	OMG	O6-C6	-2.11	1.18	1.23
1	S2	166	A2M	C2-N3	2.11	1.35	1.32
1	S2	121	OMU	O4-C4	-2.11	1.20	1.24
1	S2	644	OMG	O6-C6	-2.05	1.18	1.23
1	S2	121	OMU	C5-C4	2.05	1.48	1.43
1	S2	1243	PSU	O4'-C1'	-2.04	1.41	1.43
1	S2	159	A2M	C2-N3	2.03	1.35	1.32

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	1850	MA6	N1-C6-N6	-13.46	101.28	116.83
1	S2	1851	MA6	N1-C6-N6	-12.96	101.85	116.83
1	S2	1806	M7A	C5-C6-N6	10.92	142.30	123.75
1	S2	668	A2M	C1'-N9-C4	-10.43	108.31	126.64
1	S2	1806	M7A	N6-C6-N1	-9.32	97.62	118.38
1	S2	814	5MU	C5-C4-N3	9.19	123.31	115.32
1	S2	668	A2M	C5-C6-N6	8.84	133.78	120.31
1	S2	159	A2M	C1'-N9-C4	-8.71	111.34	126.64
1	S2	484	A2M	C5-C6-N6	8.68	133.53	120.31
1	S2	27	A2M	C5-C6-N6	8.47	133.22	120.31
1	S2	1031	A2M	C1'-N9-C4	-8.47	111.77	126.64
1	S2	1031	A2M	C5-C6-N6	8.43	133.15	120.31
1	S2	1830	UR3	C4-N3-C2	-8.22	117.97	124.58
1	S2	484	A2M	C1'-N9-C4	-8.17	112.29	126.64
1	S2	166	A2M	C5-C6-N6	8.13	132.70	120.31
1	S2	27	A2M	C1'-N9-C4	-8.12	112.38	126.64
1	S2	814	5MU	C5-C6-N1	-8.02	114.60	123.31
1	S2	1678	A2M	C1'-N9-C4	-7.89	112.79	126.64
1	S2	159	A2M	C5-C6-N6	7.86	132.28	120.31
1	S2	166	A2M	C1'-N9-C4	-7.79	112.96	126.64
1	S2	484	A2M	C4'-O4'-C1'	-7.42	103.13	109.92
1	S2	668	A2M	C4'-O4'-C1'	-7.41	103.14	109.92
1	S2	568	E3C	C1'-N1-C2	7.32	129.02	117.04
1	S2	1678	A2M	C5-C6-N6	7.16	131.22	120.31
1	S2	814	5MU	C4-N3-C2	-7.03	118.12	127.34
1	S2	668	A2M	N3-C2-N1	-6.79	119.45	128.67
1	S2	1851	MA6	N3-C2-N1	-6.75	119.52	128.67
1	S2	1830	UR3	C1'-N1-C2	6.45	127.61	117.04
1	S2	1031	A2M	N3-C2-N1	-6.42	119.96	128.67
1	S2	159	A2M	N3-C2-N1	-6.42	119.96	128.67
1	S2	166	A2M	N3-C2-N1	-6.41	119.97	128.67
1	S2	27	A2M	N3-C2-N1	-6.37	120.03	128.67
1	S2	484	A2M	N3-C2-N1	-6.30	120.12	128.67
1	S2	1806	M7A	N3-C4-N9	6.28	134.74	126.88
1	S2	166	A2M	C4'-O4'-C1'	-6.19	104.26	109.92
1	S2	1678	A2M	N3-C2-N1	-6.17	120.29	128.67
1	S2	1031	A2M	C4'-O4'-C1'	-6.08	104.36	109.92
1	S2	668	A2M	N6-C6-N1	-6.08	105.35	118.33
1	S2	1850	MA6	N3-C2-N1	-6.03	120.48	128.67
1	S2	121	OMU	C4-N3-C2	-5.94	119.23	126.61
1	S2	1832	6MZ	N3-C2-N1	-5.94	120.61	128.67
1	S2	27	A2M	N6-C6-N1	-5.74	106.07	118.33
1	S2	484	A2M	N6-C6-N1	-5.64	106.28	118.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	1806	M7A	N3-C2-N1	-5.56	120.17	128.58
1	S2	814	5MU	N3-C2-N1	5.48	122.03	114.89
1	S2	568	E3C	O2-C2-N3	-5.46	115.11	122.10
1	S2	1031	A2M	N6-C6-N1	-5.38	106.85	118.33
1	S2	1248	B8N	C5-C4-N3	5.31	125.80	116.15
1	S2	116	OMU	C4-N3-C2	-5.24	120.10	126.61
1	S2	1081	PSU	C4-N3-C2	-5.17	119.25	126.37
1	S2	814	5MU	C5M-C5-C6	-5.15	115.88	122.85
1	S2	1830	UR3	O2-C2-N3	-5.12	114.26	121.33
1	S2	166	A2M	N6-C6-N1	-5.08	107.47	118.33
1	S2	159	A2M	N6-C6-N1	-5.04	107.56	118.33
1	S2	1248	B8N	C4-N3-C2	-5.03	119.43	125.62
1	S2	159	A2M	C4'-O4'-C1'	-5.01	105.34	109.92
1	S2	822	PSU	C4-N3-C2	-4.93	119.58	126.37
1	S2	1219	B8Q	N3-C2-N1	4.93	124.02	117.16
1	S2	119	PSU	C4-N3-C2	-4.84	119.71	126.37
1	S2	1850	MA6	C1'-N9-C4	4.82	135.12	126.64
1	S2	612	PSU	C4-N3-C2	-4.68	119.92	126.37
1	S2	822	PSU	N1-C2-N3	4.66	120.08	115.17
1	S2	1851	MA6	C2-N1-C6	4.65	121.40	116.84
1	S2	568	E3C	C6-N1-C2	-4.61	118.03	121.80
1	S2	823	PSU	N1-C2-N3	4.60	120.02	115.17
1	S2	1678	A2M	C4'-O4'-C1'	-4.52	105.79	109.92
1	S2	1081	PSU	N1-C2-N3	4.45	119.86	115.17
1	S2	823	PSU	C4-N3-C2	-4.40	120.31	126.37
1	S2	1806	M7A	C4-N9-C1'	-4.37	116.45	126.63
1	S2	823	PSU	O2-C2-N1	-4.36	118.30	122.79
1	S2	612	PSU	N1-C2-N3	4.35	119.75	115.17
1	S2	119	PSU	N1-C2-N3	4.35	119.75	115.17
1	S2	1830	UR3	C6-N1-C2	-4.33	118.26	121.80
1	S2	27	A2M	C4'-O4'-C1'	-4.32	105.97	109.92
1	S2	1678	A2M	N6-C6-N1	-4.32	109.11	118.33
1	S2	814	5MU	C6-C5-C4	4.31	121.57	118.02
1	S2	823	PSU	C6-N1-C2	-4.30	118.70	122.69
1	S2	116	OMU	N3-C2-N1	4.29	120.47	114.89
1	S2	121	OMU	N3-C2-N1	4.26	120.44	114.89
1	S2	568	E3C	C31-N3-C2	4.24	122.81	117.49
1	S2	1243	PSU	C4-N3-C2	-4.11	120.71	126.37
1	S2	1243	PSU	N1-C2-N3	3.98	119.37	115.17
1	S2	814	5MU	O4-C4-C5	-3.90	120.45	124.92
1	S2	612	PSU	C6-C5-C4	3.89	120.80	118.17
1	S2	1830	UR3	C3U-N3-C4	3.85	123.20	117.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	159	A2M	O2'-C2'-C1'	3.84	116.43	109.00
1	S2	1248	B8N	N3-C2-N1	3.84	121.41	116.72
1	S2	1219	B8Q	C31-N3-C4	3.81	121.35	114.76
1	S2	1248	B8N	C31-N3-C4	3.76	122.51	117.18
1	S2	1851	MA6	C1'-N9-C4	3.71	133.17	126.64
1	S2	1806	M7A	C71-N7-C5	-3.71	107.99	123.44
1	S2	1374	5MC	C5-C6-N1	-3.67	119.33	123.31
1	S2	568	E3C	C1'-N1-C6	-3.66	112.95	120.78
1	S2	568	E3C	C4-N3-C2	-3.66	115.41	122.00
1	S2	121	OMU	C5-C4-N3	3.66	119.92	114.80
1	S2	1243	PSU	C6-N1-C2	-3.64	119.31	122.69
1	S2	612	PSU	O2-C2-N1	-3.59	119.09	122.79
1	S2	159	A2M	C2'-C1'-N9	-3.57	104.63	112.56
1	S2	814	5MU	O2-C2-N1	-3.57	118.15	122.80
1	S2	1832	6MZ	C2-N1-C6	3.56	119.36	116.60
1	S2	814	5MU	C5M-C5-C4	3.52	122.54	118.78
1	S2	116	OMU	C5-C4-N3	3.49	119.69	114.80
1	S2	121	OMU	O4-C4-C5	-3.45	119.21	125.16
1	S2	1248	B8N	C1'-C5-C4	3.44	122.83	117.61
1	S2	1850	MA6	C2-N1-C6	3.43	120.20	116.84
1	S2	644	OMG	C2-N1-C6	-3.41	118.87	125.11
1	S2	509	OMG	C2-N1-C6	-3.41	118.87	125.11
1	S2	612	PSU	C6-N1-C2	-3.32	119.61	122.69
1	S2	119	PSU	C6-N1-C2	-3.30	119.63	122.69
1	S2	509	OMG	C8-N7-C5	3.30	108.16	102.55
1	S2	166	A2M	O4'-C1'-C2'	-3.29	101.00	106.61
1	S2	116	OMU	O4-C4-C5	-3.26	119.53	125.16
1	S2	683	OMG	C5-C6-N1	3.24	120.24	114.07
1	S2	1806	M7A	C2-N3-C4	3.22	119.70	111.83
1	S2	822	PSU	C6-N1-C2	-3.20	119.72	122.69
1	S2	1219	B8Q	O2-C2-N3	-3.14	118.54	122.95
1	S2	1830	UR3	C1'-N1-C6	-3.12	114.11	120.78
1	S2	509	OMG	C5-C6-N1	3.12	120.02	114.07
1	S2	644	OMG	C5-C6-N1	3.11	120.01	114.07
1	S2	644	OMG	C8-N7-C5	3.09	107.82	102.55
1	S2	1842	4AC	C6-C5-C4	3.08	120.71	117.00
1	S2	119	PSU	O2-C2-N1	-3.01	119.69	122.79
1	S2	668	A2M	C3'-C2'-C1'	2.97	108.49	102.81
1	S2	1248	B8N	O4-C4-C5	-2.88	117.59	122.58
1	S2	1806	M7A	C5-C4-N3	-2.88	119.91	126.56
1	S2	1337	4AC	C5-C4-N3	-2.86	118.12	122.60
1	S2	1842	4AC	O7-C7-CM7	-2.85	116.98	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	1243	PSU	O2-C2-N1	-2.85	119.85	122.79
1	S2	683	OMG	C2-N1-C6	-2.82	119.94	125.11
1	S2	1081	PSU	C6-N1-C2	-2.81	120.08	122.69
1	S2	822	PSU	O2-C2-N1	-2.80	119.90	122.79
1	S2	121	OMU	O2-C2-N1	-2.78	119.18	122.80
1	S2	116	OMU	C6-N1-C2	-2.78	117.62	121.00
1	S2	1031	A2M	O4'-C1'-C2'	-2.77	101.88	106.61
1	S2	1081	PSU	O2-C2-N1	-2.70	120.01	122.79
1	S2	1830	UR3	C5-C4-N3	2.66	118.54	115.04
1	S2	1337	4AC	C6-C5-C4	2.65	120.19	117.00
1	S2	823	PSU	C6-C5-C4	2.61	119.94	118.17
1	S2	683	OMG	C8-N7-C5	2.59	106.96	102.55
1	S2	814	5MU	O3'-C3'-C2'	2.58	120.10	111.82
1	S2	1248	B8N	O2-C2-N3	-2.58	118.51	121.98
1	S2	1678	A2M	C3'-C2'-C1'	2.56	107.70	102.81
1	S2	1842	4AC	N4-C4-N3	2.54	118.00	113.87
1	S2	1337	4AC	O7-C7-CM7	-2.53	117.55	122.05
1	S2	1830	UR3	O4-C4-N3	2.52	122.72	119.66
1	S2	1219	B8Q	C31-N3-C2	2.49	121.62	117.70
1	S2	683	OMG	O6-C6-C5	-2.42	119.53	124.32
1	S2	1337	4AC	N4-C4-N3	2.41	117.78	113.87
1	S2	1219	B8Q	O2-C2-N1	-2.40	117.44	122.78
1	S2	1081	PSU	C6-C5-C4	2.32	119.74	118.17
1	S2	1842	4AC	C5-C4-N3	-2.28	119.03	122.60
1	S2	1832	6MZ	C6-C5-C4	2.28	120.09	117.68
1	S2	612	PSU	O4'-C1'-C2'	2.26	108.28	105.15
1	S2	159	A2M	C2'-C3'-C4'	2.24	106.81	101.99
1	S2	644	OMG	O6-C6-C5	-2.23	119.91	124.32
1	S2	159	A2M	CM'-O2'-C2'	2.22	120.17	114.47
1	S2	1248	B8N	O36-C34-O35	-2.19	119.10	124.08
1	S2	668	A2M	C5'-C4'-C3'	-2.19	107.34	115.21
1	S2	1374	5MC	CM5-C5-C6	-2.18	119.90	122.85
1	S2	1248	B8N	O4-C4-N3	-2.08	116.60	119.99
1	S2	814	5MU	O4-C4-N3	-2.06	116.24	120.11
1	S2	668	A2M	C2'-C3'-C4'	2.05	106.41	101.99
1	S2	517	OMC	O2-C2-N3	-2.05	119.10	122.33
1	S2	509	OMG	O6-C6-C5	-2.04	120.27	124.32
1	S2	1703	OMC	C1'-N1-C6	2.04	125.13	120.78
1	S2	1842	4AC	O7-C7-N4	2.03	125.10	121.90
1	S2	1374	5MC	C5-C4-N3	-2.03	119.67	121.75
1	S2	1374	5MC	O2-C2-N3	-2.00	119.17	122.33

