



Full wwPDB EM Validation Report ⓘ

Nov 9, 2024 – 01:46 PM EST

PDB ID : 6OLI
EMDB ID : EMD-0526
Title : Structure of human ribosome nascent chain complex selectively stalled by a drug-like small molecule (USO1-RNC)
Authors : Li, W.; Cate, J.H.D.
Deposited on : 2019-04-16
Resolution : 3.50 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) : 2.39

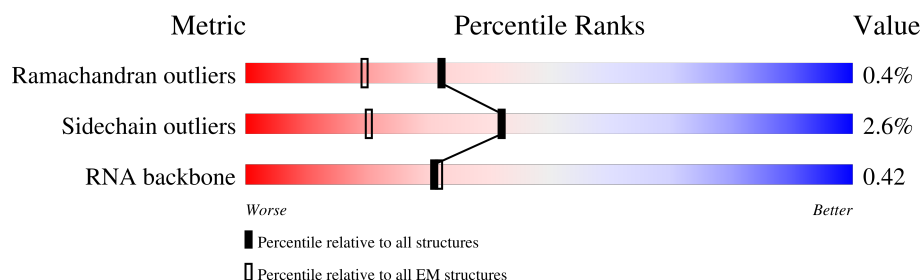
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	S2	1714	
2	SA	221	
3	SB	214	
4	SD	226	
5	SE	259	
6	SF	189	
7	SH	189	
8	SI	204	

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Mol	Chain	Length	Quality of chain
9	SK	98	<div>58%</div> <div>93%</div> <div>7%</div>
10	SL	153	<div>22%</div> <div>96%</div> <div>.</div>
11	SP	127	<div>36%</div> <div>97%</div> <div>.</div>
12	SQ	146	<div>31%</div> <div>96%</div> <div>..</div>
13	SR	134	<div>48%</div> <div>97%</div> <div>.</div>
14	SS	145	<div>31%</div> <div>98%</div> <div>.</div>
15	ST	143	<div>24%</div> <div>97%</div> <div>..</div>
16	SU	104	<div>53%</div> <div>95%</div> <div>5%</div>
17	SV	82	<div>24%</div> <div>96%</div> <div>.</div>
18	SX	141	<div>14%</div> <div>98%</div> <div>.</div>
19	Sa	102	<div>17%</div> <div>96%</div> <div>.</div>
20	Sc	64	<div>61%</div> <div>100%</div>
21	Sd	55	<div>16%</div> <div>91%</div> <div>9%</div>
22	Sg	312	<div>72%</div> <div>98%</div> <div>.</div>
23	SC	220	<div>17%</div> <div>98%</div> <div>.</div>
24	SG	237	<div>54%</div> <div>97%</div> <div>.</div>
25	SJ	185	<div>29%</div> <div>95%</div> <div>5%</div>
26	SM	118	<div>96%</div> <div>97%</div> <div>.</div>
27	SN	150	<div>21%</div> <div>98%</div> <div>.</div>
28	SO	137	<div>21%</div> <div>100%</div>
29	SW	129	<div>8%</div> <div>97%</div> <div>.</div>
30	SY	131	<div>44%</div> <div>96%</div> <div>..</div>
31	SZ	73	<div>49%</div> <div>96%</div> <div>.</div>
32	Sb	82	<div>43%</div> <div>100%</div>
33	Se	57	<div>37%</div> <div>100%</div>

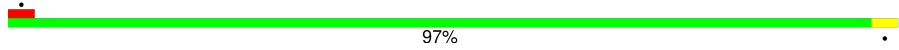
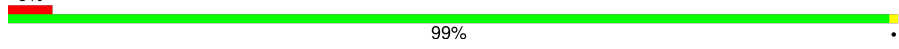
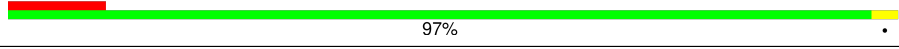
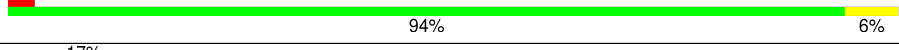

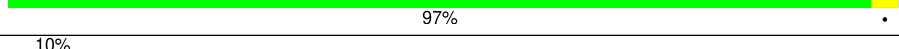
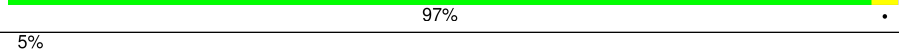
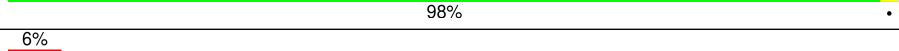
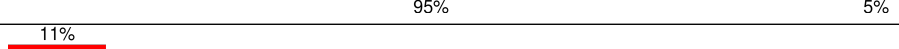
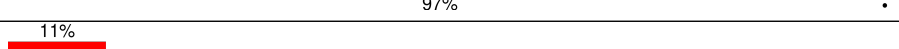
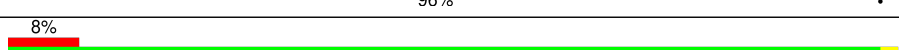
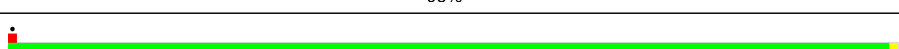
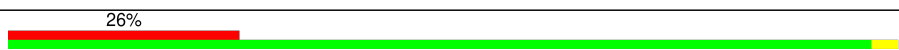
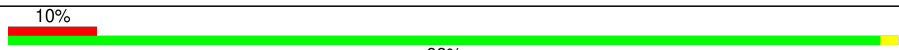
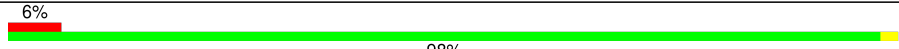
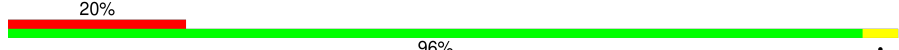
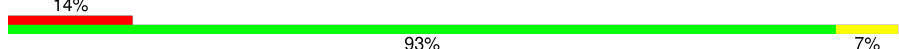
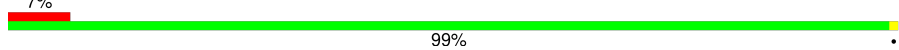
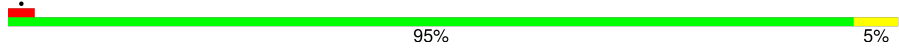


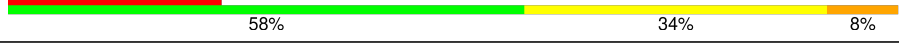

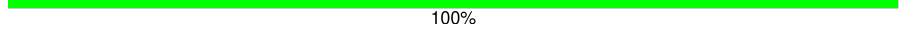

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Mol	Chain	Length	Quality of chain
34	Sf	67	96%
35	A	252	6% 97%
36	B	397	7% 96%
37	C	363	6% 96%
38	D	157	9% 71% 25%
39	E	121	77% 20%
40	F	294	12% 97%
41	G	247	18% 91%
42	H	225	5% 96%
43	I	234	19% 100%
44	J	191	14% 97%
45	K	211	11% 95%
46	L	169	14% 98%
47	M	205	13% 94% 5%
48	N	139	11% 98%
49	O	203	97%
50	P	195	95%
51	Q	153	97%
52	R	187	5% 95%
53	S	181	18% 98%
54	T	175	97%
55	U	157	6% 95% 5%
56	V	99	21% 94% 6%
57	W	129	8% 100%
58	X	61	8% 98%

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Mol	Chain	Length	Quality of chain
59	Y	117	
60	Z	134	
61	a	134	
62	b	147	
63	c	121	
64	d	103	
65	e	106	
66	f	129	
67	g	109	
68	h	114	
69	i	122	
70	j	97	
71	k	84	
72	l	69	
73	m	50	
74	n	50	
75	o	25	
76	p	105	
77	q	91	
78	r	122	
79	t	3607	
80	u	76	
81	v	76	
82	w	10	
83	y	36	

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 214867 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
1	S2	1714	Total	C	N	O	P	0	0
			36501	16306	6533	11949	1713		

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

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

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

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

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

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

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

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

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

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

- 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	61	Total	C	N	O	S	0	0
			511	327	100	82	2		

- 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 L27.

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

- Molecule 62 is a protein called 60S ribosomal protein L27a.

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

- Molecule 63 is a protein called 60S ribosomal protein L29.

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

- Molecule 64 is a protein called 60S ribosomal protein L30.

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

- Molecule 65 is a protein called 60S ribosomal protein L31.

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

- Molecule 66 is a protein called 60S ribosomal protein L32.

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

- Molecule 67 is a protein called 60S ribosomal protein L35a.

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

- Molecule 68 is a protein called 60S ribosomal protein L34.

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

- Molecule 69 is a protein called 60S ribosomal protein L35.

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

- Molecule 70 is a protein called 60S ribosomal protein L36.

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

- Molecule 71 is a protein called 60S ribosomal protein L37.

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

- Molecule 72 is a protein called 60S ribosomal protein L38.

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

- Molecule 73 is a protein called 60S ribosomal protein L39.

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

- Molecule 74 is a protein called 60S ribosomal protein L40.

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

- Molecule 75 is a protein called 60S ribosomal protein L41.

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

- Molecule 76 is a protein called 60S ribosomal protein L36a.

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

- Molecule 77 is a protein called 60S ribosomal protein L37a.

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

- Molecule 78 is a protein called 60S ribosomal protein L28.

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

- Molecule 79 is a RNA chain called 28S ribosomal RNA.

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

- Molecule 80 is a RNA chain called tRNA.

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

- Molecule 81 is a RNA chain called tRNA.

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

- Molecule 82 is a RNA chain called mRNA.

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

- Molecule 83 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
83	y	36	Total	C	N	O	0	0
			178	106	36	36		

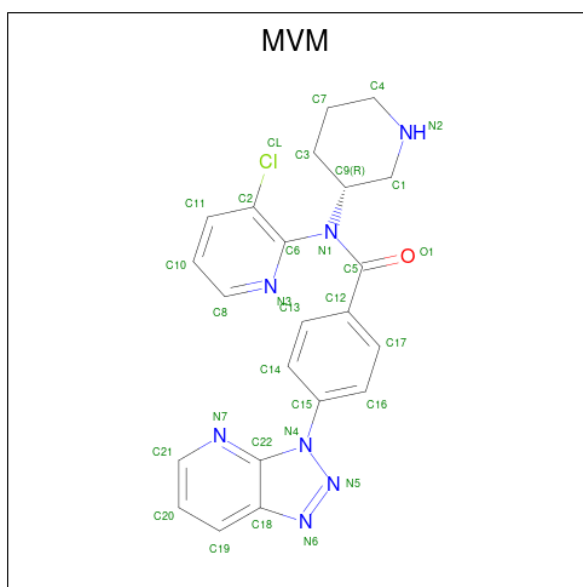
- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	S2	2	Total	Mg	0
			2	2	
84	B	1	Total	Mg	0
			1	1	
84	D	7	Total	Mg	0
			7	7	
84	E	9	Total	Mg	0
			9	9	
84	O	1	Total	Mg	0
			1	1	
84	b	1	Total	Mg	0
			1	1	
84	o	1	Total	Mg	0
			1	1	
84	t	9	Total	Mg	0
			9	9	

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- 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: C₂₂H₂₀ClN₇O).



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

- Molecule 87 is water.

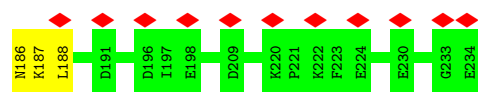
Mol	Chain	Residues	Atoms		AltConf
87	S2	5	Total	O	0
			5	5	
87	SP	1	Total	O	0
			1	1	
87	SQ	1	Total	O	0
			1	1	
87	SR	1	Total	O	0
			1	1	
87	SS	1	Total	O	0
			1	1	
87	SC	1	Total	O	0
			1	1	
87	SJ	1	Total	O	0
			1	1	
87	Sb	1	Total	O	0
			1	1	
87	Sf	1	Total	O	0
			1	1	
87	u	1	Total	O	0
			1	1	

3 Residue-property plots

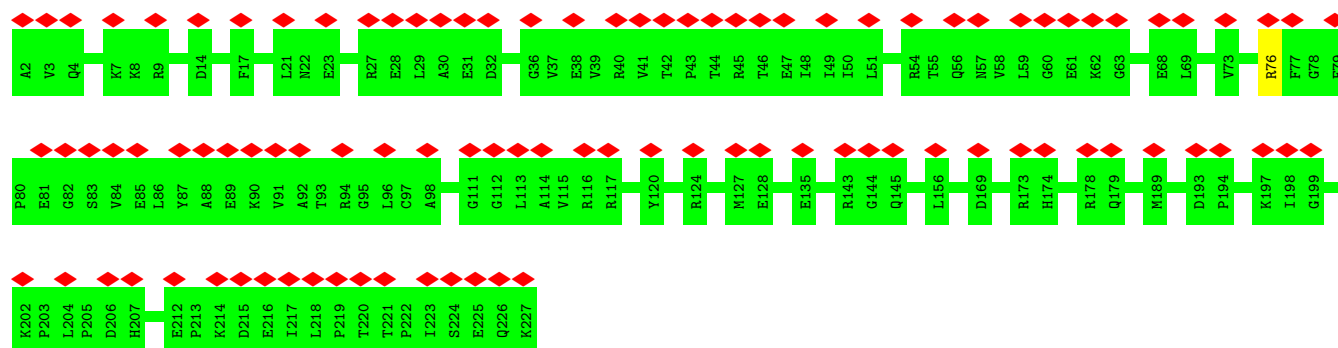
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

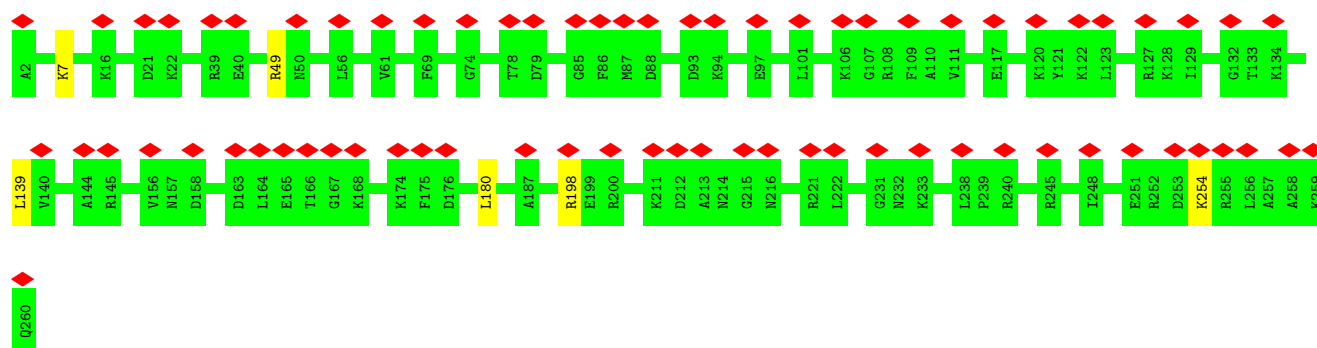




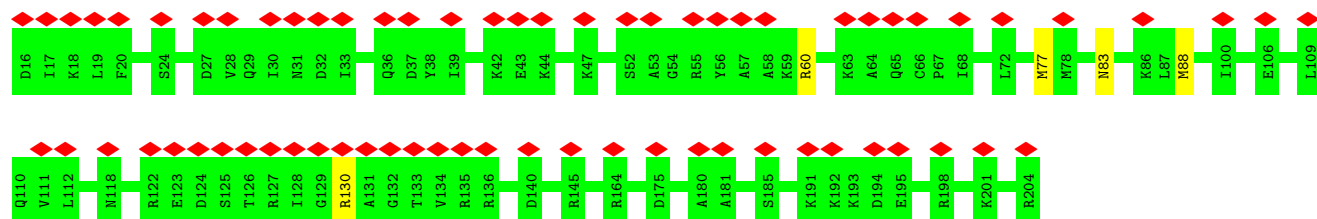
• Molecule 4: 40S ribosomal protein S3



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

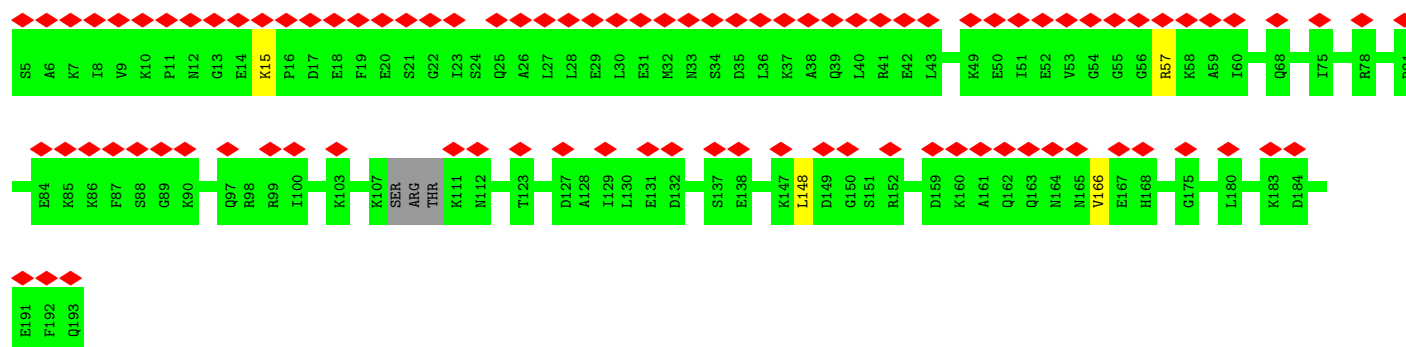


• Molecule 6: 40S ribosomal protein S5

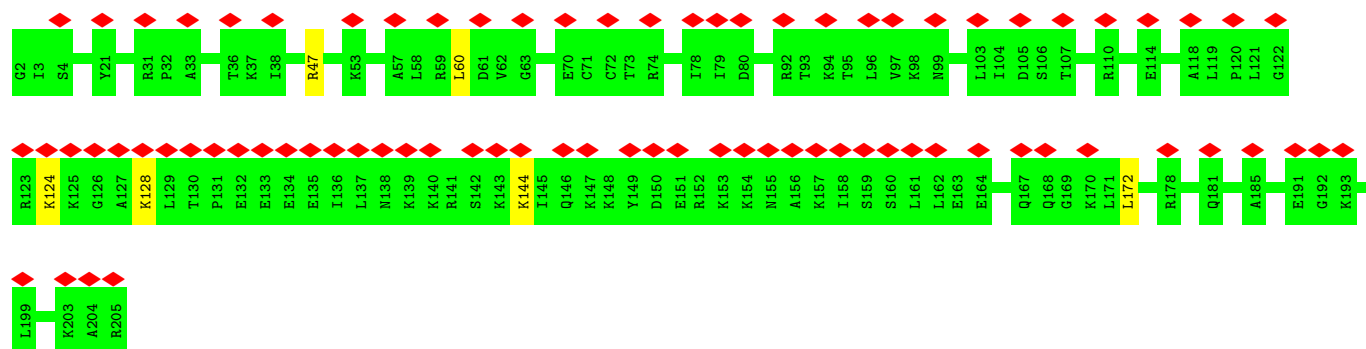
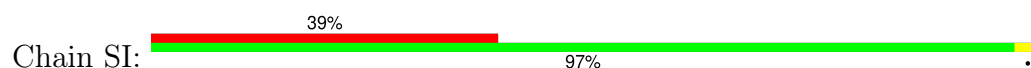


• Molecule 7: 40S ribosomal protein S7

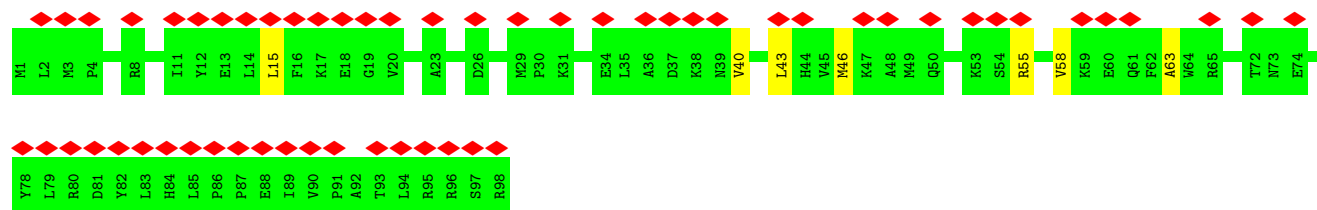




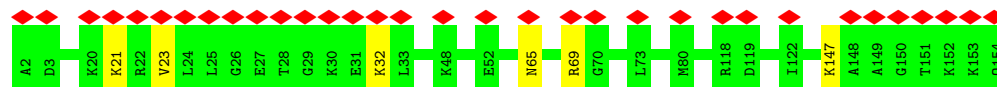
• Molecule 8: 40S ribosomal protein S8



• Molecule 9: 40S ribosomal protein S10

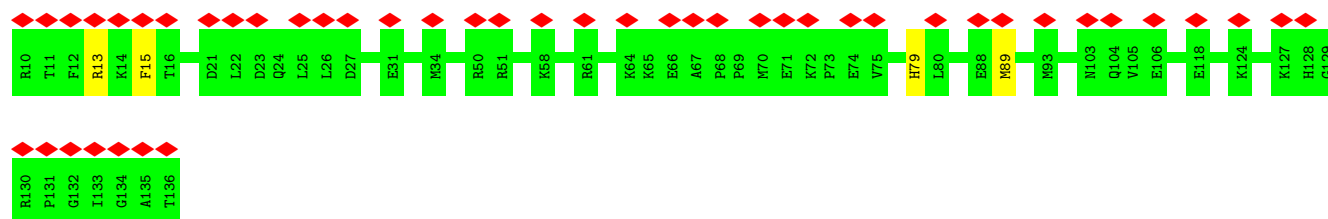


• Molecule 10: 40S ribosomal protein S11

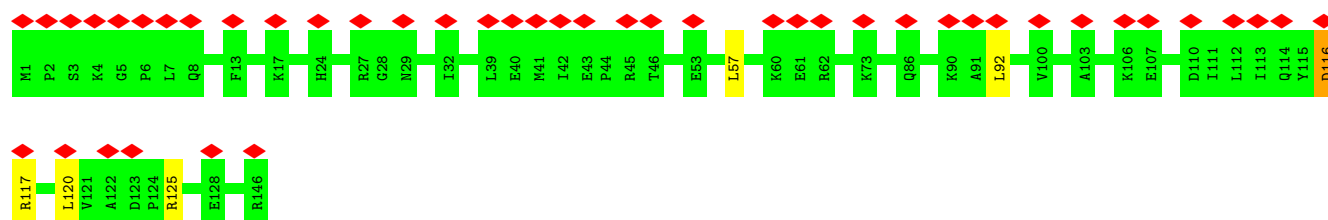


• Molecule 11: 40S ribosomal protein S15

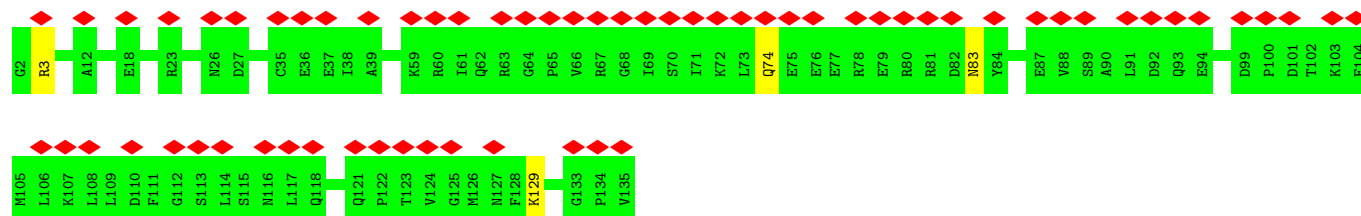




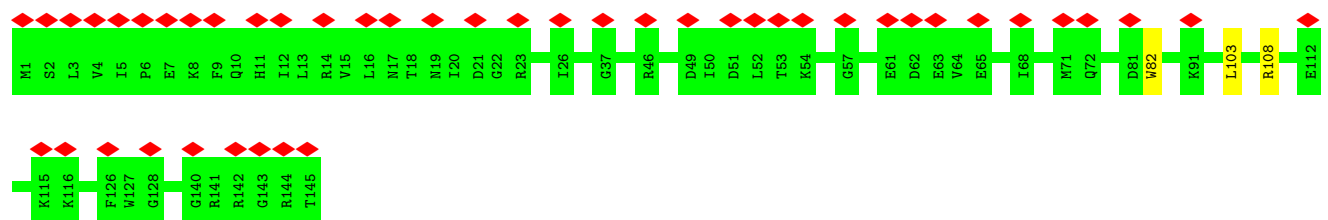
- Molecule 12: 40S ribosomal protein S16



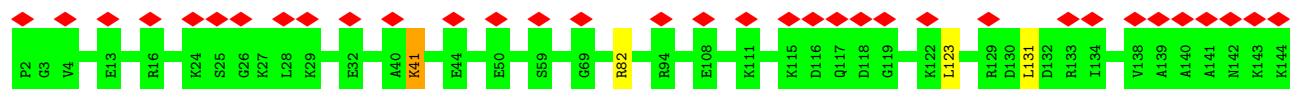
- Molecule 13: 40S ribosomal protein S17



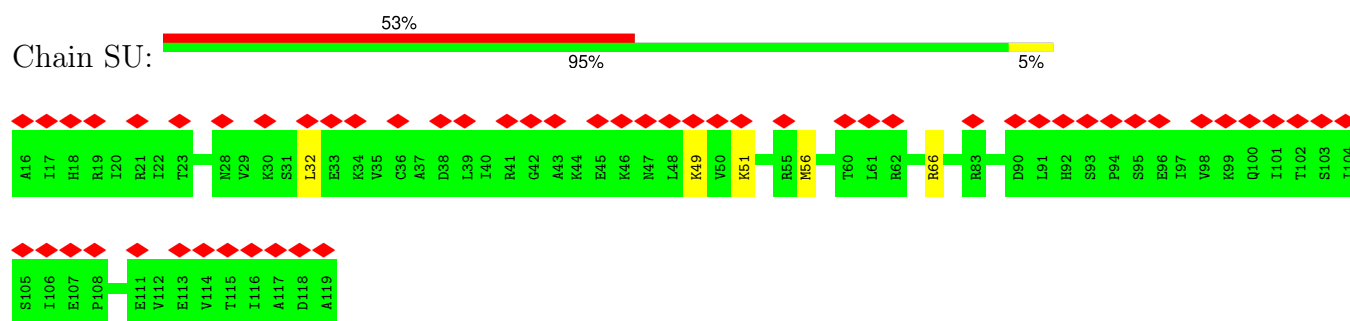
- Molecule 14: 40S ribosomal protein S18



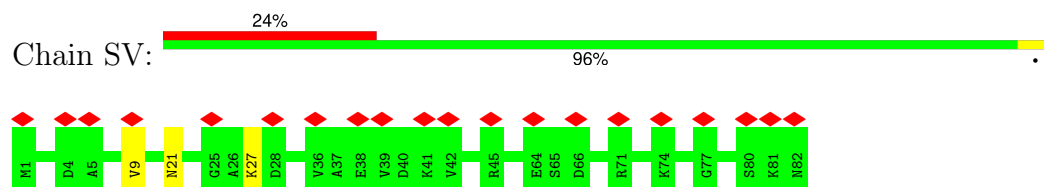
- Molecule 15: 40S ribosomal protein S19



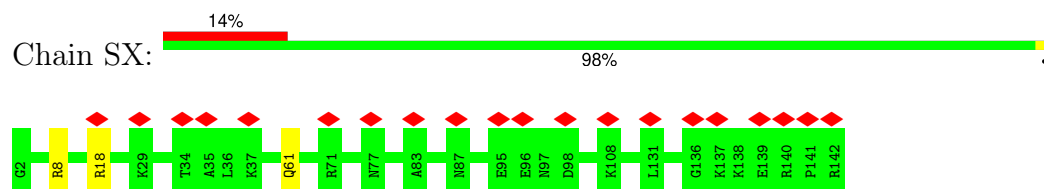
- Molecule 16: 40S ribosomal protein S20



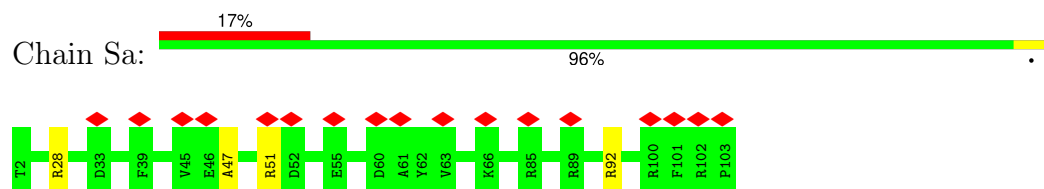
- Molecule 17: 40S ribosomal protein S21



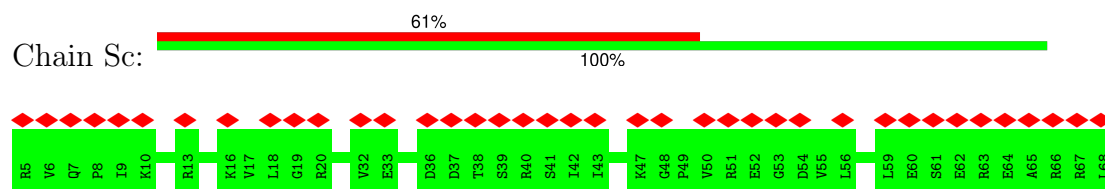
- Molecule 18: 40S ribosomal protein S23



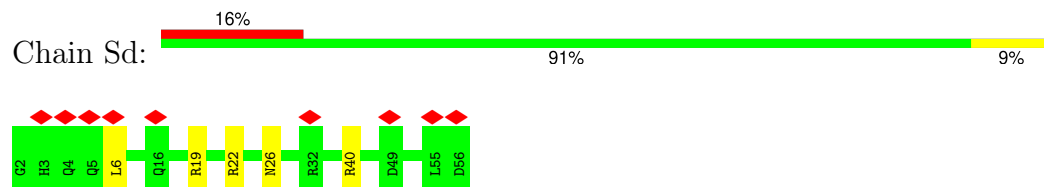
- Molecule 19: 40S ribosomal protein S26



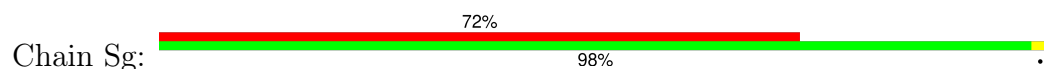
- Molecule 20: 40S ribosomal protein S28

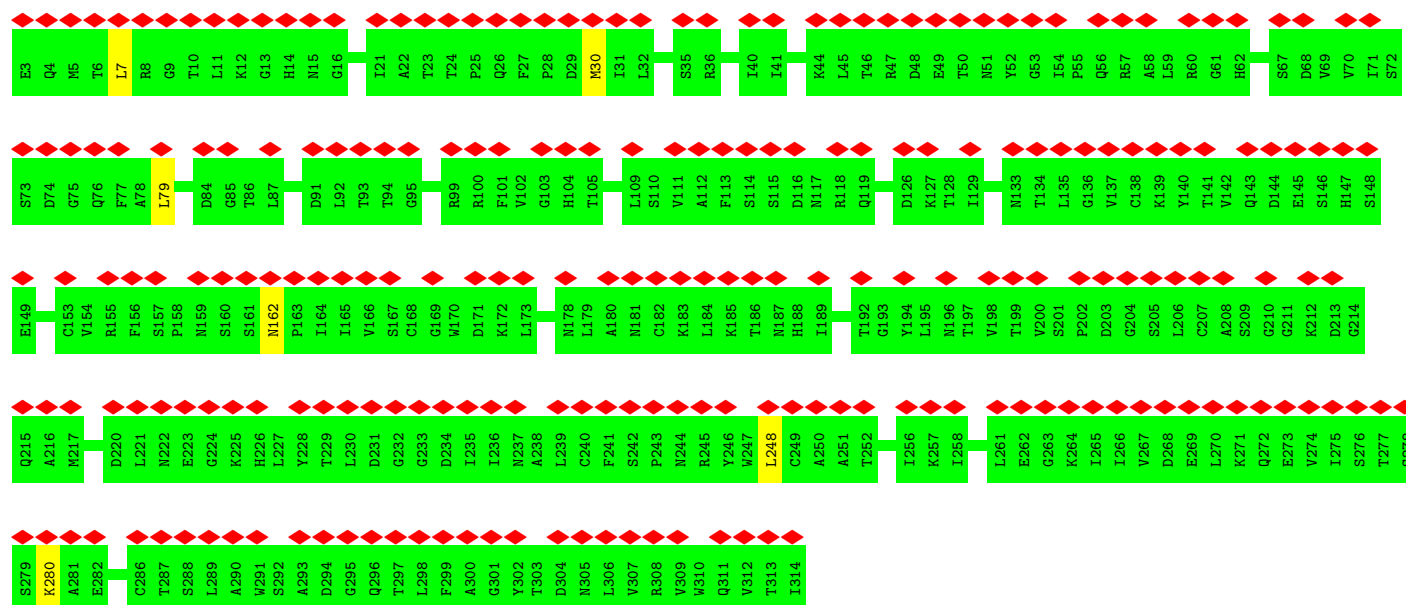


- Molecule 21: 40S ribosomal protein S29



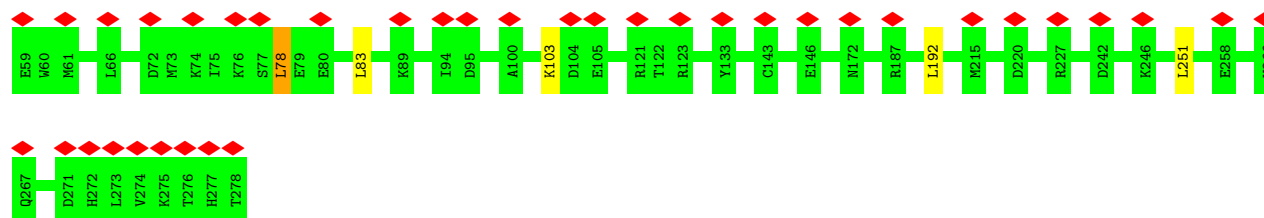
- Molecule 22: Receptor of activated protein C kinase 1