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S2	27	A2M	C1'-C2'-O2'-CM'
1	S2	116	OMU	C3'-C4'-C5'-O5'
1	S2	116	OMU	O4'-C4'-C5'-O5'
1	S2	159	A2M	O4'-C4'-C5'-O5'
1	S2	159	A2M	C1'-C2'-O2'-CM'
1	S2	509	OMG	C1'-C2'-O2'-CM2
1	S2	568	E3C	O4'-C1'-N1-C2
1	S2	568	E3C	O4'-C1'-N1-C6
1	S2	644	OMG	C1'-C2'-O2'-CM2
1	S2	668	A2M	O4'-C4'-C5'-O5'
1	S2	668	A2M	C3'-C4'-C5'-O5'
1	S2	683	OMG	O4'-C4'-C5'-O5'
1	S2	683	OMG	C3'-C4'-C5'-O5'
1	S2	822	PSU	O4'-C4'-C5'-O5'
1	S2	1031	A2M	C1'-C2'-O2'-CM'
1	S2	1830	UR3	O4'-C1'-N1-C6
1	S2	1830	UR3	O4'-C1'-N1-C2
1	S2	1832	6MZ	C5-C6-N6-C9
1	S2	1832	6MZ	N1-C6-N6-C9
1	S2	1850	MA6	O4'-C4'-C5'-O5'
1	S2	1850	MA6	C3'-C4'-C5'-O5'
1	S2	1850	MA6	C5-C6-N6-C9
1	S2	1851	MA6	O4'-C4'-C5'-O5'
1	S2	1851	MA6	C3'-C4'-C5'-O5'
1	S2	159	A2M	C3'-C4'-C5'-O5'
1	S2	568	E3C	C3'-C4'-C5'-O5'
1	S2	568	E3C	O4'-C4'-C5'-O5'
1	S2	517	OMC	O4'-C4'-C5'-O5'
1	S2	823	PSU	O4'-C4'-C5'-O5'
1	S2	1031	A2M	C3'-C4'-C5'-O5'
1	S2	1850	MA6	N1-C6-N6-C9
1	S2	1830	UR3	C2'-C1'-N1-C6
1	S2	823	PSU	C3'-C4'-C5'-O5'
1	S2	1830	UR3	O4'-C4'-C5'-O5'
1	S2	1830	UR3	C3'-C4'-C5'-O5'
1	S2	121	OMU	C3'-C4'-C5'-O5'
1	S2	517	OMC	C3'-C4'-C5'-O5'
1	S2	822	PSU	C3'-C4'-C5'-O5'
1	S2	1031	A2M	O4'-C4'-C5'-O5'
1	S2	1806	M7A	C3'-C4'-C5'-O5'
1	S2	1806	M7A	O4'-C4'-C5'-O5'
1	S2	121	OMU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	S2	121	OMU	O4'-C4'-C5'-O5'
1	S2	1243	PSU	O4'-C4'-C5'-O5'
1	S2	1703	OMC	O4'-C4'-C5'-O5'
1	S2	484	A2M	O4'-C4'-C5'-O5'
1	S2	1243	PSU	C3'-C4'-C5'-O5'
1	S2	1830	UR3	C2'-C1'-N1-C2
1	S2	1806	M7A	C2'-C1'-N9-C8
1	S2	1081	PSU	C3'-C4'-C5'-O5'
1	S2	1851	MA6	C5-C6-N6-C9
1	S2	159	A2M	C4'-C5'-O5'-P
1	S2	119	PSU	O4'-C1'-C5-C4
1	S2	823	PSU	O4'-C1'-C5-C4
1	S2	1830	UR3	C4'-C5'-O5'-P
1	S2	1851	MA6	C4'-C5'-O5'-P
1	S2	1081	PSU	O4'-C4'-C5'-O5'
1	S2	644	OMG	C4'-C5'-O5'-P
1	S2	612	PSU	O4'-C4'-C5'-O5'
1	S2	1374	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 37 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	$\#\|Z\| > 2$
86	MVM	t	5112	-	32,35,35	1.79	4 (12%)	39,49,49	2.29	16 (41%)