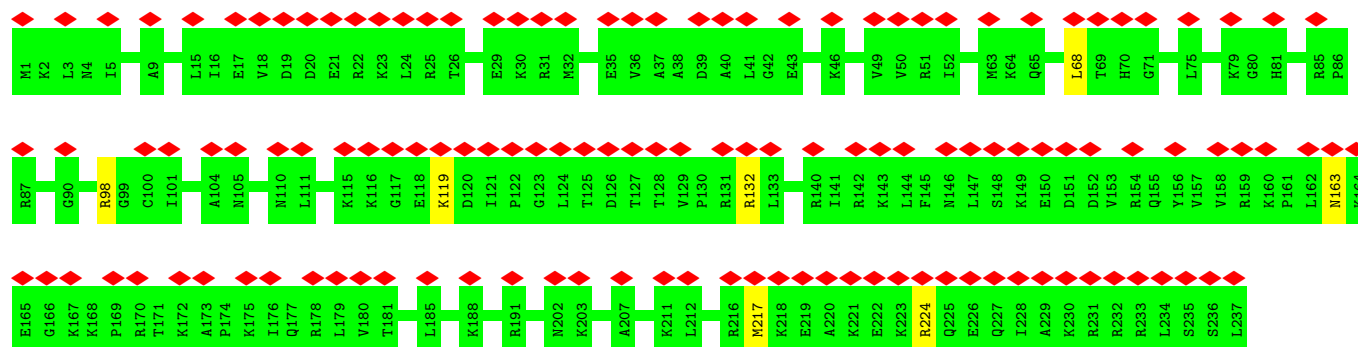
• Molecule 23: 40S ribosomal protein S2

Chain SC: 17% 98%



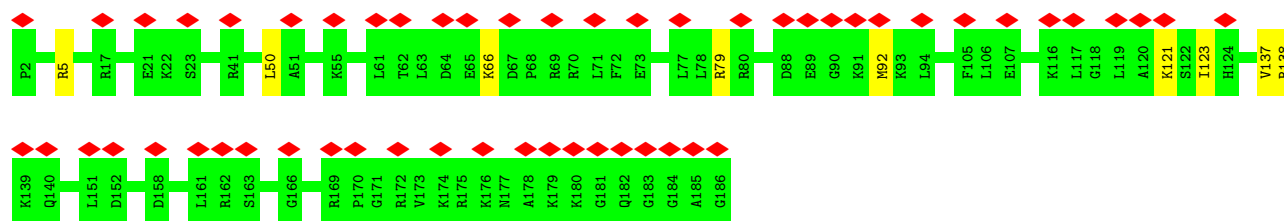
• Molecule 24: 40S ribosomal protein S6

Chain SG: 54% 97%

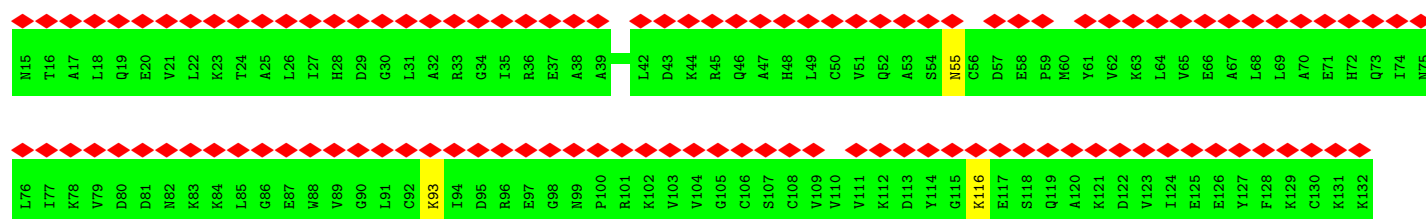


• Molecule 25: 40S ribosomal protein S9

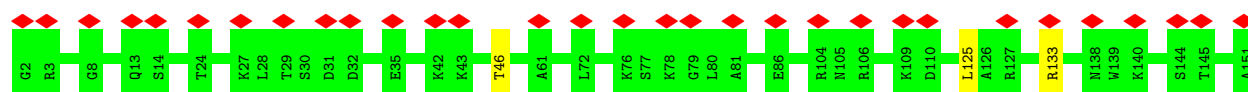
Chain SJ: 29% 95% 5%



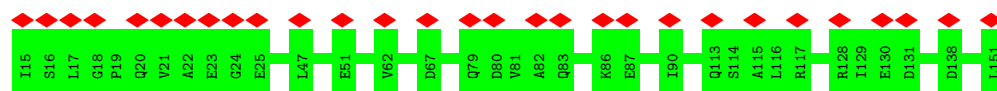
• Molecule 26: 40S ribosomal protein S12



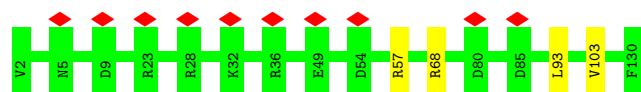
• Molecule 27: 40S ribosomal protein S13



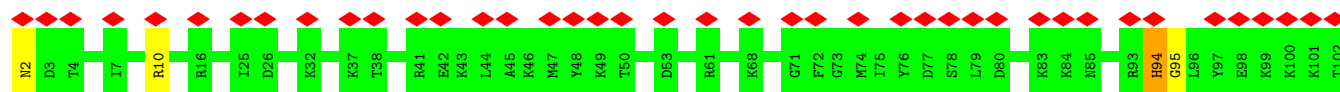
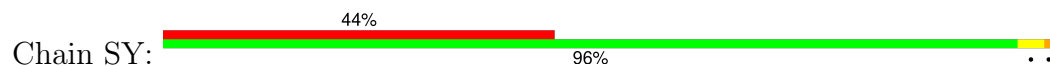
• Molecule 28: 40S ribosomal protein S14

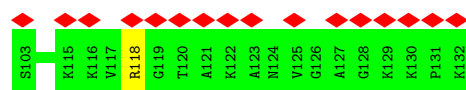


• Molecule 29: 40S ribosomal protein S15a

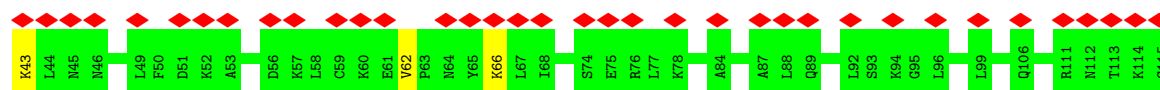


• Molecule 30: 40S ribosomal protein S24

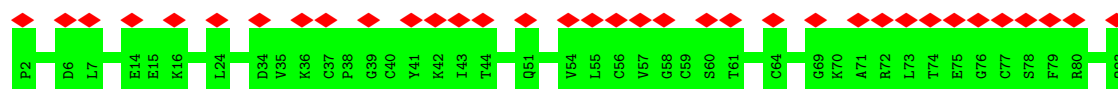




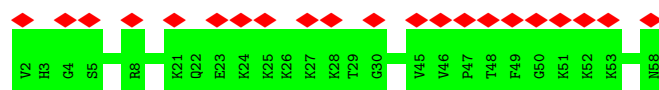
- Molecule 31: 40S ribosomal protein S25



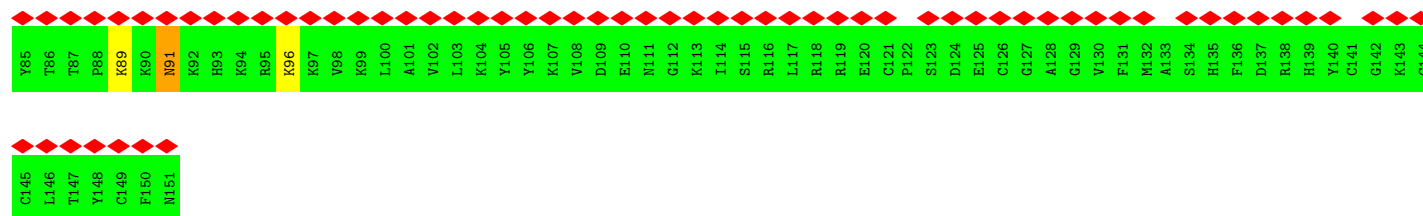
- Molecule 32: 40S ribosomal protein S27



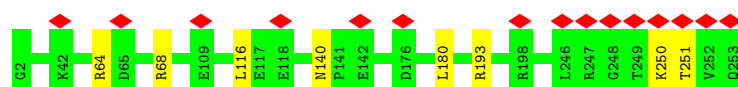
- Molecule 33: 40S ribosomal protein S30



- Molecule 34: 40S ribosomal protein S27a

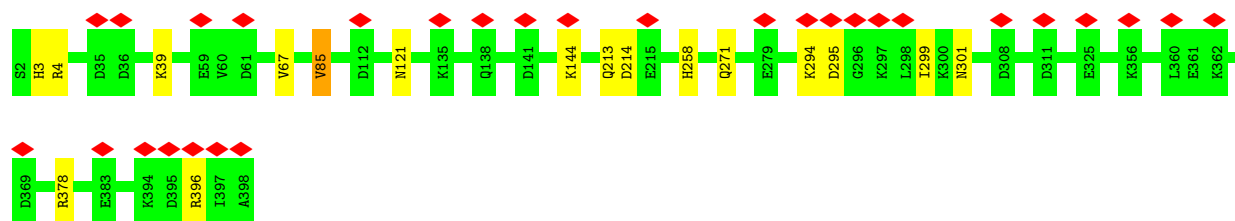


- Molecule 35: 60S ribosomal protein L8



- Molecule 36: 60S ribosomal protein L3

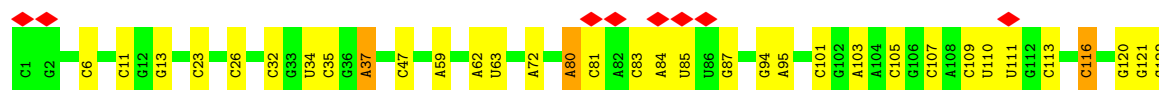




- Molecule 37: 60S ribosomal protein L4



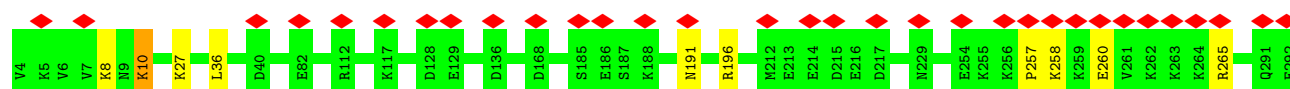
- Molecule 38: 5.8S ribosomal RNA



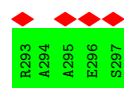
- Molecule 39: 5S ribosomal RNA

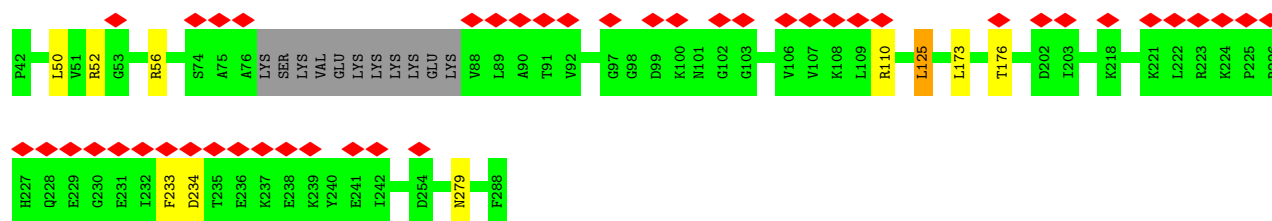


- Molecule 40: 60S ribosomal protein L5

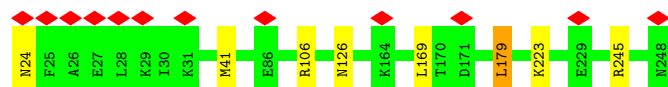


- Molecule 41: 60S ribosomal protein L6

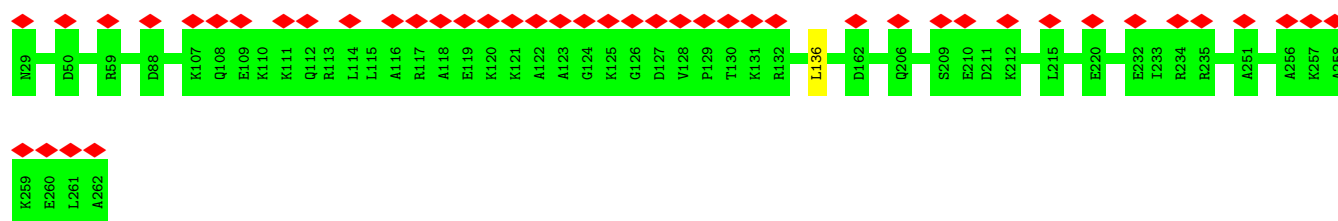




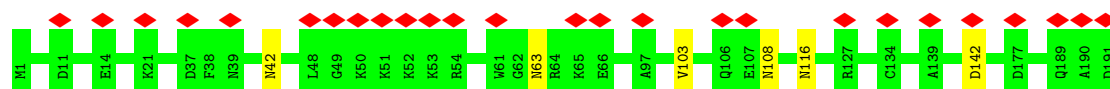
- Molecule 42: 60S ribosomal protein L7



- Molecule 43: 60S ribosomal protein L7a



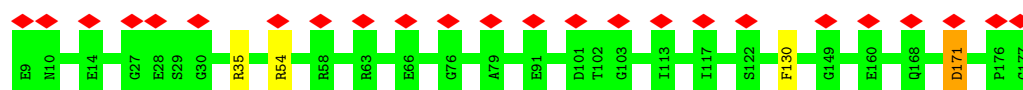
- Molecule 44: 60S ribosomal protein L9



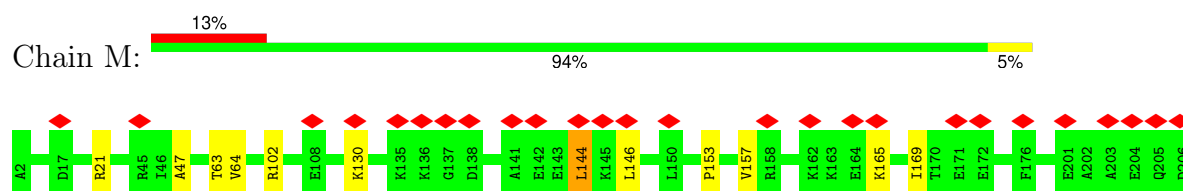
- Molecule 45: 60S ribosomal protein L10



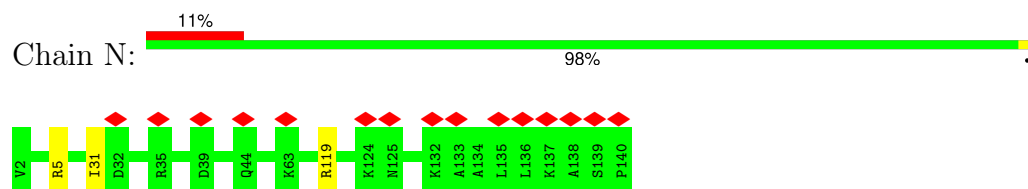
- Molecule 46: 60S ribosomal protein L11



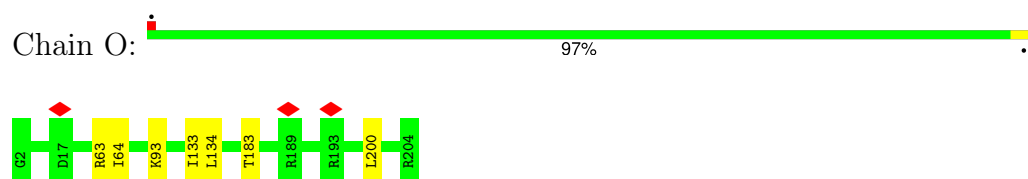
- Molecule 47: 60S ribosomal protein L13



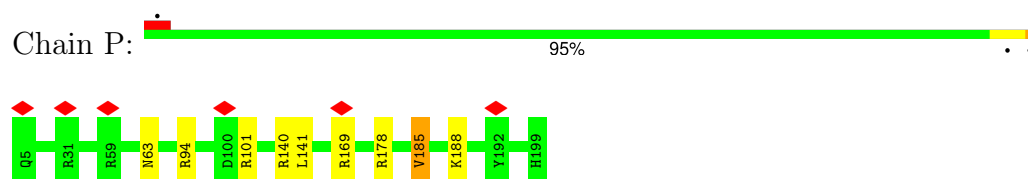
- Molecule 48: 60S ribosomal protein L14



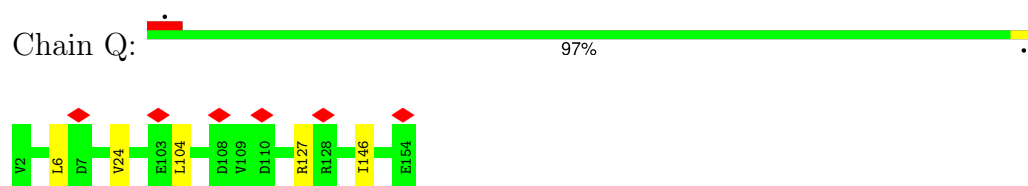
- Molecule 49: 60S ribosomal protein L15



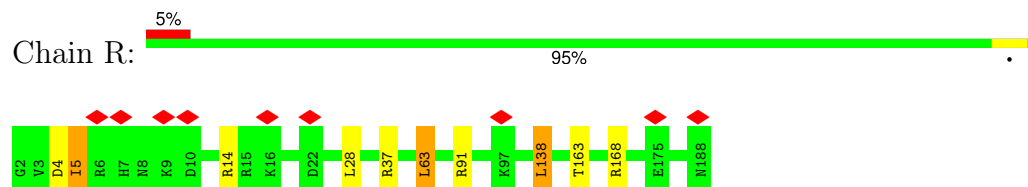
- Molecule 50: 60S ribosomal protein L13a



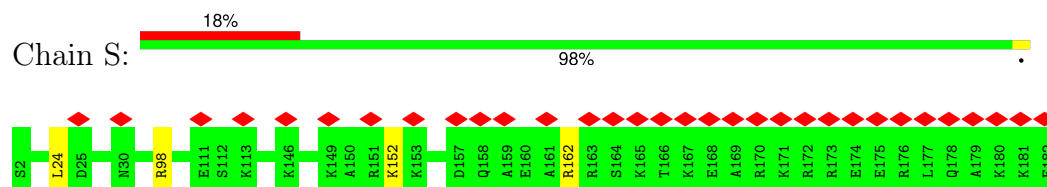
- Molecule 51: 60S ribosomal protein L17



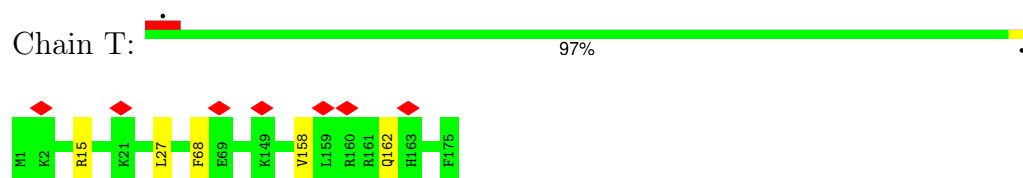
- Molecule 52: 60S ribosomal protein L18



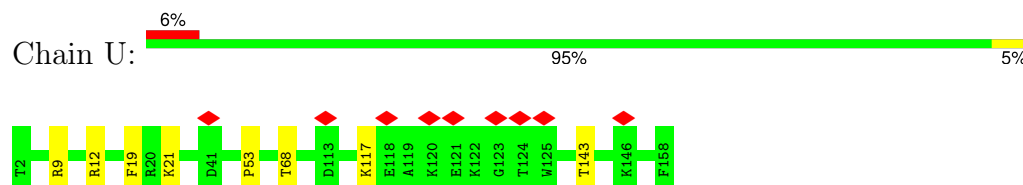
- Molecule 53: 60S ribosomal protein L19



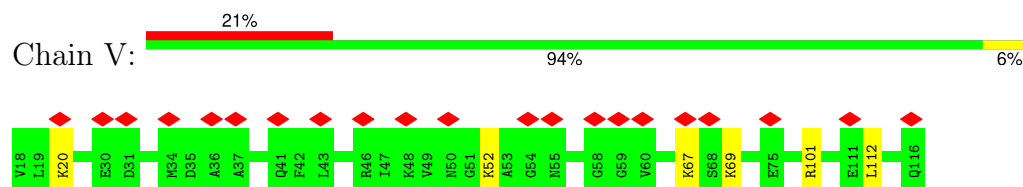
• Molecule 54: 60S ribosomal protein L18a



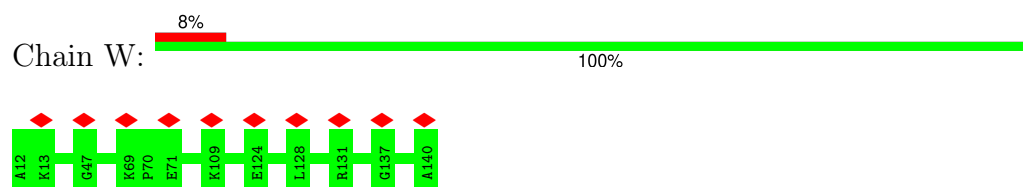
• Molecule 55: 60S ribosomal protein L21



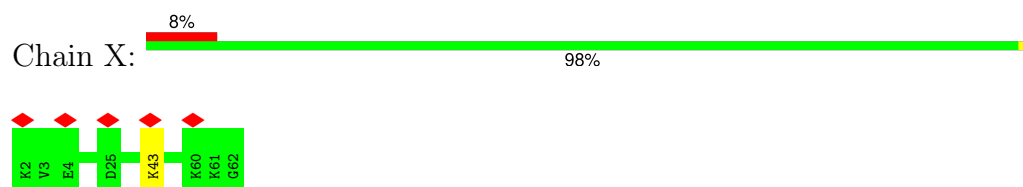
• Molecule 56: 60S ribosomal protein L22



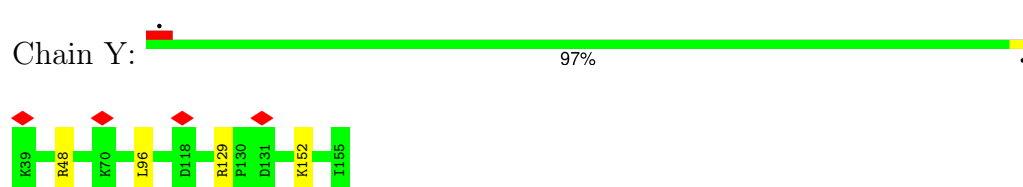
• Molecule 57: 60S ribosomal protein L23



• Molecule 58: 60S ribosomal protein L24

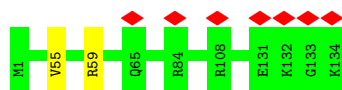


• Molecule 59: 60S ribosomal protein L23a

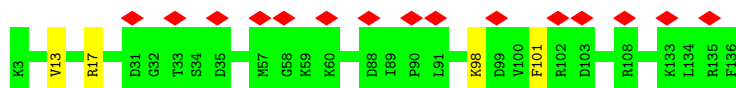


• Molecule 60: 60S ribosomal protein L26

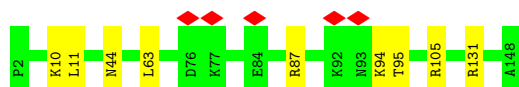




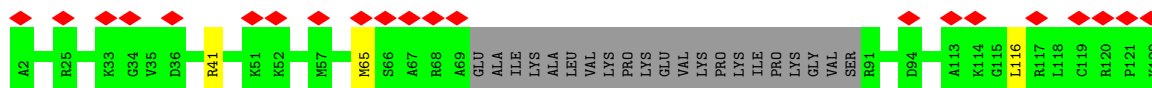
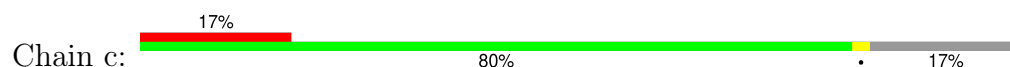
- Molecule 61: 60S ribosomal protein L27



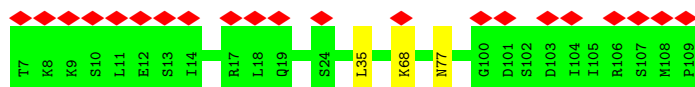
- Molecule 62: 60S ribosomal protein L27a



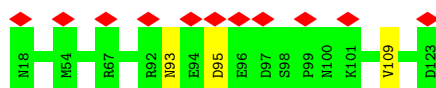
- Molecule 63: 60S ribosomal protein L29



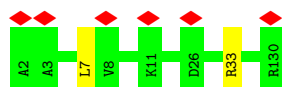
- Molecule 64: 60S ribosomal protein L30



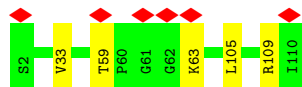
- Molecule 65: 60S ribosomal protein L31



- Molecule 66: 60S ribosomal protein L32



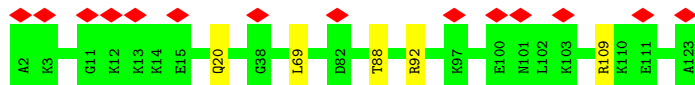
- Molecule 67: 60S ribosomal protein L35a



- Molecule 68: 60S ribosomal protein L34



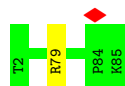
- Molecule 69: 60S ribosomal protein L35



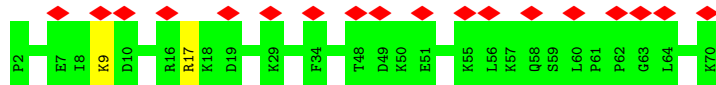
- Molecule 70: 60S ribosomal protein L36



- Molecule 71: 60S ribosomal protein L37



- Molecule 72: 60S ribosomal protein L38

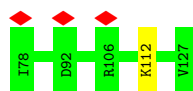


- Molecule 73: 60S ribosomal protein L39

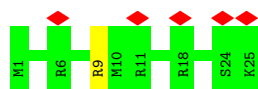




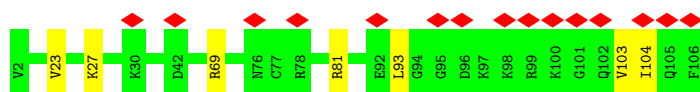
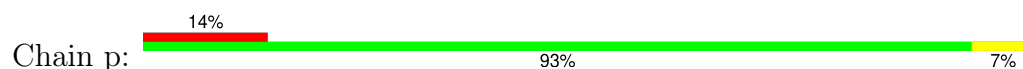
- Molecule 74: 60S ribosomal protein L40



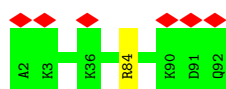
- Molecule 75: 60S ribosomal protein L41



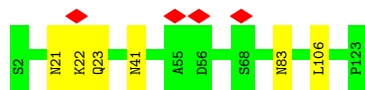
- Molecule 76: 60S ribosomal protein L36a



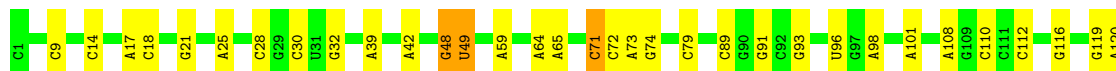
- Molecule 77: 60S ribosomal protein L37a



- Molecule 78: 60S ribosomal protein L28

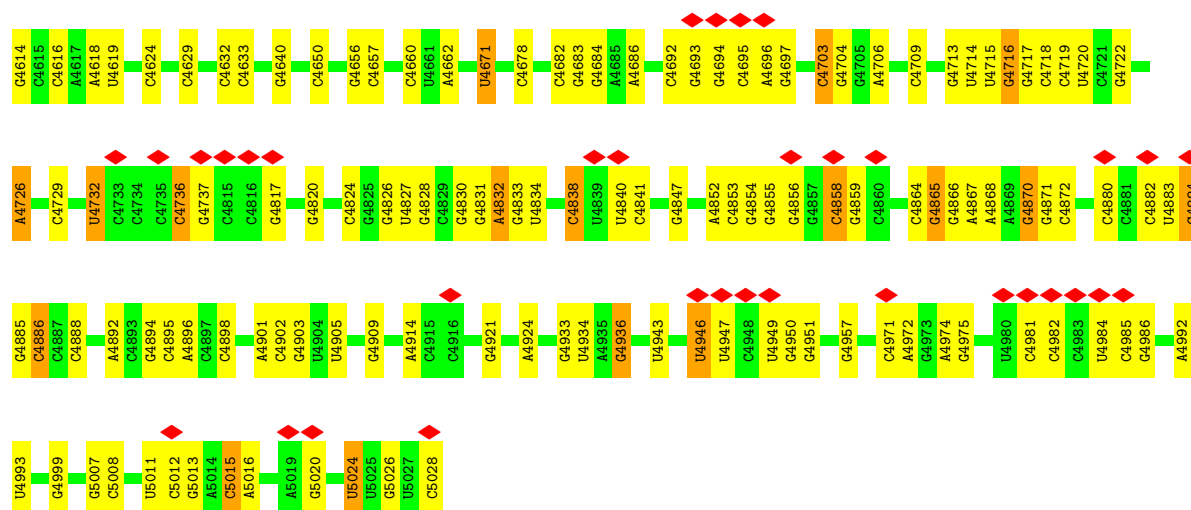


- Molecule 79: 28S ribosomal RNA

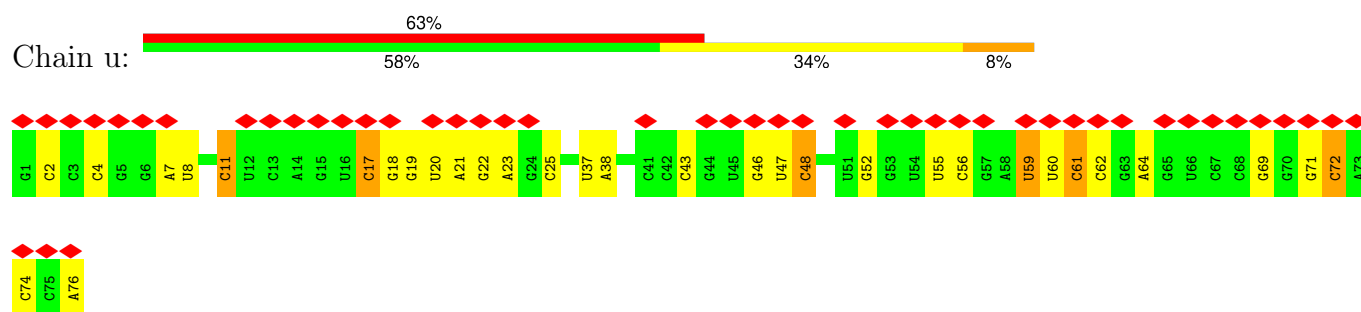




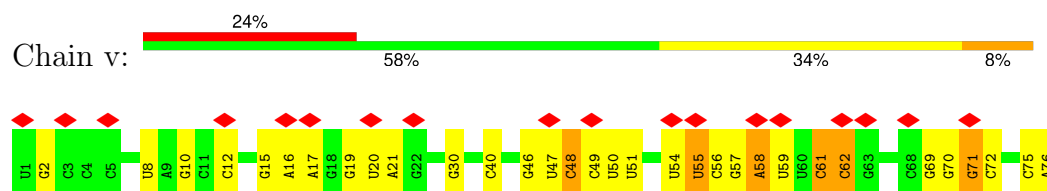
G4437	G4453	G4454	G4455	U4460	G4461	U4462	U4463	C4464	U4472	U4473	U4474	U4475	U4476	U4477	U4480	U4485	U4486	U4490	U4501	A4510	C4511	U4517	C4522	C4529	A4530	U4531	G4537	C4545	A4551	A4552	A4561	G4562	C4570	C4575	U4578	C4595	U4598	C4599	U4600	G4601															
C4294	A4296	G4299	C4300	A4301	C4311	C4312	U4313	U4316	U4322	U4326	C4327	G4333	G4334	A4338	G4339	A4340	A4341	A4342	A4343	G4344	C4349	G4353	A4356	U4357	A4358	A4359	C4360	G4367	U4381	A4384	C4388	C4391	U4401	G4402	C4406	U4414	A4426	U4427	C4428																
C4139	C4145	C4146	C4153	C4158	A4165	C4166	A4167	A4174	A4175	A4176	C4177	C4185	A4186	C4187	A4190	U4191	A4195	C4205	C4211	C4212	A4213	C4216	A4217	C4228	C4229	A4230	C4234	A4235	A4242	A4243	C4250	C4253	A4266	C4267	C4276	C4289	C4290	C4291	C4292	G4293															
G4054	C4058	G4062	G4063	G4064	G4065	C4066	G4067	A4068	G4069	C4070	C4071	C4072	G4073	A4074	G4075	G4076	G4077	G4078	C4079	U4080	C4081	U4082	C4083	G4084	C4085	U4086	U4087	C4088	G4093	A4096	C4099	G4100	C4101	G4104	C4105	C4106	C4107	G4108	C4109	C4110	C4111	A4119	C4124	U4125	C4126	G4130	G4131	A4132							
G3790	A3795	A3796	C3797	C3798	A3799	C3805	U3809	C3810	U3811	U3822	A3838	A3847	A3848	C3849	G3850	G3851	G3852	C3858	G3859	G3860	U3863	C3864	A3865	C3866	C3867	G3868	G3869	A3872	A3876	A3877	G3878	A3879	C3880	U3886	C3887	A3894	C3897	G3909	G3917	A3918	U4037	G4046													
G3657	C3671	U3680	G3681	A3682	U3683	U3684	U3700	A3707	A3719	G3722	C3723	G3724	G3725	G3728	U3729	A3730	C3731	C3732	U3733	C3734	U3741	C3742	U3743	U3744	A3745	G3748	G3751	A3754	A3755	A3756	U3757	C3758	C3759	C3762	C3765	C3781	G3782	C3783	A3784	U3785	A3788	U3789													
A2858	U2859	A2860	G2863	C2871	U2879	G2880	G2881	C3569	A3570	G3571	C3572	C3573	U3577	U3587	G3588	C3589	G3590	A3595	G3596	G3597	A3606	C3607	U3612	U3615	C3616	A3617	A3618	A3619	A3624	A3633	A3634	G3635	C3638	G3643	C3644	U3651	C3656	U3659	G3660	U3661	G3662	A3663													
G2714	C2718	U2719	A2722	A2723	U2726	C2727	G2733	G2737	G2741	A2745	U2748	C2759	A2766	U2767	A2768	U2769	C2773	A2774	G2775	A2777	G2778	A2785	C2793	U2798	C2799	U2805	G2806	G2809	A2814	G2817	G2821	A2824	G2834	C2835	G2836	U2839	G2855																		
G2542	G2543	A2544	C2562	G2565	A2566	C2567	C2568	C2574	A2580	G2581	C2582	G2585	C2606	U2607	C2608	G2617	U2618	C2632	G2637	U2640	U2644	U2645	G2646	C2648	G2652	G2665	U2666	G2673	A2674	A2675	U2686	U2687	C2688	C2689	G2690	G2691	G2698	C2699	G2700	G2705															
G2421	U2426	G2429	A2430	G2431	A2432	G2442	U2446	U2447	C2448	C2449	C2457	G2458	C2461	A2462	A2463	U2464	G2465	G2466	C2467	C2468	U2469	C2470	A2471	G2472	U2473	U2474	G2475	C2476	G2477	G2482	C2483	C2484	G2485	A2490	A2491	A2492	C2499	G2523	U2524	G2525	G2526	A2532	U2533	G2538	C2539	C2540	G2541								
C2348	G2349	A2364	G2365	C2368	G2378	A2379	C2381	C2382	G2385	A2392	G2395	G2321	G2322	U2323	G2324	C2325	A2326	G2327	C2330	G2340	G2343	C2344	U2350	A2358	G2373	A2374	A2375	U2388	C2389	C2390	A2391	A2396	A2397	C2398	A2399	G2400	C2401	U2404	U2405	C2416															
A2028	U2029	C2032	G2036	G2037	C2043	G2043	U2051	C2054	C2064	C2065	G2066	G2067	C2068	G2069	U2070	G2071	A2072	G2073	A2075	G2076	U2077	G2078	C2081	G2082	G2083	C2087	G2088	G2089	C2090	G2091	G2092	C2093	C2228	C2229	G2230	G2231	A2232	G2233	C2234	C2235	G2236	G2237	G2238	G2239	G2240	G2241	A2242	C2245	U2246	A2247					
G1957	C1958	C1959	A1960	U1961	G1962	G1963	A1964	A1965	G1966	U1967	C1968	G1969	G1970	A1971	A1972	U1973	C1974	G1975	G1976	C1977	U1978	A1979	A1980	G1981	G1982	A1983	G1984	U1985	G1986	U1987	G1988	U1989	A1990	A1991	C1992	A1993	A1994	C1995	U1996	C1997	A1998	C2003	C2004	G2005	A2006	A2007	U2008	C2009	A2010	A2011	C2016	A2021	U2025	G2026	G2027