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
86	MVM	t	5112	-	-	0/20/28/28	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	t	5112	MVM	C5-N1	6.27	1.46	1.37
86	t	5112	MVM	N5-N4	-4.43	1.30	1.37
86	t	5112	MVM	C6-N1	2.55	1.45	1.39
86	t	5112	MVM	C12-C5	2.42	1.54	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
86	t	5112	MVM	C21-N7-C22	4.84	122.60	116.81
86	t	5112	MVM	C15-N4-C22	-4.67	124.10	130.09
86	t	5112	MVM	C7-C3-C9	4.54	119.43	110.81
86	t	5112	MVM	C6-N1-C5	-4.30	117.79	122.94
86	t	5112	MVM	N3-C6-N1	3.80	120.41	116.35
86	t	5112	MVM	C1-C9-N1	-3.67	106.93	116.16
86	t	5112	MVM	C19-C18-N6	3.43	135.76	130.19
86	t	5112	MVM	C12-C5-N1	3.33	122.78	118.36
86	t	5112	MVM	C15-N4-N5	3.16	125.01	119.95
86	t	5112	MVM	C8-N3-C6	2.99	121.82	115.05
86	t	5112	MVM	C20-C21-N7	-2.78	119.88	123.97
86	t	5112	MVM	N6-N5-N4	2.66	109.33	106.37
86	t	5112	MVM	C11-C2-C6	2.51	120.84	118.51
86	t	5112	MVM	C6-N1-C9	2.45	122.05	118.40
86	t	5112	MVM	C2-C6-N3	-2.24	119.51	123.00
86	t	5112	MVM	C3-C9-C1	2.03	113.23	110.81

There are no chirality outliers.

There are no torsion outliers.

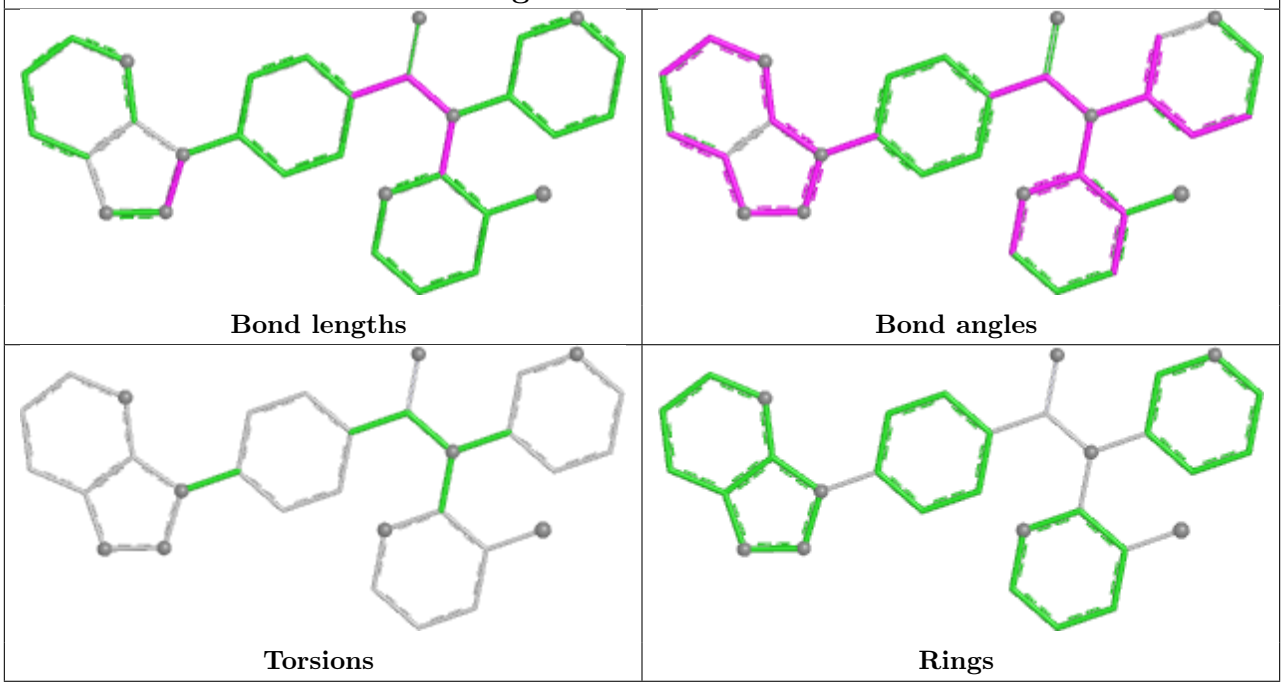
There are no ring outliers.

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 MVM t 5112



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
78	t	16
1	S2	5
79	v	4
62	c	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	26.21
1	t	750:G	O3'	890:C	P	19.49
1	t	3919:C	O3'	4035:G	P	17.88
1	t	1680:C	O3'	1699:C	P	17.58
1	t	517:C	O3'	629:G	P	17.45
1	t	2881:G	O3'	3569:C	P	16.05
1	S2	1752:C	O3'	1779:G	P	15.45
1	t	976:U	O3'	1047:G	P	15.43
1	t	1202:G	O3'	1216:G	P	15.43
1	t	4737:G	O3'	4815:C	P	15.07
1	t	2093:C	O3'	2228:C	P	14.74
1	t	1089:A	O3'	1145:G	P	14.43
1	t	1253:A	O3'	1256:G	P	13.75
1	S2	739:C	O3'	746:C	P	13.39
1	S2	698:G	O3'	730:C	P	12.80
1	S2	225:G	O3'	287:U	P	7.22
1	c	119:CYS	C	120:ARG	N	6.78
1	t	945:G	O3'	946:G	P	6.36
1	t	4734:C	O3'	4735:C	P	4.98
1	v	17:A	O3'	18:G	P	4.55
1	v	21:A	O3'	22:G	P	4.01
1	t	4817:G	O3'	4818:G	P	3.97
1	v	10:G	O3'	11:C	P	3.35
1	t	964:C	O3'	965:G	P	3.31
1	t	1938:U	O3'	1939:A	P	3.27
1	v	41:C	O3'	42:C	P	3.14

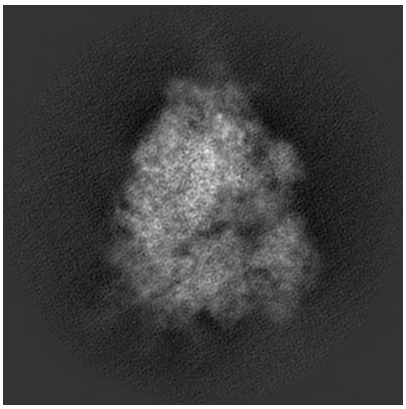
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0599. These allow visual inspection of the internal detail of the map and identification of artifacts.

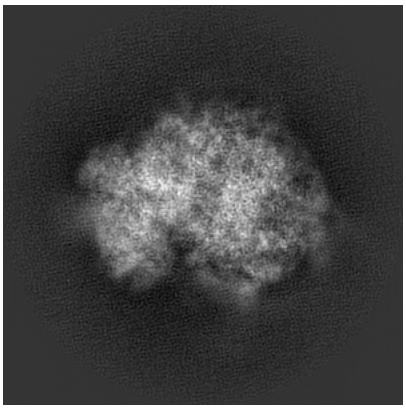
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



X



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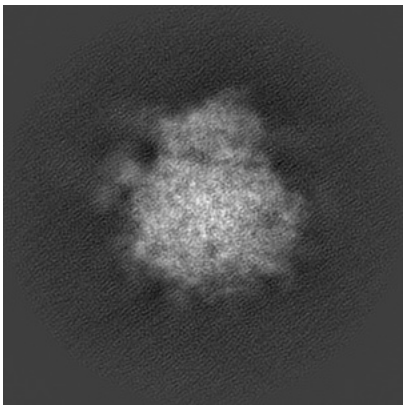
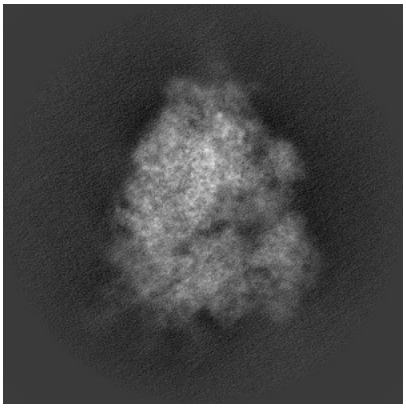
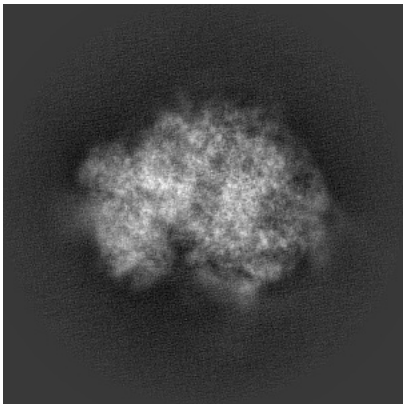


Z

6.1.2 Raw map



X



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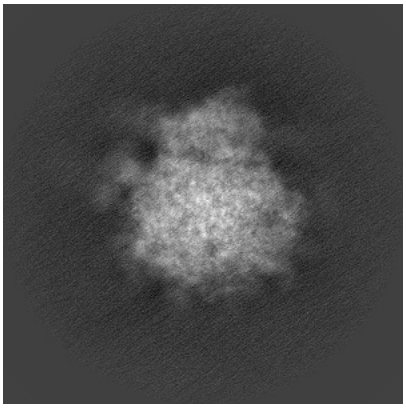
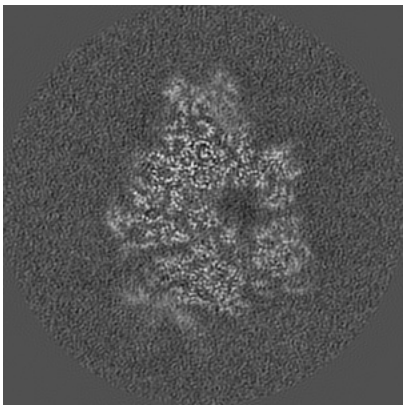


Z

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

6.2 Central slices (i)

6.2.1 Primary map



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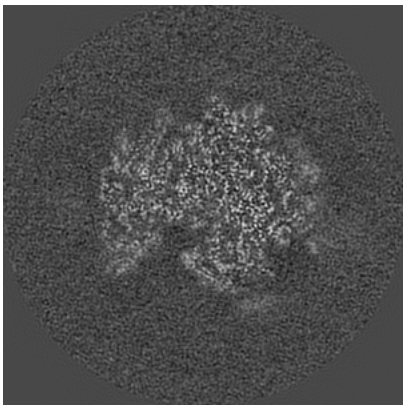
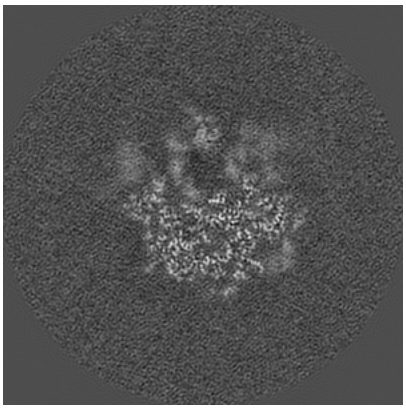
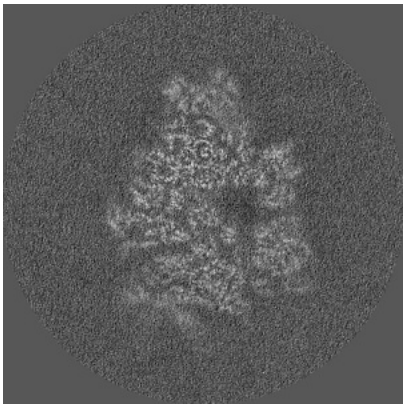


Y Index: 200

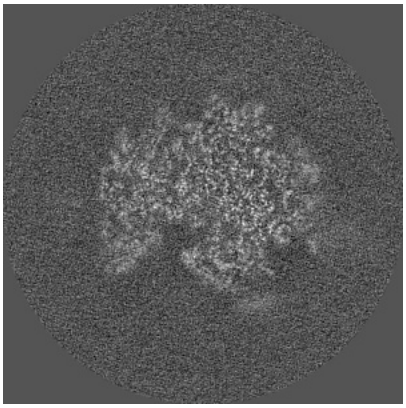


Z Index: 200

6.2.2 Raw map



X Index: 200



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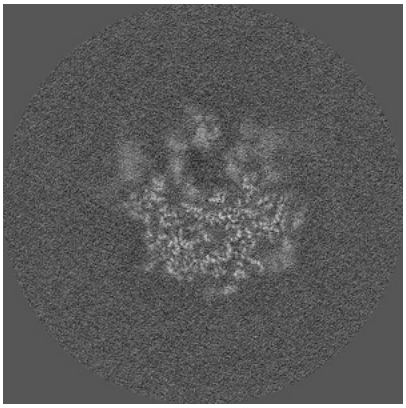
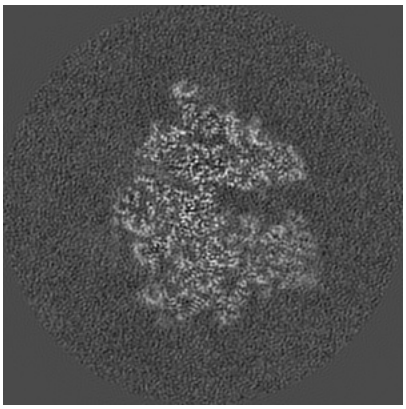


Z Index: 200

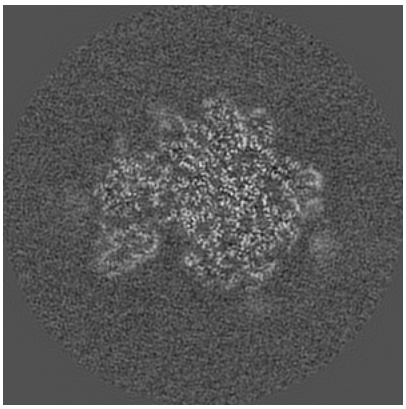
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