• Molecule 80: tRNA



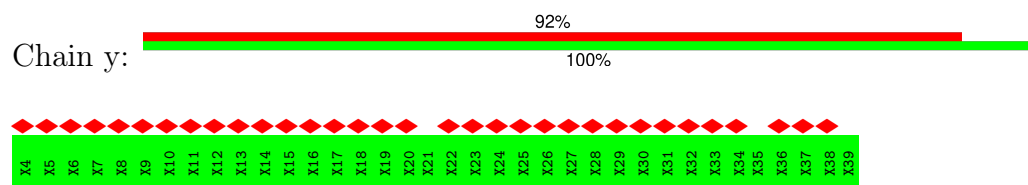
• Molecule 81: tRNA



• Molecule 82: mRNA



• Molecule 83: Nascent chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38314	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 ($e^-/\text{\AA}^2$)	55	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	0.106	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.021	Depositor
Map size (\AA)	460.0, 460.0, 460.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.15, 1.15, 1.15	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.75	1/39959 (0.0%)	1.11	196/62253 (0.3%)
2	SA	0.45	0/1778	0.71	2/2416 (0.1%)
3	SB	0.43	0/1765	0.66	1/2362 (0.0%)
4	SD	0.41	0/1785	0.69	0/2404
5	SE	0.41	0/2101	0.66	2/2828 (0.1%)
6	SF	0.41	0/1516	0.68	0/2037
7	SH	0.41	0/1519	0.70	1/2033 (0.0%)
8	SI	0.42	0/1702	0.66	1/2271 (0.0%)
9	SK	0.43	0/851	0.70	2/1147 (0.2%)
10	SL	0.44	0/1268	0.68	0/1696
11	SP	0.43	0/1065	0.65	0/1423
12	SQ	0.43	0/1177	0.76	4/1575 (0.3%)
13	SR	0.36	0/1097	0.71	0/1474
14	SS	0.42	0/1216	0.71	2/1628 (0.1%)
15	ST	0.44	0/1131	0.68	1/1515 (0.1%)
16	SU	0.37	0/831	0.71	1/1115 (0.1%)
17	SV	0.43	0/631	0.71	0/844
18	SX	0.44	0/1116	0.72	0/1490
19	Sa	0.52	0/836	0.71	1/1121 (0.1%)
20	Sc	0.36	0/508	0.73	0/680
21	Sd	0.44	0/470	0.81	1/623 (0.2%)
22	Sg	0.40	0/2486	0.74	3/3384 (0.1%)
23	SC	0.50	0/1755	0.80	5/2371 (0.2%)
24	SG	0.36	0/1946	0.66	1/2590 (0.0%)
25	SJ	0.41	0/1561	0.77	1/2083 (0.0%)
26	SM	0.34	0/922	0.68	0/1238
27	SN	0.42	0/1232	0.66	1/1656 (0.1%)
28	SO	0.41	0/1037	0.69	0/1391
29	SW	0.50	0/1051	0.71	0/1406
30	SY	0.39	0/1094	0.68	1/1452 (0.1%)
31	SZ	0.41	0/585	0.80	0/785

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Sb	0.40	0/653	0.62	0/876
33	Se	0.36	0/458	0.69	0/604
34	Sf	0.44	1/560 (0.2%)	0.79	0/745
35	A	0.56	0/1968	0.72	2/2639 (0.1%)
36	B	0.53	0/3270	0.75	2/4377 (0.0%)
37	C	0.57	0/2942	0.77	2/3951 (0.1%)
38	D	0.96	2/3726 (0.1%)	1.17	24/5804 (0.4%)
39	E	0.90	1/2839 (0.0%)	1.05	10/4425 (0.2%)
40	F	0.50	0/2437	0.70	1/3262 (0.0%)
41	G	0.48	0/1942	0.81	5/2606 (0.2%)
42	H	0.61	0/1905	0.75	2/2539 (0.1%)
43	I	0.51	0/1913	0.71	1/2576 (0.0%)
44	J	0.46	0/1545	0.68	1/2077 (0.0%)
45	K	0.52	0/1730	0.69	2/2311 (0.1%)
46	L	0.46	0/1376	0.72	2/1841 (0.1%)
47	M	0.50	0/1688	0.75	2/2260 (0.1%)
48	N	0.51	0/1161	0.67	0/1554
49	O	0.62	0/1746	0.79	2/2338 (0.1%)
50	P	0.51	0/1638	0.71	1/2191 (0.0%)
51	Q	0.55	0/1268	0.74	2/1701 (0.1%)
52	R	0.57	0/1537	0.77	3/2052 (0.1%)
53	S	0.47	0/1533	0.72	1/2025 (0.0%)
54	T	0.55	0/1488	0.68	1/1997 (0.1%)
55	U	0.55	0/1312	0.71	0/1753
56	V	0.43	0/822	0.64	0/1103
57	W	0.54	0/983	0.66	0/1319
58	X	0.53	0/524	0.67	0/698
59	Y	0.51	0/975	0.70	0/1312
60	Z	0.55	0/1132	0.68	0/1504
61	a	0.52	0/1126	0.71	1/1502 (0.1%)
62	b	0.57	0/1191	0.80	2/1591 (0.1%)
63	c	0.44	0/826	0.70	1/1088 (0.1%)
64	d	0.50	0/812	0.75	0/1089
65	e	0.50	0/894	0.72	1/1204 (0.1%)
66	f	0.55	0/1082	0.71	0/1443
67	g	0.58	0/895	0.75	1/1198 (0.1%)
68	h	0.53	0/916	0.80	0/1220
69	i	0.48	0/1023	0.72	1/1351 (0.1%)
70	j	0.45	0/805	0.71	0/1065
71	k	0.55	0/703	0.71	0/929
72	l	0.46	0/575	0.68	0/761
73	m	0.52	0/454	0.76	0/599
74	n	0.41	0/417	0.71	0/553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	o	0.40	0/241	0.73	0/305
76	p	0.55	0/877	0.76	0/1156
77	q	0.60	0/718	0.72	0/953
78	r	0.58	0/995	0.85	1/1334 (0.1%)
79	t	0.95	10/86502 (0.0%)	1.16	539/134927 (0.4%)
80	u	0.52	0/1799	1.34	24/2800 (0.9%)
81	v	0.66	1/1802 (0.1%)	1.30	24/2797 (0.9%)
82	w	0.80	0/235	1.50	8/365 (2.2%)
All	All	0.75	16/229950 (0.0%)	1.01	896/337961 (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
25	SJ	0	1
40	F	0	1
47	M	0	1
76	p	0	1
All	All	0	4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1495	G	C2-N3	-6.58	1.27	1.32
79	t	1221	A	N9-C4	-6.56	1.33	1.37
38	D	37	A	N9-C4	-6.53	1.33	1.37
79	t	1321	G	N9-C4	-6.51	1.32	1.38
79	t	148	G	N9-C4	-6.30	1.32	1.38
79	t	4234	G	N9-C4	-5.93	1.33	1.38
79	t	930	A	N9-C4	-5.60	1.34	1.37
79	t	2067	G	N7-C5	-5.47	1.35	1.39
79	t	2067	G	N9-C4	-5.45	1.33	1.38
34	Sf	91	ASN	CA-C	5.42	1.67	1.52
39	E	7	G	C8-N7	-5.33	1.27	1.30
79	t	4298	A	N9-C4	-5.33	1.34	1.37
79	t	714	A	N9-C4	-5.20	1.34	1.37
38	D	62	A	N9-C4	-5.09	1.34	1.37
79	t	1320	A	N9-C4	-5.05	1.34	1.37
81	v	58	A	N9-C4	-5.03	1.34	1.37

All (896) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	115	U	C2-N3-C4	21.07	139.65	127.00
80	u	55	U	N3-C2-O2	-14.70	111.91	122.20
81	v	61	C	C2-N1-C1'	14.12	134.33	118.80
1	S2	65	C	N1-C2-O2	14.06	127.33	118.90
81	v	61	C	N1-C2-O2	13.79	127.17	118.90
1	S2	65	C	C2-N1-C1'	13.32	133.46	118.80
80	u	55	U	N1-C2-O2	13.01	131.91	122.80
1	S2	1283	C	N1-C2-O2	11.92	126.06	118.90
1	S2	1865	C	C6-N1-C2	-11.56	115.68	120.30
1	S2	1453	C	N1-C2-O2	11.52	125.81	118.90
1	S2	115	U	N3-C4-C5	11.27	121.36	114.60
79	t	2323	U	N3-C2-O2	-11.19	114.37	122.20
1	S2	501	C	C2-N1-C1'	11.08	130.99	118.80
38	D	26	C	C6-N1-C2	-11.08	115.87	120.30
80	u	55	U	C2-N1-C1'	10.88	130.75	117.70
1	S2	1453	C	C2-N1-C1'	10.85	130.74	118.80
79	t	918	C	N1-C2-O2	10.80	125.38	118.90
1	S2	65	C	N3-C2-O2	-10.76	114.37	121.90
81	v	61	C	C6-N1-C1'	-10.67	108.00	120.80
1	S2	1341	C	N1-C2-O2	10.58	125.25	118.90
79	t	2323	U	N1-C2-O2	10.37	130.06	122.80
79	t	4480	A	C8-N9-C4	10.13	109.85	105.80
1	S2	65	C	C6-N1-C1'	-10.06	108.73	120.80
1	S2	1139	C	N1-C2-O2	10.04	124.92	118.90
1	S2	118	C	C2-N1-C1'	9.99	129.79	118.80
38	D	126	C	C2-N1-C1'	9.96	129.75	118.80
79	t	4545	C	N1-C2-O2	9.87	124.82	118.90
1	S2	1283	C	N3-C2-O2	-9.86	115.00	121.90
79	t	2330	C	N1-C2-O2	9.86	124.81	118.90
23	SC	78	LEU	CA-CB-CG	9.84	137.93	115.30
79	t	233	G	N3-C2-N2	-9.82	113.03	119.90
1	S2	1139	C	N3-C2-O2	-9.81	115.04	121.90
38	D	126	C	N1-C2-O2	9.69	124.71	118.90
1	S2	578	C	N1-C2-O2	9.67	124.70	118.90
79	t	2447	U	N3-C2-O2	-9.66	115.44	122.20
1	S2	356	C	N1-C2-O2	9.60	124.66	118.90
1	S2	501	C	N1-C2-O2	9.53	124.62	118.90
1	S2	1341	C	N3-C2-O2	-9.41	115.31	121.90
79	t	148	G	N3-C4-N9	-9.37	120.38	126.00
81	v	61	C	N3-C2-O2	-9.34	115.36	121.90
79	t	225	C	C5-C6-N1	9.29	125.65	121.00
1	S2	53	C	C6-N1-C2	-9.19	116.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	t	1930	U	N3-C2-O2	-9.17	115.78	122.20
1	S2	115	U	N1-C2-N3	9.16	120.40	114.90
79	t	148	G	N3-C4-C5	9.16	133.18	128.60
1	S2	1495	G	N3-C2-N2	-9.13	113.51	119.90
79	t	4234	G	N3-C4-N9	-8.93	120.64	126.00
79	t	1321	G	N3-C4-C5	8.92	133.06	128.60
1	S2	356	C	C2-N1-C1'	8.90	128.59	118.80
1	S2	1139	C	C2-N1-C1'	8.88	128.57	118.80
79	t	4736	C	N1-C2-O2	8.76	124.15	118.90
1	S2	1453	C	N3-C2-O2	-8.74	115.78	121.90
79	t	1930	U	C2-N1-C1'	8.64	128.06	117.70
79	t	3616	U	N3-C2-O2	-8.53	116.23	122.20
1	S2	1341	C	C2-N1-C1'	8.52	128.17	118.80
54	T	27	LEU	CA-CB-CG	8.51	134.88	115.30
79	t	225	C	C6-N1-C2	-8.50	116.90	120.30
79	t	1564	U	C2-N1-C1'	8.48	127.88	117.70
79	t	918	C	N3-C2-O2	-8.46	115.98	121.90
79	t	918	C	C2-N1-C1'	8.44	128.08	118.80
1	S2	118	C	N1-C2-O2	8.43	123.96	118.90
79	t	2727	C	C2-N1-C1'	8.39	128.03	118.80
1	S2	501	C	C6-N1-C2	-8.35	116.96	120.30
1	S2	1265	A	C2-N3-C4	8.34	114.77	110.60
1	S2	118	C	C6-N1-C1'	-8.30	110.84	120.80
1	S2	1283	C	C2-N1-C1'	8.28	127.91	118.80
81	v	61	C	C5-C6-N1	8.20	125.10	121.00
79	t	1989	U	C2-N1-C1'	8.19	127.53	117.70
79	t	197	U	C2-N1-C1'	8.18	127.51	117.70
79	t	4736	C	C2-N1-C1'	8.16	127.77	118.80
1	S2	501	C	C5-C6-N1	8.14	125.07	121.00
79	t	2793	C	N1-C2-O2	8.14	123.78	118.90
1	S2	1495	G	N1-C2-N2	8.13	123.52	116.20
79	t	49	U	N1-C2-O2	8.12	128.48	122.80
51	Q	6	LEU	CA-CB-CG	8.10	133.94	115.30
78	r	106	LEU	CA-CB-CG	8.08	133.88	115.30
79	t	302	G	C5-N7-C8	-8.08	100.26	104.30
79	t	4545	C	C2-N1-C1'	8.08	127.69	118.80
79	t	219	C	C2-N1-C1'	8.04	127.64	118.80
79	t	236	C	N1-C2-O2	8.04	123.72	118.90
79	t	4480	A	N7-C8-N9	-8.04	109.78	113.80
79	t	905	G	C4-N9-C1'	8.02	136.92	126.50
1	S2	1520	G	C4-N9-C1'	8.01	136.92	126.50
1	S2	1453	C	C6-N1-C1'	-7.99	111.22	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	t	4480	A	N9-C4-C5	-7.99	102.61	105.80
81	v	71	G	N3-C4-N9	7.98	130.79	126.00
81	v	71	G	C4-N9-C1'	7.95	136.84	126.50
1	S2	578	C	N3-C2-O2	-7.92	116.36	121.90
79	t	2388	U	N1-C2-O2	7.91	128.34	122.80
1	S2	1495	G	O5'-P-OP1	-7.87	98.61	105.70
41	G	234	ASP	CB-CG-OD1	7.87	125.38	118.30
42	H	179	LEU	CA-CB-CG	7.84	133.33	115.30
79	t	3849	C	N1-C2-O2	7.83	123.60	118.90
1	S2	1307	U	N3-C2-O2	-7.82	116.72	122.20
79	t	2499	C	C2-N1-C1'	7.81	127.39	118.80
79	t	1466	G	C4-N9-C1'	7.80	136.64	126.50
38	D	126	C	N3-C2-O2	-7.78	116.46	121.90
79	t	197	U	N1-C2-O2	7.75	128.23	122.80
79	t	2447	U	N1-C2-O2	7.72	128.20	122.80
79	t	2398	C	N3-C2-O2	-7.71	116.50	121.90
79	t	1889	A	O5'-P-OP1	-7.70	98.77	105.70
79	t	1466	G	N3-C4-N9	7.70	130.62	126.00
79	t	2330	C	N3-C2-O2	-7.69	116.52	121.90
1	S2	1057	C	C6-N1-C2	-7.68	117.23	120.30
79	t	4391	C	C6-N1-C2	-7.68	117.23	120.30
79	t	1628	A	C8-N9-C4	7.66	108.86	105.80
1	S2	356	C	N3-C2-O2	-7.65	116.55	121.90
81	v	71	G	C8-N9-C1'	-7.63	117.08	127.00
79	t	197	U	N3-C2-O2	-7.60	116.88	122.20
79	t	2236	C	N1-C2-O2	7.60	123.46	118.90
82	w	17	G	N7-C8-N9	7.60	116.90	113.10
1	S2	913	A	C2-N3-C4	7.59	114.40	110.60
79	t	2373	G	N7-C8-N9	7.58	116.89	113.10
79	t	1562	C	N1-C2-O2	7.57	123.44	118.90
79	t	659	G	C4-N9-C1'	7.56	136.33	126.50
79	t	2282	C	C6-N1-C2	-7.54	117.28	120.30
38	D	26	C	C5-C6-N1	7.53	124.77	121.00
1	S2	1828	C	C6-N1-C2	-7.53	117.29	120.30
79	t	191	C	C6-N1-C2	-7.51	117.30	120.30
79	t	4736	C	N3-C2-O2	-7.50	116.65	121.90
79	t	71	C	C5-C6-N1	7.50	124.75	121.00
1	S2	1572	C	N1-C2-O2	7.49	123.39	118.90
79	t	4234	G	N3-C4-C5	7.46	132.33	128.60
79	t	715	C	N3-C2-O2	-7.44	116.69	121.90
79	t	3858	C	N1-C2-O2	7.44	123.36	118.90
79	t	444	G	O4'-C1'-N9	7.43	114.15	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	t	225	C	C2-N3-C4	7.42	123.61	119.90
1	S2	1865	C	N3-C2-O2	-7.38	116.73	121.90
80	u	43	C	C2-N1-C1'	7.37	126.91	118.80
1	S2	501	C	N3-C2-O2	-7.36	116.75	121.90
80	u	55	U	C6-N1-C2	-7.35	116.59	121.00
81	v	71	G	N3-C4-C5	-7.35	124.92	128.60
1	S2	501	C	C6-N1-C1'	-7.35	111.98	120.80
1	S2	53	C	C5-C6-N1	7.34	124.67	121.00
79	t	2727	C	N3-C2-O2	-7.33	116.77	121.90
79	t	3616	U	N1-C2-O2	7.33	127.93	122.80
79	t	956	C	C2-N1-C1'	7.32	126.85	118.80
79	t	49	U	N3-C2-O2	-7.32	117.08	122.20
79	t	3638	C	C6-N1-C2	-7.31	117.38	120.30
79	t	2373	G	C4-N9-C1'	7.29	135.98	126.50
80	u	48	C	N1-C2-O2	7.27	123.26	118.90
79	t	2388	U	C2-N1-C1'	7.25	126.40	117.70
79	t	219	C	C5-C6-N1	7.25	124.63	121.00
79	t	4832	A	O4'-C1'-N9	7.25	114.00	108.20
79	t	3897	C	C6-N1-C2	-7.25	117.40	120.30
24	SG	68	LEU	CA-CB-CG	7.24	131.96	115.30
1	S2	125	C	N1-C2-O2	7.22	123.23	118.90
79	t	905	G	N3-C4-N9	7.19	130.32	126.00
79	t	4736	C	C6-N1-C2	-7.19	117.42	120.30
79	t	302	G	C4-C5-N7	7.19	113.68	110.80
1	S2	1520	G	N3-C4-N9	7.18	130.31	126.00
1	S2	1520	G	C8-N9-C1'	-7.17	117.69	127.00
79	t	4650	C	N1-C2-O2	7.12	123.17	118.90
79	t	2398	C	N1-C2-O2	7.11	123.17	118.90
79	t	1989	U	N1-C2-O2	7.11	127.78	122.80
79	t	4880	C	C6-N1-C2	-7.11	117.46	120.30
79	t	443	C	N1-C2-O2	7.11	123.16	118.90
79	t	1466	G	N3-C4-C5	-7.11	125.05	128.60
79	t	504	U	C5-C6-N1	7.09	126.25	122.70
79	t	2646	C	C5-C6-N1	7.08	124.54	121.00
79	t	905	G	C8-N9-C1'	-7.04	117.84	127.00
1	S2	1815	A	P-O3'-C3'	7.04	128.15	119.70
79	t	1268	U	O4'-C1'-N1	7.04	113.83	108.20
79	t	1930	U	N1-C2-O2	7.03	127.72	122.80
23	SC	251	LEU	C-N-CA	7.02	139.26	121.70
79	t	4717	G	N3-C4-N9	-7.02	121.79	126.00
1	S2	1064	C	N1-C2-O2	7.01	123.11	118.90
79	t	3765	C	N1-C2-O2	7.01	123.11	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	t	493	G	C4-N9-C1'	7.01	135.61	126.50
79	t	2793	C	C2-N1-C1'	6.99	126.49	118.80
79	t	4717	G	N3-C2-N2	-6.98	115.02	119.90
79	t	214	C	N1-C2-O2	6.97	123.08	118.90
79	t	1564	U	N1-C2-O2	6.97	127.68	122.80
79	t	1746	G	C4-N9-C1'	6.96	135.54	126.50
7	SH	148	LEU	CA-CB-CG	6.96	131.30	115.30
79	t	2646	C	C6-N1-C2	-6.93	117.53	120.30
79	t	1466	G	C8-N9-C1'	-6.92	118.00	127.00
36	B	214	ASP	CB-CG-OD1	6.91	124.52	118.30
79	t	4880	C	N1-C2-O2	6.90	123.04	118.90
79	t	148	G	C4-N9-C1'	-6.89	117.54	126.50
79	t	471	C	C5-C6-N1	6.89	124.44	121.00
79	t	1321	G	N3-C4-N9	-6.89	121.87	126.00
79	t	3595	A	P-O3'-C3'	6.89	127.97	119.70
62	b	11	LEU	CA-CB-CG	6.88	131.13	115.30
79	t	2065	C	N3-C2-O2	-6.88	117.08	121.90
79	t	4545	C	N3-C2-O2	-6.88	117.08	121.90
1	S2	681	U	C6-N1-C2	-6.88	116.87	121.00
79	t	219	C	N1-C2-O2	6.87	123.02	118.90
79	t	698	C	N3-C2-O2	-6.85	117.11	121.90
79	t	4936	G	O4'-C1'-N9	6.84	113.67	108.20
79	t	4575	C	N1-C2-O2	6.83	123.00	118.90
81	v	62	C	N1-C2-O2	6.82	122.99	118.90
79	t	471	C	C6-N1-C2	-6.82	117.57	120.30
79	t	302	G	N7-C8-N9	6.82	116.51	113.10
38	D	126	C	C6-N1-C1'	-6.81	112.62	120.80
80	u	48	C	C2-N1-C1'	6.81	126.29	118.80
79	t	71	C	C6-N1-C2	-6.80	117.58	120.30
79	t	698	C	N1-C2-O2	6.79	122.97	118.90
1	S2	1572	C	C6-N1-C2	-6.76	117.60	120.30
45	K	103	LEU	CA-CB-CG	6.75	130.83	115.30
35	A	180	LEU	CA-CB-CG	6.75	130.82	115.30
1	S2	681	U	N3-C2-O2	-6.75	117.48	122.20
79	t	2373	G	C8-N9-C4	-6.74	103.70	106.40
1	S2	867	G	N3-C4-C5	-6.74	125.23	128.60
50	P	141	LEU	CA-CB-CG	6.73	130.79	115.30
1	S2	559	G	P-O3'-C3'	6.73	127.78	119.70
38	D	129	C	C6-N1-C2	-6.73	117.61	120.30
79	t	670	C	N3-C2-O2	-6.72	117.19	121.90
79	t	4234	G	C8-N9-C1'	6.72	135.73	127.00
79	t	2793	C	N3-C2-O2	-6.71	117.20	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	t	4660	C	C6-N1-C2	-6.71	117.62	120.30
38	D	126	C	C6-N1-C2	-6.70	117.62	120.30
41	G	173	LEU	CA-CB-CG	6.69	130.68	115.30
79	t	232	A	C2-N3-C4	6.68	113.94	110.60
79	t	918	C	C6-N1-C1'	-6.67	112.79	120.80
79	t	2323	U	C2-N1-C1'	6.66	125.69	117.70
1	S2	1865	C	N3-C4-C5	-6.64	119.24	121.90
79	t	1638	U	N3-C2-O2	-6.64	117.56	122.20
79	t	1335	C	C6-N1-C2	-6.63	117.65	120.30
80	u	48	C	N3-C2-O2	-6.63	117.26	121.90
79	t	901	U	P-O3'-C3'	6.62	127.65	119.70
79	t	493	G	N3-C4-C5	-6.62	125.29	128.60
81	v	61	C	C6-N1-C2	-6.62	117.65	120.30
79	t	659	G	C8-N9-C1'	-6.61	118.40	127.00
79	t	1995	C	C6-N1-C2	-6.60	117.66	120.30
81	v	12	C	N1-C2-O2	6.60	122.86	118.90
47	M	144	LEU	CA-CB-CG	6.59	130.47	115.30
79	t	2398	C	C2-N1-C1'	6.59	126.05	118.80
42	H	169	LEU	CA-CB-CG	6.59	130.46	115.30
79	t	1060	C	C6-N1-C2	-6.59	117.67	120.30
79	t	226	G	C4-N9-C1'	-6.58	117.94	126.50
79	t	4946	U	P-O3'-C3'	6.57	127.59	119.70
79	t	649	C	N1-C2-O2	6.55	122.83	118.90
79	t	238	G	N3-C4-N9	-6.54	122.07	126.00
79	t	216	G	N3-C2-N2	-6.54	115.32	119.90
79	t	1261	C	N1-C2-O2	6.54	122.82	118.90
79	t	1261	C	N3-C2-O2	-6.54	117.33	121.90
79	t	2323	U	C6-N1-C2	-6.53	117.08	121.00
79	t	1564	U	C6-N1-C1'	-6.53	112.06	121.20
79	t	2043	C	C6-N1-C2	-6.53	117.69	120.30
63	c	116	LEU	CA-CB-CG	6.53	130.31	115.30
79	t	4545	C	C6-N1-C1'	-6.52	112.97	120.80
1	S2	1341	C	C6-N1-C2	-6.51	117.70	120.30
79	t	2029	U	N3-C2-O2	-6.50	117.65	122.20
79	t	4313	U	N3-C2-O2	-6.50	117.65	122.20
79	t	3765	C	N3-C2-O2	-6.50	117.35	121.90
1	S2	356	C	C6-N1-C1'	-6.49	113.02	120.80
79	t	649	C	C5-C6-N1	6.48	124.24	121.00
1	S2	585	C	N1-C2-O2	6.48	122.79	118.90
79	t	1086	C	N1-C2-O2	6.47	122.78	118.90
79	t	470	G	N3-C4-N9	6.47	129.88	126.00
80	u	2	C	N1-C2-O2	6.47	122.78	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1053	C	N1-C2-O2	6.46	122.78	118.90
79	t	4601	G	N3-C4-N9	-6.46	122.12	126.00
79	t	956	C	N1-C2-O2	6.46	122.77	118.90
79	t	451	G	N3-C2-N2	-6.45	115.39	119.90
1	S2	1813	A	P-O3'-C3'	6.44	127.43	119.70
82	w	17	G	C6-C5-N7	-6.44	126.54	130.40
79	t	1614	A	C2-N3-C4	6.43	113.82	110.60
21	Sd	6	LEU	CA-CB-CG	6.43	130.09	115.30
23	SC	83	LEU	CA-CB-CG	6.43	130.08	115.30
79	t	2617	G	N3-C4-N9	-6.42	122.15	126.00
79	t	1260	G	N3-C2-N2	-6.41	115.41	119.90
79	t	2065	C	N1-C2-O2	6.41	122.75	118.90
1	S2	1495	G	C2-N3-C4	6.41	115.10	111.90
41	G	50	LEU	CB-CG-CD2	-6.41	100.11	111.00
79	t	4629	C	C6-N1-C2	-6.40	117.74	120.30
79	t	1746	G	N3-C4-N9	6.40	129.84	126.00
1	S2	879	C	N1-C2-O2	6.39	122.73	118.90
79	t	256	C	N1-C2-O2	6.39	122.73	118.90
79	t	2350	U	N1-C2-O2	6.38	127.27	122.80
1	S2	578	C	C2-N1-C1'	6.37	125.81	118.80
79	t	695	C	N1-C2-O2	6.37	122.72	118.90
79	t	4575	C	N3-C2-O2	-6.37	117.44	121.90
79	t	4616	C	C6-N1-C2	-6.37	117.75	120.30
79	t	2344	C	C6-N1-C2	-6.37	117.75	120.30
79	t	2373	G	C6-C5-N7	-6.37	126.58	130.40
79	t	2447	U	C6-N1-C2	-6.37	117.18	121.00
79	t	1321	G	C2-N3-C4	-6.36	108.72	111.90
79	t	4185	C	C6-N1-C2	-6.36	117.76	120.30
79	t	4946	U	OP1-P-O3'	6.36	119.19	105.20
38	D	116	C	C6-N1-C2	-6.36	117.76	120.30
79	t	1638	U	N1-C2-O2	6.36	127.25	122.80
79	t	3569	C	N1-C2-O2	6.36	122.71	118.90
79	t	1367	C	C6-N1-C2	-6.35	117.76	120.30
79	t	4880	C	C2-N1-C1'	6.35	125.78	118.80
79	t	958	U	C2-N1-C1'	6.34	125.31	117.70
79	t	2325	C	N3-C2-O2	-6.34	117.46	121.90
38	D	129	C	C2-N1-C1'	6.33	125.77	118.80
81	v	55	U	C5-C6-N1	6.33	125.87	122.70
81	v	59	U	N1-C2-O2	6.32	127.22	122.80
79	t	964	C	N1-C2-O2	6.30	122.68	118.90
79	t	2727	C	N1-C2-O2	6.29	122.68	118.90
79	t	2228	C	N1-C2-O2	6.29	122.68	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	v	50	U	P-O3'-C3'	6.29	127.25	119.70
1	S2	1566	G	C4-C5-N7	6.29	113.32	110.80
79	t	190	G	N3-C2-N2	-6.29	115.50	119.90
79	t	905	G	N3-C4-C5	-6.29	125.45	128.60
79	t	3797	C	C6-N1-C2	-6.29	117.78	120.30
40	F	36	LEU	CA-CB-CG	6.29	129.76	115.30
79	t	3762	C	N1-C2-O2	6.29	122.67	118.90
80	u	55	U	C5-C4-O4	6.29	129.67	125.90