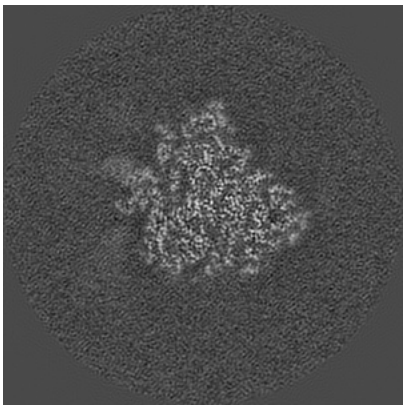
6.3.1 Primary map



X Index: 218

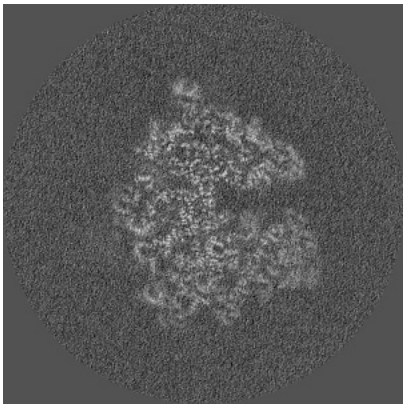


Y Index: 193

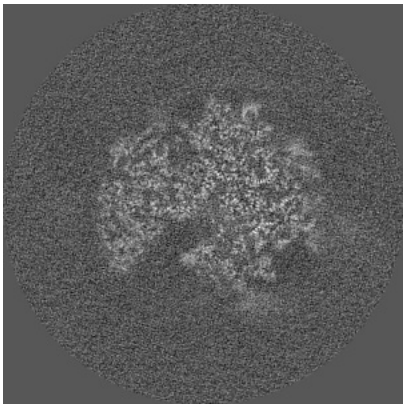


Z Index: 229

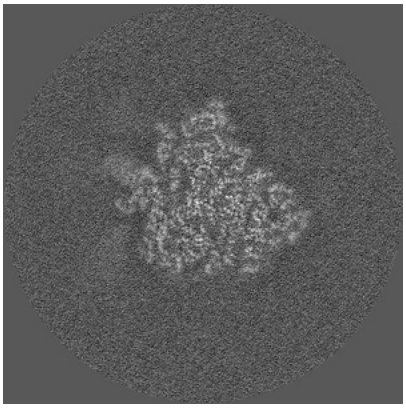
6.3.2 Raw map



X Index: 219



Y Index: 204

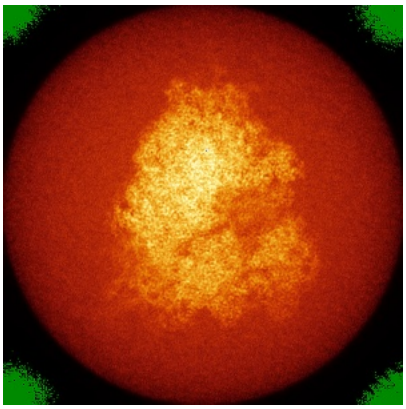


Z Index: 229

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

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map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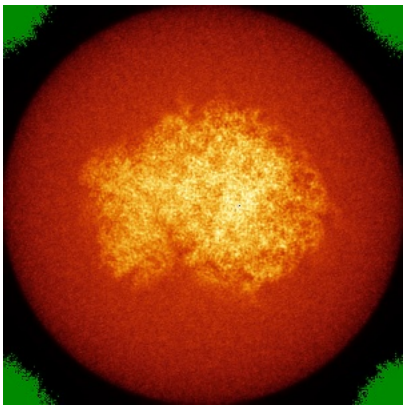
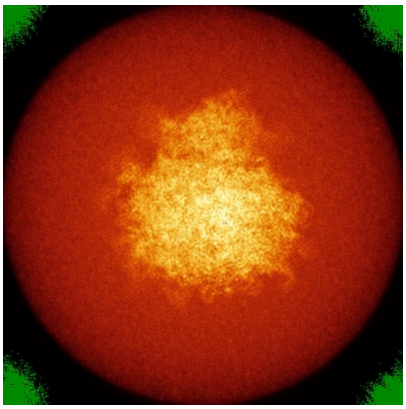
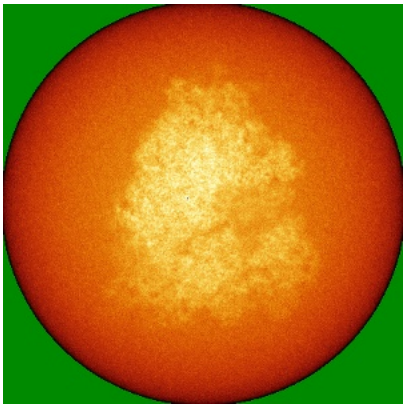
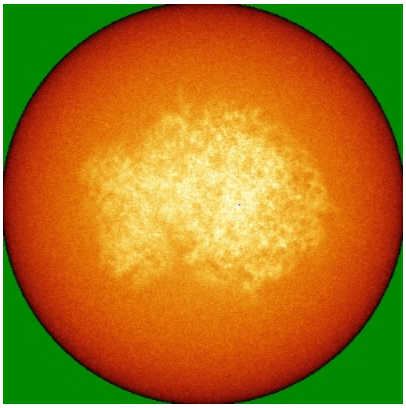
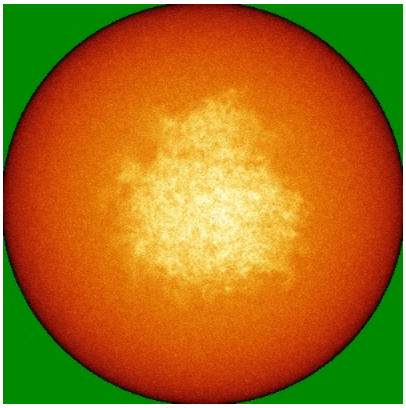

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

6.5.2 Raw map

X Y Z

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

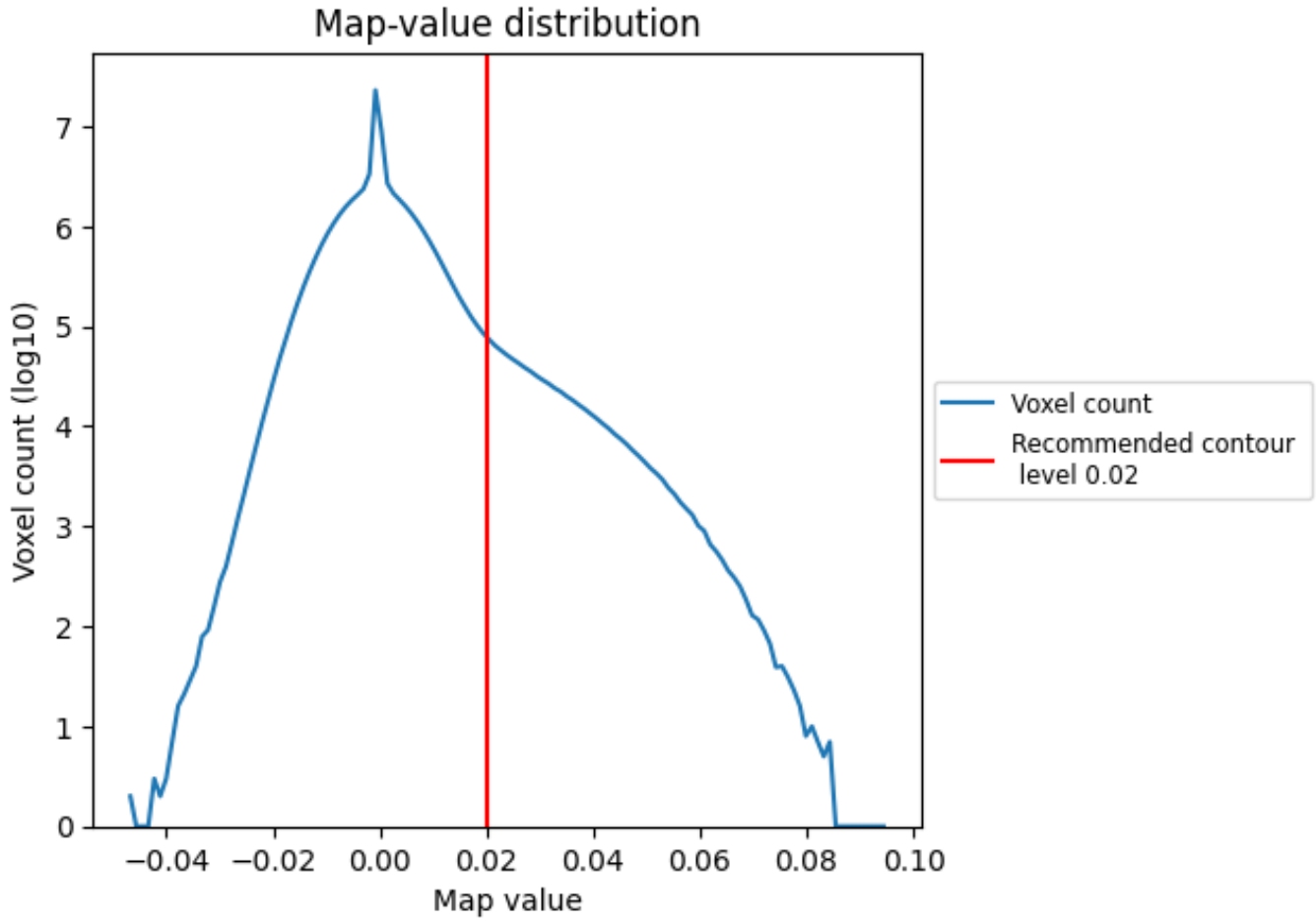
6.6 Mask visualisation (i)

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

7 Map analysis

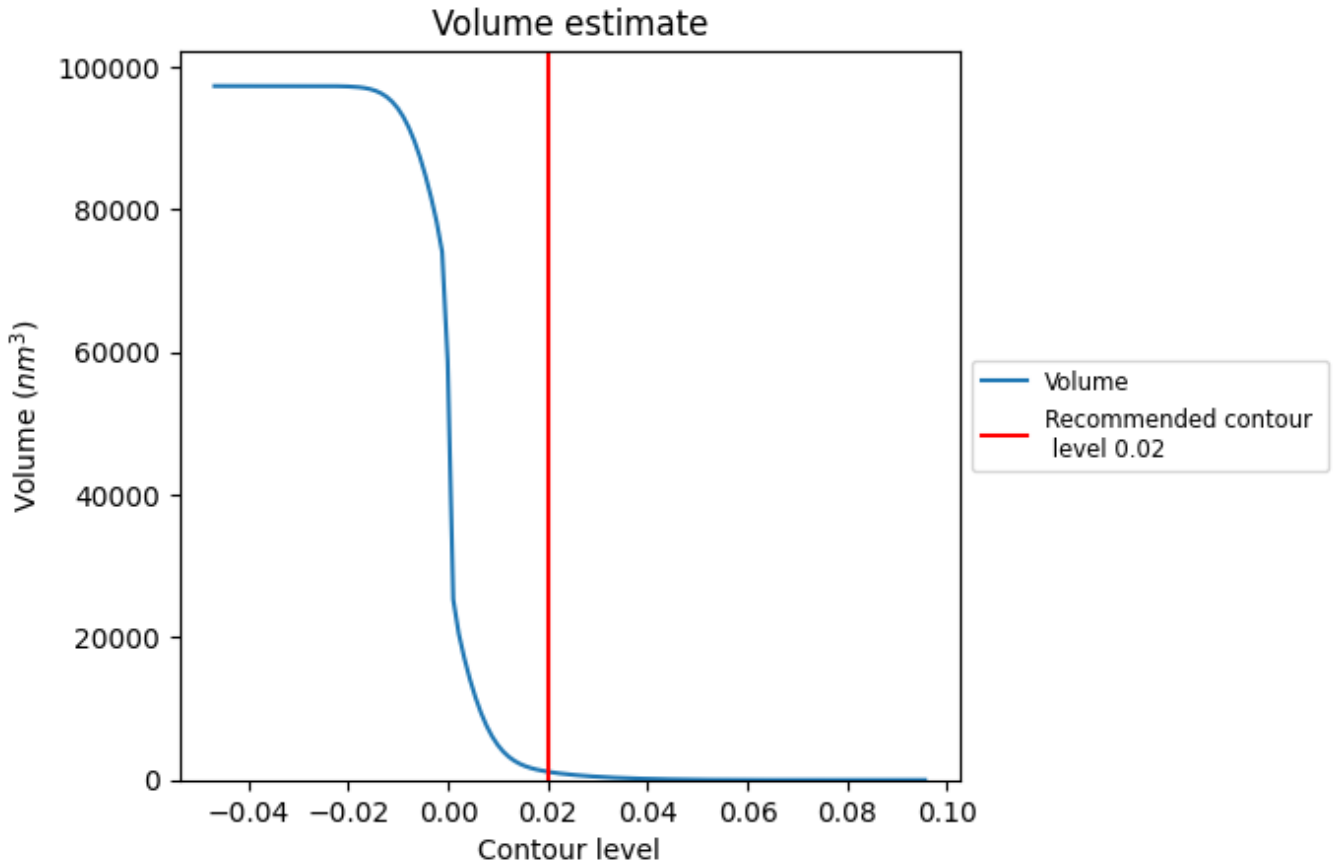
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

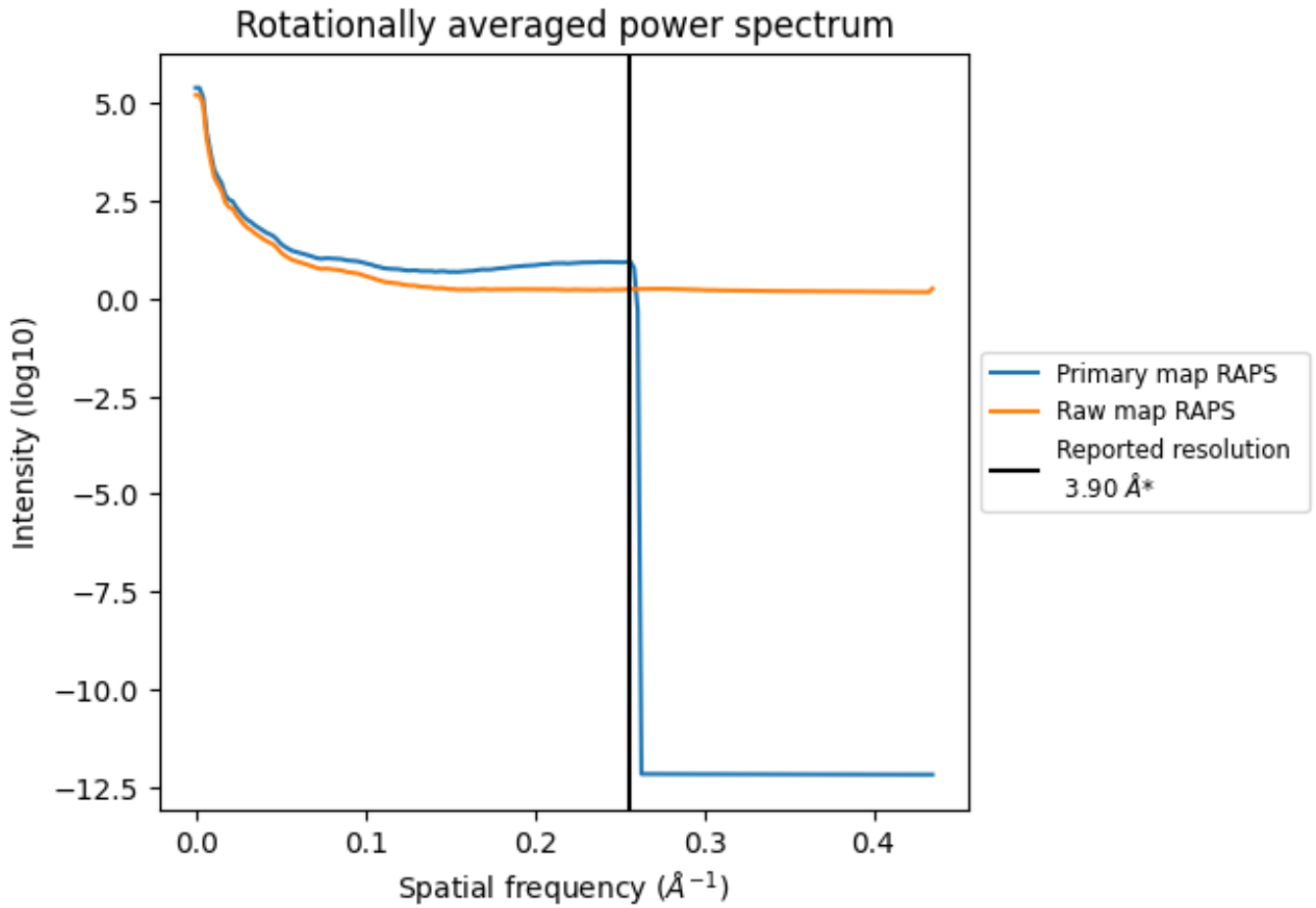
7.2 Volume estimate



The volume at the recommended contour level is 1153 nm^3; this corresponds to an approximate mass of 1042 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)