79	t	4601	G	N3-C2-N2	-6.28	115.50	119.90
79	t	2249	G	N3-C4-N9	-6.28	122.23	126.00
1	S2	456	C	C6-N1-C2	-6.28	117.79	120.30
79	t	2029	U	N1-C2-O2	6.28	127.19	122.80
79	t	4820	G	N1-C6-O6	6.28	123.67	119.90
79	t	4713	G	N3-C4-C5	6.27	131.74	128.60
79	t	2032	C	C6-N1-C2	-6.27	117.79	120.30
22	Sg	7	LEU	CA-CB-CG	6.26	129.69	115.30
79	t	690	C	N1-C2-O2	6.25	122.65	118.90
79	t	4709	C	C6-N1-C2	-6.25	117.80	120.30
79	t	727	C	C6-N1-C2	-6.24	117.81	120.30
79	t	1610	C	C6-N1-C2	-6.23	117.81	120.30
80	u	59	U	N1-C2-O2	6.23	127.16	122.80
79	t	123	C	C5-C6-N1	6.22	124.11	121.00
1	S2	30	C	C6-N1-C2	-6.22	117.81	120.30
1	S2	65	C	C6-N1-C2	-6.22	117.81	120.30
79	t	2499	C	N1-C2-O2	6.21	122.63	118.90
79	t	1562	C	N3-C2-O2	-6.21	117.55	121.90
79	t	2330	C	C2-N1-C1'	6.21	125.63	118.80
79	t	234	G	O5'-P-OP1	-6.19	100.13	105.70
79	t	49	U	O5'-P-OP2	-6.19	100.13	105.70
79	t	4826	G	N3-C2-N2	-6.19	115.57	119.90
79	t	470	G	C6-C5-N7	-6.19	126.69	130.40
79	t	3762	C	N3-C2-O2	-6.18	117.57	121.90
79	t	233	G	N1-C2-N2	6.18	121.76	116.20
79	t	2499	C	N3-C2-O2	-6.18	117.58	121.90
79	t	3849	C	N3-C2-O2	-6.18	117.58	121.90
79	t	715	C	N1-C2-O2	6.18	122.61	118.90
79	t	4974	A	N7-C8-N9	6.17	116.89	113.80
82	w	17	G	C4-N9-C1'	6.17	134.53	126.50
80	u	72	C	C6-N1-C2	-6.17	117.83	120.30
14	SS	103	LEU	CA-CB-CG	6.16	129.47	115.30
1	S2	872	A	P-O3'-C3'	6.16	127.09	119.70
79	t	1910	A	C2-N3-C4	6.16	113.68	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	t	2617	G	N3-C4-C5	6.15	131.68	128.60
79	t	493	G	N3-C4-N9	6.15	129.69	126.00
79	t	28	C	C6-N1-C2	-6.15	117.84	120.30
79	t	1176	C	N1-C2-O2	6.15	122.59	118.90
1	S2	1139	C	C6-N1-C2	-6.15	117.84	120.30
1	S2	445	A	P-O3'-C3'	6.15	127.08	119.70
79	t	1155	C	C6-N1-C2	-6.15	117.84	120.30
79	t	217	C	C6-N1-C2	-6.14	117.84	120.30
79	t	28	C	N1-C2-O2	6.14	122.58	118.90
79	t	226	G	C4-C5-N7	-6.14	108.34	110.80
79	t	1995	C	C5-C6-N1	6.14	124.07	121.00
79	t	4267	G	N3-C2-N2	-6.14	115.61	119.90
79	t	148	G	C8-N9-C1'	6.13	134.97	127.00
79	t	214	C	C2-N1-C1'	6.13	125.54	118.80
79	t	1350	C	N1-C2-O2	6.13	122.58	118.90
79	t	4601	G	N3-C4-C5	6.13	131.66	128.60
79	t	4880	C	N3-C2-O2	-6.12	117.61	121.90
80	u	43	C	N1-C2-O2	6.12	122.57	118.90
79	t	504	U	O5'-P-OP2	-6.12	100.19	105.70
79	t	289	A	N3-C4-N9	6.12	132.29	127.40
1	S2	867	G	N3-C4-N9	6.11	129.67	126.00
79	t	2325	C	N1-C2-O2	6.11	122.57	118.90
79	t	1564	U	N3-C2-O2	-6.11	117.93	122.20
80	u	55	U	C6-N1-C1'	-6.11	112.65	121.20
79	t	1618	U	N1-C2-O2	6.10	127.07	122.80
1	S2	548	C	C2-N1-C1'	6.10	125.51	118.80
79	t	4177	C	N1-C2-O2	6.10	122.56	118.90
1	S2	65	C	C5-C6-N1	6.09	124.05	121.00
79	t	1614	A	C4-N9-C1'	6.09	137.27	126.30
1	S2	424	C	C6-N1-C2	-6.09	117.86	120.30
16	SU	32	LEU	CA-CB-CG	6.08	129.29	115.30
15	ST	123	LEU	CA-CB-CG	6.08	129.28	115.30
1	S2	1572	C	C5-C6-N1	6.08	124.04	121.00
39	E	47	G	O4'-C1'-N9	6.07	113.06	108.20
79	t	48	G	O4'-C1'-N9	6.06	113.05	108.20
79	t	1989	U	N3-C2-O2	-6.06	117.96	122.20
1	S2	1261	C	C5-C6-N1	6.06	124.03	121.00
79	t	1321	G	N3-C2-N2	-6.05	115.66	119.90
80	u	17	C	N1-C2-O2	6.05	122.53	118.90
79	t	2249	G	N9-C4-C5	6.05	107.82	105.40
79	t	3659	U	C5-C6-N1	6.05	125.72	122.70
1	S2	1252	C	C5-C6-N1	6.05	124.02	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	t	905	G	C6-C5-N7	-6.05	126.77	130.40
79	t	2447	U	C2-N1-C1'	6.05	124.95	117.70
79	t	5026	G	C4-N9-C1'	6.05	134.36	126.50
79	t	1909	C	C6-N1-C2	6.04	122.72	120.30
79	t	2236	C	C2-N1-C1'	6.04	125.45	118.80
79	t	2344	C	C5-C6-N1	6.04	124.02	121.00
1	S2	1139	C	C6-N1-C1'	-6.03	113.56	120.80
1	S2	1265	A	N3-C4-N9	6.03	132.22	127.40
79	t	3735	U	C5-C6-N1	6.02	125.71	122.70
38	D	123	U	N1-C2-O2	6.02	127.01	122.80
82	w	19	C	C6-N1-C2	-6.01	117.90	120.30
79	t	2835	C	N1-C2-O2	5.99	122.50	118.90
1	S2	736	C	C6-N1-C2	-5.99	117.90	120.30
1	S2	1314	U	O4'-C1'-N1	5.99	112.99	108.20
1	S2	1566	G	C5-C6-O6	-5.99	125.01	128.60
79	t	4678	C	C6-N1-C2	-5.99	117.91	120.30
79	t	226	G	C8-N9-C1'	5.98	134.78	127.00
79	t	2388	U	N3-C2-O2	-5.98	118.02	122.20
79	t	229	G	C4-N9-C1'	-5.98	118.73	126.50
79	t	727	C	C5-C6-N1	5.97	123.99	121.00
79	t	3569	C	N3-C2-O2	-5.96	117.72	121.90
38	D	129	C	N3-C2-O2	-5.96	117.73	121.90
79	t	2389	C	N1-C2-O2	5.96	122.48	118.90
1	S2	1283	C	C6-N1-C2	-5.96	117.92	120.30
1	S2	1307	U	C2-N1-C1'	5.96	124.85	117.70
44	J	142	ASP	CB-CG-OD1	5.96	123.66	118.30
79	t	443	C	C6-N1-C2	-5.96	117.92	120.30
1	S2	115	U	C5-C4-O4	-5.96	122.33	125.90
53	S	24	LEU	CA-CB-CG	5.96	129.00	115.30
79	t	28	C	N3-C2-O2	-5.96	117.73	121.90
79	t	1746	G	C8-N9-C1'	-5.95	119.27	127.00
79	t	1413	C	C5-C6-N1	5.95	123.97	121.00
81	v	58	A	N3-C4-N9	-5.94	122.65	127.40
1	S2	1289	U	N1-C2-O2	5.93	126.95	122.80
79	t	470	G	C4-N9-C1'	5.93	134.22	126.50
80	u	59	U	N3-C2-O2	-5.93	118.05	122.20
79	t	463	C	N1-C2-O2	5.93	122.46	118.90
81	v	12	C	N3-C2-O2	-5.93	117.75	121.90
1	S2	1572	C	N3-C2-O2	-5.92	117.75	121.90
79	t	2608	C	C6-N1-C2	-5.92	117.93	120.30
79	t	700	C	N3-C2-O2	-5.92	117.76	121.90
79	t	243	G	N3-C4-N9	-5.91	122.45	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	SE	139	LEU	CA-CB-CG	5.91	128.88	115.30
79	t	1221	A	N3-C4-N9	-5.90	122.68	127.40
35	A	116	LEU	CA-CB-CG	5.89	128.85	115.30
79	t	1648	C	C6-N1-C2	-5.89	117.94	120.30
79	t	930	A	C6-N1-C2	5.89	122.13	118.60
79	t	4234	G	C4-N9-C1'	-5.89	118.84	126.50
79	t	493	G	C8-N9-C1'	-5.88	119.35	127.00
79	t	1260	G	N3-C4-N9	-5.88	122.47	126.00
52	R	63	LEU	CA-CB-CG	5.88	128.83	115.30
79	t	462	U	N3-C2-O2	-5.87	118.09	122.20
79	t	207	C	N1-C2-O2	5.87	122.42	118.90
79	t	509	C	C5-C6-N1	5.86	123.93	121.00
79	t	669	G	N3-C4-N9	-5.86	122.48	126.00
79	t	1910	A	N3-C4-N9	5.86	132.09	127.40
79	t	927	C	C2-N1-C1'	5.86	125.24	118.80
79	t	3659	U	N3-C2-O2	-5.85	118.11	122.20
79	t	5026	G	N3-C4-N9	5.85	129.51	126.00
79	t	3858	C	N3-C2-O2	-5.85	117.81	121.90
79	t	1176	C	N3-C2-O2	-5.84	117.81	121.90
79	t	4333	G	P-O3'-C3'	5.84	126.71	119.70
79	t	2727	C	C6-N1-C2	-5.83	117.97	120.30
79	t	2539	C	C6-N1-C2	-5.83	117.97	120.30
79	t	298	C	C6-N1-C2	-5.83	117.97	120.30
38	D	6	C	C5-C6-N1	5.83	123.91	121.00
1	S2	1106	C	C5-C6-N1	5.82	123.91	121.00
79	t	1413	C	C6-N1-C2	-5.82	117.97	120.30
1	S2	387	C	C6-N1-C2	-5.82	117.97	120.30
79	t	470	G	N1-C2-N2	-5.82	110.97	116.20
3	SB	74	LEU	CA-CB-CG	5.82	128.68	115.30
79	t	236	C	N3-C2-O2	-5.82	117.83	121.90
79	t	4716	G	N3-C2-N2	-5.82	115.83	119.90
79	t	966	C	C6-N1-C2	-5.81	117.98	120.30
1	S2	1707	U	C2-N1-C1'	5.80	124.67	117.70
79	t	489	C	N3-C2-O2	-5.80	117.84	121.90
79	t	3659	U	C6-N1-C2	-5.80	117.52	121.00
80	u	37	U	N3-C2-O2	-5.80	118.14	122.20
46	L	171	ASP	CB-CG-OD1	5.79	123.51	118.30
1	S2	682	U	C5-C6-N1	5.79	125.59	122.70
79	t	4391	C	C5-C6-N1	5.79	123.89	121.00
79	t	4616	C	C5-C6-N1	5.79	123.89	121.00
79	t	1618	U	N3-C2-O2	-5.78	118.15	122.20
79	t	2234	C	C2-N1-C1'	5.78	125.16	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	t	219	C	C6-N1-C1'	-5.78	113.86	120.80
79	t	4250	C	C6-N1-C2	-5.78	117.99	120.30
79	t	1489	C	C6-N1-C2	-5.78	117.99	120.30
79	t	649	C	C2-N1-C1'	5.77	125.15	118.80
1	S2	1520	G	N3-C4-C5	-5.77	125.72	128.60
1	S2	1314	U	C2-N1-C1'	5.77	124.62	117.70
1	S2	1661	A	P-O3'-C3'	5.76	126.61	119.70
30	SY	94	HIS	N-CA-C	-5.76	95.46	111.00
52	R	138	LEU	CA-CB-CG	5.75	128.52	115.30
79	t	4660	C	C5-C6-N1	5.75	123.87	121.00
79	t	4888	C	N3-C2-O2	-5.75	117.88	121.90
79	t	4713	G	N3-C4-N9	-5.75	122.55	126.00
39	E	47	G	N7-C8-N9	5.74	115.97	113.10
1	S2	358	C	N3-C2-O2	-5.74	117.88	121.90
79	t	2236	C	N3-C2-O2	-5.74	117.88	121.90
1	S2	1265	A	N3-C4-C5	-5.73	122.79	126.80
79	t	344	C	N1-C2-O2	5.73	122.34	118.90
79	t	2330	C	C6-N1-C2	-5.73	118.01	120.30
79	t	5015	C	C6-N1-C2	-5.73	118.01	120.30
79	t	4820	G	C5-C6-O6	-5.73	125.16	128.60
9	SK	43	LEU	CA-CB-CG	5.72	128.47	115.30
79	t	2727	C	C6-N1-C1'	-5.72	113.93	120.80
79	t	4069	G	OP2-P-O3'	5.72	117.79	105.20
1	S2	346	C	C6-N1-C2	-5.72	118.01	120.30
79	t	659	G	N3-C4-N9	5.72	129.43	126.00
49	O	134	LEU	CA-CB-CG	5.72	128.45	115.30
79	t	407	G	C4-N9-C1'	5.72	133.94	126.50
79	t	216	G	N1-C2-N3	5.72	127.33	123.90
49	O	200	LEU	CA-CB-CG	5.72	128.45	115.30
79	t	71	C	P-O3'-C3'	5.72	126.56	119.70
36	B	85	VAL	CG1-CB-CG2	-5.71	101.76	110.90
79	t	123	C	C6-N1-C2	-5.71	118.01	120.30
79	t	474	C	N3-C2-O2	-5.71	117.90	121.90
1	S2	749	U	C5-C6-N1	5.70	125.55	122.70
79	t	289	A	N9-C4-C5	-5.70	103.52	105.80
79	t	2076	G	C4-N9-C1'	5.70	133.91	126.50
79	t	2373	G	C5-N7-C8	-5.70	101.45	104.30
45	K	48	LEU	CA-CB-CG	5.70	128.41	115.30
81	v	62	C	N3-C2-O2	-5.70	117.91	121.90
80	u	59	U	C2-N1-C1'	5.69	124.53	117.70
1	S2	125	C	N3-C2-O2	-5.69	117.92	121.90
1	S2	1520	G	C6-C5-N7	-5.69	126.99	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	t	4650	C	N3-C2-O2	-5.69	117.92	121.90
79	t	352	C	N1-C2-O2	5.68	122.31	118.90
79	t	1746	G	N3-C4-C5	-5.68	125.76	128.60
1	S2	387	C	C5-C6-N1	5.68	123.84	121.00
12	SQ	92	LEU	CA-CB-CG	5.68	128.36	115.30
79	t	462	U	N1-C2-O2	5.67	126.77	122.80
79	t	2350	U	N3-C2-O2	-5.67	118.23	122.20
1	S2	144	U	N1-C2-O2	5.67	126.77	122.80
47	M	146	LEU	CA-CB-CG	5.67	128.33	115.30
79	t	288	G	C4-N9-C1'	5.67	133.87	126.50
79	t	1176	C	C6-N1-C2	-5.67	118.03	120.30
79	t	1989	U	C6-N1-C1'	-5.67	113.27	121.20
79	t	4069	G	P-O3'-C3'	5.67	126.50	119.70
1	S2	751	G	C4-N9-C1'	5.67	133.86	126.50
79	t	1647	C	C6-N1-C2	-5.66	118.03	120.30
1	S2	973	C	N1-C2-O2	5.66	122.30	118.90
1	S2	427	U	C2-N1-C1'	5.66	124.49	117.70
1	S2	1289	U	N3-C2-O2	-5.66	118.24	122.20
79	t	2766	A	N7-C8-N9	5.66	116.63	113.80
1	S2	736	C	C5-C6-N1	5.66	123.83	121.00
79	t	4838	C	N1-C2-O2	5.65	122.29	118.90
1	S2	1689	C	C6-N1-C2	-5.65	118.04	120.30
1	S2	144	U	C5-C6-N1	5.65	125.53	122.70
1	S2	106	C	C6-N1-C2	-5.65	118.04	120.30
79	t	2799	C	N1-C2-O2	5.65	122.29	118.90
82	w	17	G	C8-N9-C4	-5.65	104.14	106.40
1	S2	1453	C	C5-C6-N1	5.64	123.82	121.00
14	SS	82	TRP	CA-CB-CG	5.64	124.42	113.70
41	G	233	PHE	C-N-CA	5.64	135.80	121.70
1	S2	79	A	P-O3'-C3'	5.64	126.47	119.70
1	S2	1453	C	C6-N1-C2	-5.64	118.05	120.30
79	t	49	U	C2-N1-C1'	5.63	124.46	117.70
79	t	2373	G	O4'-C1'-N9	5.63	112.71	108.20
1	S2	1005	G	N3-C4-N9	5.63	129.38	126.00
79	t	489	C	N1-C2-O2	5.63	122.28	118.90
82	w	20	G	P-O3'-C3'	5.62	126.44	119.70
79	t	2241	G	C4-N9-C1'	5.61	133.80	126.50
79	t	4401	U	C5-C6-N1	5.61	125.51	122.70
43	I	136	LEU	CA-CB-CG	5.61	128.21	115.30
79	t	2718	C	C6-N1-C2	5.61	122.55	120.30
1	S2	35	C	C6-N1-C2	-5.61	118.06	120.30
79	t	443	C	C5-C6-N1	5.61	123.80	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1252	C	C6-N1-C2	-5.59	118.06	120.30
79	t	197	U	C6-N1-C1'	-5.59	113.37	121.20
79	t	4703	C	N1-C2-O2	5.59	122.25	118.90
1	S2	492	C	C6-N1-C2	5.59	122.54	120.30
79	t	1234	C	N1-C2-O2	5.59	122.25	118.90
79	t	352	C	N3-C2-O2	-5.58	117.99	121.90
1	S2	1341	C	C6-N1-C1'	-5.58	114.11	120.80
79	t	1378	U	C5-C6-N1	5.58	125.49	122.70
1	S2	1864	U	N3-C2-O2	-5.58	118.30	122.20
79	t	2582	C	C6-N1-C2	-5.58	118.07	120.30
79	t	4267	G	N3-C4-N9	5.58	129.35	126.00
79	t	14	C	N1-C2-O2	5.57	122.24	118.90
79	t	2499	C	C6-N1-C2	-5.57	118.07	120.30
79	t	4099	C	N1-C2-O2	5.57	122.24	118.90
79	t	1594	G	C4-N9-C1'	5.57	133.74	126.50
79	t	4992	A	N7-C8-N9	5.57	116.58	113.80
79	t	3762	C	C2-N1-C1'	5.57	124.92	118.80
79	t	2239	C	N1-C2-O2	5.56	122.24	118.90
79	t	1910	A	C4-N9-C1'	5.55	136.30	126.30
79	t	1912	C	N1-C2-O2	5.55	122.23	118.90
79	t	710	C	N3-C2-O2	-5.55	118.01	121.90
79	t	2632	C	C6-N1-C2	-5.55	118.08	120.30
79	t	196	G	N3-C4-N9	-5.54	122.67	126.00
80	u	11	C	C6-N1-C2	-5.54	118.08	120.30
1	S2	1786	U	C5-C6-N1	5.54	125.47	122.70
65	e	95	ASP	CB-CG-OD1	5.53	123.28	118.30
39	E	57	C	C6-N1-C2	-5.53	118.09	120.30
79	t	4820	G	C6-C5-N7	-5.53	127.08	130.40
1	S2	96	C	C6-N1-C2	-5.52	118.09	120.30
79	t	2249	G	C8-N9-C4	-5.52	104.19	106.40
79	t	4951	G	N3-C4-C5	5.52	131.36	128.60
1	S2	303	C	N1-C2-O2	5.52	122.21	118.90
38	D	126	C	C5-C6-N1	5.52	123.76	121.00
1	S2	1283	C	C6-N1-C1'	-5.52	114.18	120.80
1	S2	1660	C	C2-N1-C1'	5.52	124.87	118.80
79	t	930	A	N1-C2-N3	-5.52	126.54	129.30
79	t	2373	G	C4-C5-N7	5.51	113.01	110.80
79	t	226	G	N3-C4-N9	-5.51	122.69	126.00
79	t	2484	C	C5-C6-N1	5.51	123.75	121.00
79	t	2652	G	O4'-C1'-N9	-5.51	103.80	108.20
79	t	226	G	C6-C5-N7	5.50	133.70	130.40
41	G	125	LEU	CA-CB-CG	5.50	127.95	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	t	1262	A	C2-N3-C4	-5.50	107.85	110.60
79	t	4717	G	C8-N9-C1'	5.50	134.14	127.00
79	t	2229	C	N1-C2-O2	5.49	122.20	118.90
79	t	2759	C	C5-C6-N1	5.49	123.75	121.00
79	t	4717	G	C4-N9-C1'	-5.49	119.36	126.50
38	D	80	A	C2-N3-C4	5.49	113.34	110.60
79	t	470	G	C8-N9-C1'	-5.49	119.87	127.00
1	S2	1261	C	C6-N1-C2	-5.48	118.11	120.30
1	S2	1591	C	C6-N1-C2	-5.48	118.11	120.30
1	S2	867	G	C4-N9-C1'	5.48	133.62	126.50
79	t	2016	C	C6-N1-C2	-5.47	118.11	120.30
1	S2	1694	U	C5-C6-N1	5.47	125.43	122.70
23	SC	78	LEU	CB-CG-CD1	-5.46	101.72	111.00
79	t	207	C	N3-C2-O2	-5.46	118.08	121.90
79	t	2032	C	N3-C2-O2	-5.46	118.08	121.90
79	t	940	C	N3-C2-O2	-5.45	118.08	121.90
79	t	4313	U	N1-C2-O2	5.45	126.62	122.80
79	t	4267	G	N3-C4-C5	-5.45	125.88	128.60