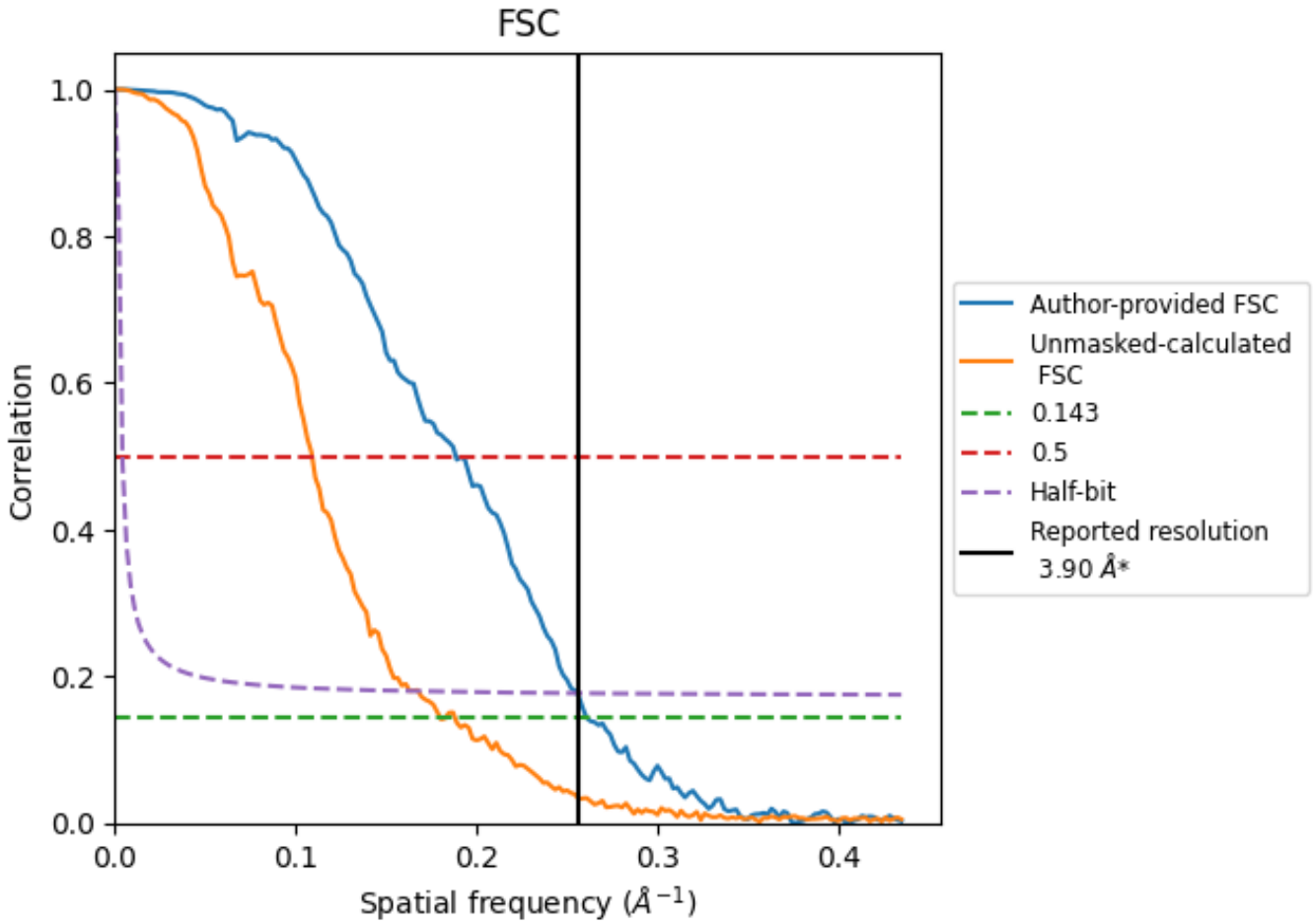


*Reported resolution corresponds to spatial frequency of 0.256 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

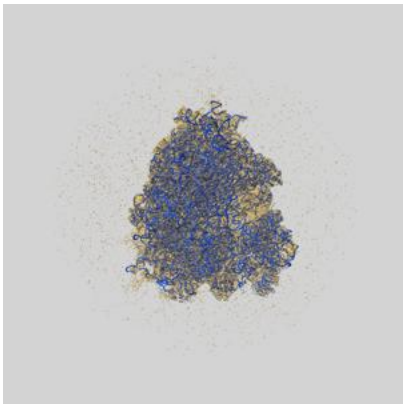
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.83	5.31	3.92
Unmasked-calculated*	5.56	9.17	5.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.56 differs from the reported value 3.9 by more than 10 %

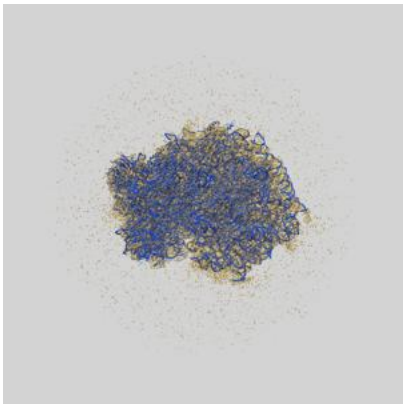
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0599 and PDB model 6OLF. Per-residue inclusion information can be found in section 3 on page 20.

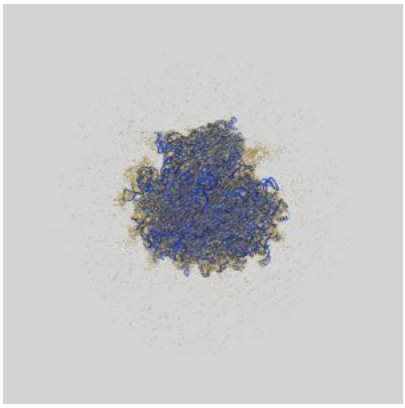
9.1 Map-model overlay



X



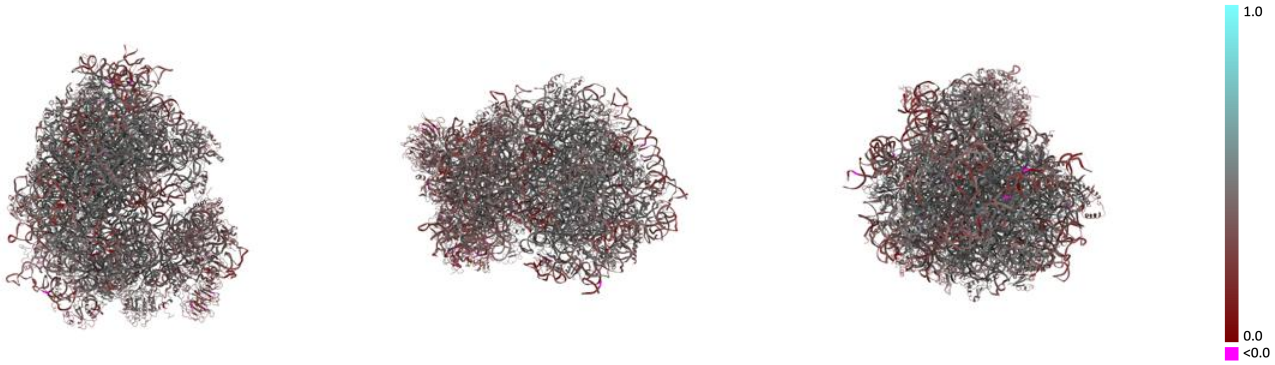
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

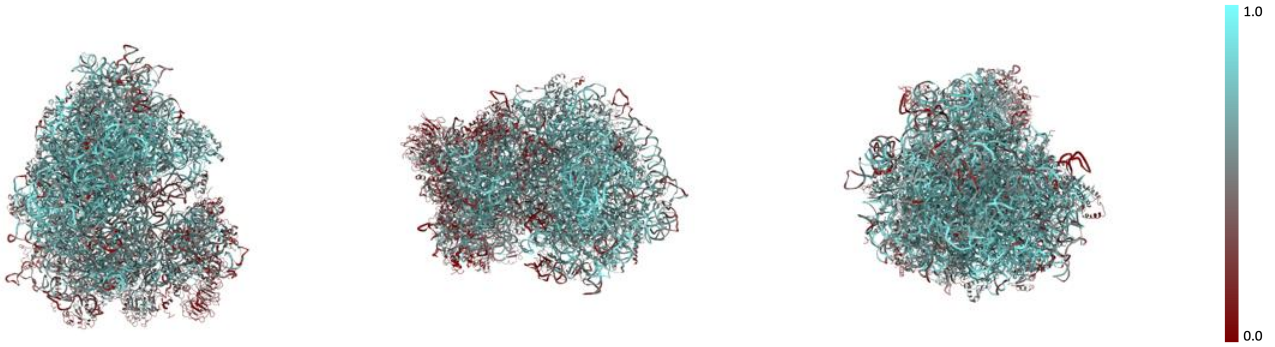
9.2 Q-score mapped to coordinate model (i)



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.

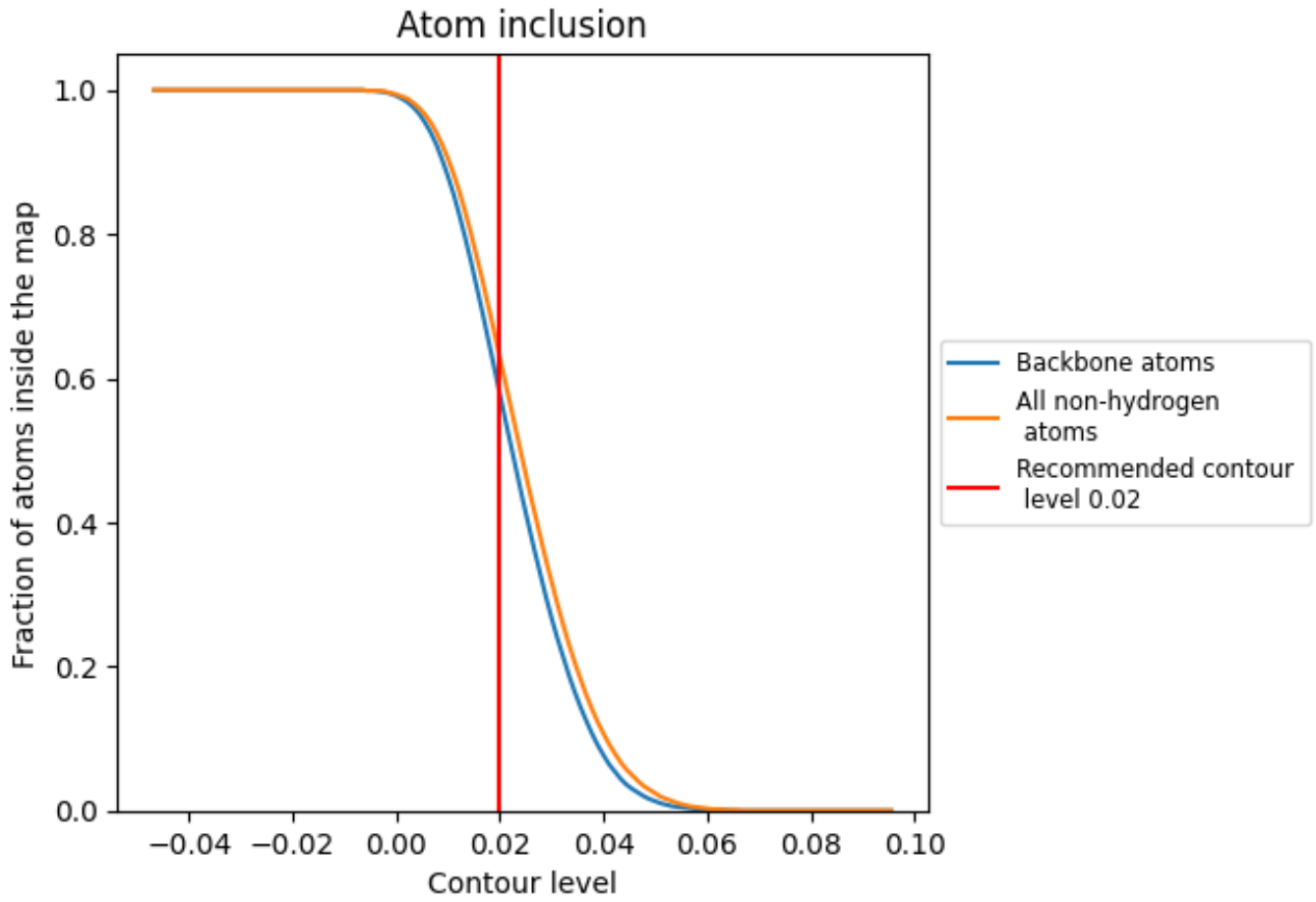
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 58% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6280	0.4070
A	0.6380	0.4810
B	0.6080	0.4550
C	0.6370	0.4590
D	0.7640	0.4230
E	0.8510	0.4420
F	0.5970	0.4180
G	0.5380	0.4070
H	0.6460	0.4600
I	0.5590	0.4220
J	0.5330	0.4310
K	0.6050	0.4520
L	0.5520	0.4140
M	0.5970	0.4250
N	0.6120	0.4410
O	0.6910	0.4830
P	0.6420	0.4600
Q	0.6500	0.4620
R	0.6260	0.4660
S	0.5680	0.4280
S2	0.6710	0.3900
SA	0.4590	0.4080
SB	0.4140	0.3990
SC	0.5060	0.4180
SD	0.3400	0.3550
SE	0.4150	0.3680
SF	0.3310	0.3550
SG	0.3350	0.3370
SH	0.3600	0.3410
SI	0.4260	0.3780
SJ	0.4290	0.3710
SK	0.3130	0.3370
SL	0.4600	0.3950
SM	0.1020	0.2340
SN	0.5070	0.4250

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Chain	Atom inclusion	Q-score
SO	0.4350	0.4040
SP	0.4300	0.3590
SQ	0.3810	0.3640
SR	0.3360	0.3670
SS	0.3860	0.3620
ST	0.3960	0.3630
SU	0.3390	0.3470
SV	0.4780	0.3850
SW	0.5470	0.4430
SX	0.5070	0.4150
SY	0.4090	0.3570
SZ	0.2830	0.3230
Sa	0.5310	0.4160
Sb	0.3840	0.3790
Sc	0.2720	0.3370
Sd	0.5350	0.4090
Se	0.3750	0.3740
Sf	0.1440	0.2410
Sg	0.2310	0.3030
T	0.6180	0.4550
U	0.6070	0.4540
V	0.5380	0.3890
W	0.5790	0.4650
X	0.3400	0.3120
Y	0.6050	0.4440
Z	0.6170	0.4420
a	0.5960	0.4350
b	0.6670	0.4700
c	0.5580	0.4300
d	0.5620	0.4200
e	0.5940	0.4400
f	0.6510	0.4670
g	0.6890	0.4790
h	0.6100	0.4630
i	0.5890	0.4170
j	0.5840	0.4220
k	0.7280	0.4870
l	0.4880	0.3950
m	0.6150	0.4560
n	0.6020	0.4420
o	0.5570	0.4410
p	0.5440	0.4490

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Chain	Atom inclusion	Q-score
q	0.6270	0.4670
r	0.6620	0.4560
t	0.7560	0.4140
u	0.3390	0.2500
v	0.4060	0.3060
w	0.5920	0.4150
y	0.1150	0.2570