79	t	691	G	N3-C2-N2	-5.45	116.09	119.90
79	t	714	A	C5-N7-C8	-5.45	101.18	103.90
79	t	1083	U	N1-C2-O2	5.45	126.61	122.80
79	t	669	G	N3-C2-N2	-5.45	116.09	119.90
39	E	105	C	N1-C2-O2	5.44	122.17	118.90
1	S2	751	G	N3-C4-N9	5.44	129.27	126.00
1	S2	1375	G	P-O3'-C3'	5.44	126.23	119.70
79	t	289	A	C4-C5-N7	5.44	113.42	110.70
79	t	4729	C	N3-C2-O2	-5.44	118.09	121.90
79	t	690	C	C5-C6-N1	5.44	123.72	121.00
1	S2	1495	G	C4-C5-C6	-5.44	115.54	118.80
79	t	4709	C	C5-C6-N1	5.43	123.72	121.00
1	S2	1259	A	N1-C6-N6	5.43	121.86	118.60
12	SQ	57	LEU	CA-CB-CG	5.43	127.79	115.30
38	D	147	G	O4'-C1'-N9	5.43	112.54	108.20
79	t	4732	U	C5-C6-N1	5.43	125.42	122.70
79	t	4936	G	C4-N9-C1'	5.43	133.56	126.50
38	D	6	C	C6-N1-C2	-5.42	118.13	120.30
1	S2	570	C	N1-C2-O2	5.42	122.15	118.90
79	t	1163	C	C2-N1-C1'	5.42	124.76	118.80
79	t	288	G	C8-N9-C1'	-5.42	119.96	127.00
79	t	4678	C	C5-C6-N1	5.42	123.71	121.00
79	t	4858	C	N1-C2-O2	5.42	122.15	118.90
79	t	1335	C	C5-C6-N1	5.41	123.70	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	t	1060	C	N3-C4-N4	5.41	121.78	118.00
79	t	3638	C	C5-C6-N1	5.41	123.70	121.00
79	t	4624	C	C6-N1-C2	-5.41	118.14	120.30
79	t	1910	A	N3-C4-C5	-5.40	123.02	126.80
1	S2	559	G	C4-N9-C1'	-5.40	119.48	126.50
38	D	11	C	C6-N1-C2	-5.40	118.14	120.30
79	t	249	C	N3-C2-O2	-5.40	118.12	121.90
1	S2	563	G	P-O3'-C3'	5.40	126.17	119.70
79	t	1771	C	C6-N1-C2	-5.39	118.14	120.30
79	t	4480	A	C5-N7-C8	5.39	106.60	103.90
79	t	2009	C	C6-N1-C2	-5.39	118.14	120.30
79	t	4884	C	C6-N1-C2	-5.39	118.14	120.30
1	S2	427	U	N3-C2-O2	-5.38	118.43	122.20
1	S2	53	C	P-O3'-C3'	5.38	126.16	119.70
1	S2	1805	G	N3-C4-N9	5.38	129.23	126.00
79	t	894	C	C6-N1-C2	-5.38	118.15	120.30
79	t	79	C	C6-N1-C2	-5.38	118.15	120.30
79	t	229	G	N3-C4-N9	-5.38	122.77	126.00
61	a	101	PHE	C-N-CA	5.37	135.12	121.70
1	S2	317	C	P-O3'-C3'	5.37	126.14	119.70
79	t	1388	C	C6-N1-C2	-5.37	118.15	120.30
79	t	2637	G	N7-C8-N9	5.37	115.78	113.10
79	t	4216	G	C4-N9-C1'	5.36	133.47	126.50
52	R	5	ILE	N-CA-C	-5.36	96.53	111.00
79	t	1930	U	C6-N1-C1'	-5.36	113.69	121.20
79	t	2474	U	N3-C2-O2	-5.36	118.45	122.20
1	S2	456	C	C5-C6-N1	5.36	123.68	121.00
79	t	3732	C	P-O3'-C3'	5.36	126.13	119.70
39	E	48	G	C4-N9-C1'	5.36	133.46	126.50
79	t	4716	G	N3-C4-N9	-5.36	122.79	126.00
79	t	670	C	N1-C2-O2	5.35	122.11	118.90
79	t	4633	C	N1-C2-O2	5.35	122.11	118.90
79	t	4093	G	N3-C4-C5	5.35	131.28	128.60
79	t	3741	U	N1-C2-O2	5.35	126.55	122.80
79	t	3757	U	N3-C2-O2	-5.35	118.46	122.20
79	t	695	C	N3-C2-O2	-5.35	118.16	121.90
79	t	2064	C	C5-C6-N1	5.34	123.67	121.00
79	t	1882	C	N1-C2-O2	5.34	122.10	118.90
79	t	461	U	N1-C2-O2	5.34	126.54	122.80
1	S2	1514	G	C5-C6-O6	-5.34	125.40	128.60
38	D	47	C	C5-C6-N1	5.34	123.67	121.00
79	t	3656	C	C6-N1-C2	-5.34	118.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1261	C	P-O3'-C3'	5.33	126.10	119.70
1	S2	197	U	N1-C2-O2	5.33	126.53	122.80
79	t	205	A	C2-N3-C4	5.33	113.27	110.60
1	S2	585	C	N3-C2-O2	-5.33	118.17	121.90
79	t	4185	C	C5-C6-N1	5.33	123.67	121.00
80	u	48	C	C6-N1-C2	-5.33	118.17	120.30
1	S2	1057	C	C5-C6-N1	5.33	123.66	121.00
79	t	509	C	C6-N1-C2	-5.33	118.17	120.30
1	S2	1670	C	N1-C2-O2	5.32	122.09	118.90
1	S2	1812	U	N1-C2-O2	5.32	126.53	122.80
38	D	129	C	N1-C2-O2	5.32	122.09	118.90
62	b	131	ARG	NE-CZ-NH2	-5.32	117.64	120.30
79	t	2617	G	N3-C2-N2	-5.32	116.17	119.90
1	S2	1289	U	C2-N1-C1'	5.32	124.09	117.70
79	t	2766	A	C8-N9-C4	-5.32	103.67	105.80
38	D	123	U	N3-C2-O2	-5.32	118.48	122.20
23	SC	192	LEU	CA-CB-CG	5.32	127.53	115.30
79	t	2054	C	C6-N1-C2	-5.32	118.17	120.30
79	t	4865	G	P-O3'-C3'	5.31	126.08	119.70
1	S2	583	C	N1-C2-O2	5.31	122.09	118.90
79	t	463	C	N3-C2-O2	-5.31	118.18	121.90
19	Sa	92	ARG	NE-CZ-NH2	-5.31	117.64	120.30
80	u	55	U	C5-C6-N1	5.31	125.36	122.70
1	S2	197	U	N3-C2-O2	-5.31	118.48	122.20
8	SI	172	LEU	CA-CB-CG	5.31	127.51	115.30
79	t	1912	C	N3-C2-O2	-5.31	118.19	121.90
79	t	2574	C	C6-N1-C2	-5.30	118.18	120.30
1	S2	144	U	N3-C2-O2	-5.30	118.49	122.20
79	t	3659	U	N1-C2-O2	5.30	126.51	122.80
79	t	4660	C	N1-C2-O2	5.30	122.08	118.90
79	t	2241	G	N3-C4-N9	5.30	129.18	126.00
79	t	2388	U	C6-N1-C1'	-5.30	113.78	121.20
1	S2	1578	U	C2-N1-C1'	5.30	124.06	117.70
79	t	962	C	C6-N1-C2	-5.30	118.18	120.30
79	t	5026	G	C6-C5-N7	-5.29	127.22	130.40
79	t	3797	C	C5-C6-N1	5.29	123.65	121.00
38	D	123	U	OP1-P-O3'	5.29	116.83	105.20
79	t	3643	G	N3-C4-C5	5.29	131.24	128.60
1	S2	53	C	N1-C2-O2	5.29	122.07	118.90
79	t	4298	A	N3-C4-N9	-5.28	123.17	127.40
79	t	4624	C	N1-C2-O2	5.28	122.07	118.90
27	SN	125	LEU	CA-CB-CG	5.28	127.44	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	t	1638	U	C2-N1-C1'	5.28	124.03	117.70
79	t	4177	C	N3-C2-O2	-5.28	118.20	121.90
80	u	61	C	N1-C2-O2	5.28	122.07	118.90
1	S2	183	G	C2-N3-C4	5.27	114.54	111.90
79	t	89	C	C5-C6-N1	5.27	123.64	121.00
1	S2	1307	U	N1-C2-O2	5.27	126.49	122.80
79	t	205	A	N3-C4-N9	5.27	131.62	127.40
1	S2	1064	C	N3-C2-O2	-5.27	118.21	121.90
80	u	17	C	N3-C2-O2	-5.27	118.21	121.90
1	S2	1053	C	N3-C2-O2	-5.26	118.22	121.90
39	E	67	C	C6-N1-C2	-5.26	118.19	120.30
79	t	956	C	C6-N1-C2	-5.26	118.19	120.30
79	t	4886	C	C5-C6-N1	5.26	123.63	121.00
79	t	451	G	N1-C2-N2	5.26	120.93	116.20
79	t	4951	G	N3-C4-N9	-5.26	122.84	126.00
79	t	3671	C	N1-C2-O2	5.26	122.05	118.90
1	S2	125	C	C2-N1-C1'	5.25	124.58	118.80
1	S2	1707	U	C5-C6-N1	5.25	125.33	122.70
22	Sg	248	LEU	CA-CB-CG	5.25	127.38	115.30
79	t	166	G	N3-C2-N2	-5.25	116.22	119.90
79	t	2373	G	C8-N9-C1'	-5.25	120.17	127.00
38	D	113	C	N1-C2-O2	5.25	122.05	118.90
81	v	40	C	N1-C2-O2	5.25	122.05	118.90
12	SQ	116	ASP	CB-CG-OD1	5.24	123.02	118.30
1	S2	1154	U	C2-N1-C1'	5.24	123.99	117.70
46	L	130	PHE	CB-CG-CD1	5.24	124.47	120.80
79	t	1466	G	C6-C5-N7	-5.24	127.25	130.40
79	t	2499	C	C6-N1-C1'	-5.24	114.51	120.80
79	t	3741	U	C2-N1-C1'	5.24	123.99	117.70
79	t	3805	C	N1-C2-O2	5.24	122.04	118.90
1	S2	402	C	C5-C6-N1	5.23	123.62	121.00
79	t	1218	G	N3-C2-N2	-5.23	116.24	119.90
79	t	2241	G	N3-C4-C5	-5.23	125.98	128.60
79	t	4992	A	C5-N7-C8	-5.23	101.28	103.90
1	S2	424	C	N1-C2-O2	5.23	122.04	118.90
1	S2	1802	C	P-O3'-C3'	5.23	125.98	119.70
79	t	1350	C	N3-C2-O2	-5.23	118.24	121.90
79	t	1267	G	C4-C5-N7	5.22	112.89	110.80
79	t	2239	C	N3-C2-O2	-5.22	118.24	121.90
79	t	4289	C	N1-C2-O2	5.22	122.03	118.90
79	t	474	C	N1-C2-O2	5.22	122.03	118.90
79	t	1446	C	C6-N1-C2	-5.22	118.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	v	48	C	OP2-P-O3'	5.22	116.69	105.20
79	t	1829	C	C6-N1-C2	-5.22	118.21	120.30
79	t	288	G	N3-C4-N9	5.22	129.13	126.00
79	t	461	U	N3-C2-O2	-5.22	118.55	122.20
82	w	17	G	N3-C4-N9	5.22	129.13	126.00
1	S2	1495	G	C5-C6-N1	5.21	114.11	111.50
79	t	4820	G	C4-C5-N7	5.21	112.88	110.80
39	E	67	C	O5'-P-OP1	-5.21	101.01	105.70
79	t	4736	C	C5-C6-N1	5.21	123.60	121.00
79	t	1538	C	C6-N1-C2	-5.20	118.22	120.30
1	S2	1567	G	P-O3'-C3'	5.20	125.94	119.70
5	SE	180	LEU	CA-CB-CG	5.20	127.26	115.30
79	t	1221	A	N3-C4-C5	5.20	130.44	126.80
79	t	2330	C	C5-C6-N1	5.20	123.60	121.00
79	t	2282	C	C5-C6-N1	5.20	123.60	121.00
79	t	3757	U	C2-N1-C1'	5.20	123.93	117.70
79	t	4633	C	C2-N1-C1'	5.20	124.52	118.80
79	t	1502	C	C6-N1-C2	-5.19	118.22	120.30
79	t	2064	C	C6-N1-C2	-5.19	118.22	120.30
1	S2	867	G	C2-N3-C4	5.19	114.50	111.90
1	S2	1797	U	N1-C2-O2	5.19	126.44	122.80
1	S2	570	C	N3-C2-O2	-5.19	118.27	121.90
79	t	219	C	O4'-C1'-N1	5.19	112.35	108.20
79	t	1394	C	C6-N1-C2	-5.19	118.22	120.30
79	t	229	G	C8-N9-C1'	5.18	133.74	127.00
79	t	96	U	N3-C2-O2	-5.18	118.58	122.20
67	g	105	LEU	CA-CB-CG	5.17	127.19	115.30
79	t	189	G	N3-C4-N9	-5.17	122.90	126.00
79	t	344	C	N3-C2-O2	-5.17	118.28	121.90
79	t	4058	C	C6-N1-C2	-5.17	118.23	120.30
79	t	4870	G	P-O3'-C3'	5.17	125.90	119.70
79	t	177	C	C6-N1-C2	-5.16	118.23	120.30
2	SA	147	LEU	CA-CB-CG	5.16	127.17	115.30
79	t	1187	C	N3-C2-O2	-5.16	118.29	121.90
79	t	1086	C	C2-N1-C1'	5.16	124.48	118.80
79	t	1894	C	C6-N1-C2	-5.16	118.24	120.30
79	t	1442	C	C6-N1-C2	-5.16	118.24	120.30
79	t	2759	C	C6-N1-C2	-5.15	118.24	120.30
1	S2	1496	U	C2-N1-C1'	5.15	123.88	117.70
79	t	4562	G	C4-C5-N7	5.15	112.86	110.80
79	t	4858	C	C6-N1-C2	-5.15	118.24	120.30
79	t	4886	C	C2-N1-C1'	5.14	124.46	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	t	4905	U	N3-C2-O2	-5.14	118.60	122.20
79	t	1086	C	N3-C2-O2	-5.14	118.30	121.90
1	S2	666	U	C5-C6-N1	5.14	125.27	122.70
79	t	196	G	N3-C4-C5	5.14	131.17	128.60
79	t	453	C	C6-N1-C2	-5.14	118.24	120.30
79	t	5026	G	C8-N9-C1'	-5.14	120.32	127.00
1	S2	1157	G	N3-C4-C5	-5.14	126.03	128.60
81	v	59	U	N3-C2-O2	-5.14	118.61	122.20
79	t	1250	C	O4'-C1'-N1	5.13	112.31	108.20
1	S2	292	A	P-O3'-C3'	5.13	125.86	119.70
1	S2	42	A	P-O3'-C3'	5.13	125.86	119.70
1	S2	751	G	N3-C4-C5	-5.13	126.03	128.60
79	t	3756	A	C8-N9-C4	5.13	107.85	105.80
79	t	4624	C	N3-C2-O2	-5.13	118.31	121.90
37	C	289	LEU	CA-CB-CG	5.13	127.09	115.30
1	S2	358	C	C6-N1-C2	-5.12	118.25	120.30
2	SA	159	ILE	CG1-CB-CG2	-5.12	100.14	111.40
1	S2	879	C	N3-C2-O2	-5.12	118.32	121.90
79	t	4726	A	C4-C5-N7	5.12	113.26	110.70
1	S2	118	C	N3-C2-O2	-5.11	118.32	121.90
1	S2	1689	C	N3-C2-O2	-5.11	118.32	121.90
51	Q	104	LEU	CA-CB-CG	5.11	127.06	115.30
79	t	226	G	N7-C8-N9	-5.11	110.55	113.10
39	E	92	C	C5-C6-N1	5.11	123.55	121.00
1	S2	1109	C	C6-N1-C2	-5.10	118.26	120.30
1	S2	358	C	N1-C2-O2	5.10	121.96	118.90
1	S2	1130	G	C2-N3-C4	5.10	114.45	111.90
79	t	226	G	N9-C4-C5	5.10	107.44	105.40
79	t	4993	U	N1-C2-O2	5.10	126.37	122.80
79	t	4367	G	N3-C4-N9	5.10	129.06	126.00
79	t	4267	G	C4-C5-N7	5.10	112.84	110.80
79	t	1267	G	N7-C8-N9	5.09	115.65	113.10
79	t	3607	C	C6-N1-C2	-5.09	118.26	120.30
79	t	5024	U	N3-C2-O2	-5.09	118.64	122.20
1	S2	115	U	N3-C2-O2	-5.09	118.64	122.20
79	t	2805	U	N1-C2-O2	5.09	126.36	122.80
22	Sg	79	LEU	CA-CB-CG	5.09	127.00	115.30
81	v	71	G	N1-C6-O6	-5.09	116.85	119.90
79	t	907	C	N1-C2-O2	5.09	121.95	118.90
79	t	2644	U	N3-C2-O2	-5.09	118.64	122.20
79	t	4719	C	C6-N1-C2	-5.09	118.27	120.30
79	t	1262	A	N1-C2-N3	5.08	131.84	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	t	1394	C	C5-C6-N1	5.08	123.54	121.00
37	C	319	LEU	CA-CB-CG	5.08	126.99	115.30
79	t	1268	U	C5-C6-N1	-5.08	120.16	122.70
1	S2	1538	C	C2-N1-C1'	5.08	124.39	118.80
79	t	232	A	N1-C2-N3	-5.08	126.76	129.30
79	t	668	C	C5-C6-N1	5.08	123.54	121.00
79	t	1275	C	N1-C2-O2	5.08	121.95	118.90
1	S2	418	A	O5'-P-OP1	-5.08	101.13	105.70
1	S2	632	C	C6-N1-C2	-5.07	118.27	120.30
79	t	4234	G	N3-C2-N2	-5.07	116.35	119.90
80	u	43	C	C6-N1-C1'	-5.07	114.72	120.80
1	S2	1005	G	C4-N9-C1'	5.07	133.09	126.50
79	t	4974	A	C8-N9-C4	-5.07	103.77	105.80
38	D	116	C	C5-C6-N1	5.07	123.53	121.00
1	S2	1566	G	C6-C5-N7	-5.06	127.36	130.40
79	t	1180	C	N3-C2-O2	-5.06	118.36	121.90
1	S2	427	U	N1-C2-O2	5.06	126.34	122.80
69	i	69	LEU	CA-CB-CG	5.06	126.94	115.30
79	t	956	C	C5-C6-N1	5.06	123.53	121.00
79	t	2009	C	N3-C2-O2	-5.06	118.36	121.90
79	t	964	C	N3-C2-O2	-5.05	118.36	121.90
1	S2	900	C	N1-C2-O2	5.05	121.93	118.90
79	t	4629	C	N1-C2-O2	5.05	121.93	118.90
1	S2	1644	C	C6-N1-C2	-5.05	118.28	120.30
39	E	66	G	C4-N9-C1'	5.05	133.06	126.50
79	t	504	U	C2-N1-C1'	5.04	123.75	117.70
81	v	50	U	OP1-P-O3'	5.04	116.30	105.20
25	SJ	50	LEU	CA-CB-CG	5.04	126.89	115.30
79	t	216	G	C2-N3-C4	-5.04	109.38	111.90
9	SK	15	LEU	CA-CB-CG	5.04	126.89	115.30
79	t	2249	G	N3-C2-N2	-5.04	116.37	119.90
79	t	4671	U	C5-C6-N1	5.04	125.22	122.70
39	E	78	C	C6-N1-C2	-5.04	118.28	120.30
12	SQ	120	LEU	CA-CB-CG	5.04	126.88	115.30
79	t	273	A	N1-C2-N3	-5.03	126.78	129.30
79	t	4327	C	C6-N1-C2	-5.03	118.29	120.30
79	t	4629	C	N3-C2-O2	-5.03	118.38	121.90
79	t	1966	G	C4-N9-C1'	5.03	133.04	126.50
81	v	61	C	C2-N3-C4	5.03	122.42	119.90
79	t	1614	A	C8-N9-C4	-5.03	103.79	105.80
79	t	2389	C	N3-C2-O2	-5.03	118.38	121.90
79	t	1656	C	C5-C6-N1	5.02	123.51	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	t	4974	A	O4'-C1'-N9	5.02	112.22	108.20
79	t	1538	C	N3-C2-O2	-5.02	118.38	121.90
79	t	2532	A	O4'-C1'-N9	5.02	112.22	108.20
79	t	4217	A	O4'-C1'-N9	5.02	112.22	108.20
79	t	1561	C	C6-N1-C2	-5.02	118.29	120.30
79	t	1829	C	N1-C2-O2	5.02	121.91	118.90
82	w	19	C	N3-C2-O2	-5.01	118.39	121.90
1	S2	337	C	N1-C2-O2	5.01	121.90	118.90
1	S2	803	C	C6-N1-C2	-5.01	118.30	120.30
79	t	1717	U	N3-C2-O2	-5.01	118.69	122.20
79	t	154	U	N3-C2-O2	-5.00	118.70	122.20
79	t	1610	C	C5-C6-N1	5.00	123.50	121.00
79	t	126	C	N3-C2-O2	-5.00	118.40	121.90
79	t	4736	C	C6-N1-C1'	-5.00	114.80	120.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	F	257	PRO	Peptide
47	M	130	LYS	Peptide
25	SJ	137	VAL	Peptide
76	p	103	VAL	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%)	192 (88%)	26 (12%)	1 (0%)	25 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	SB	212/214 (99%)	191 (90%)	21 (10%)	0	100	100
4	SD	224/226 (99%)	194 (87%)	30 (13%)	0	100	100
5	SE	257/259 (99%)	241 (94%)	16 (6%)	0	100	100
6	SF	187/189 (99%)	171 (91%)	16 (9%)	0	100	100
7	SH	182/189 (96%)	163 (90%)	19 (10%)	0	100	100
8	SI	202/204 (99%)	182 (90%)	20 (10%)	0	100	100
9	SK	96/98 (98%)	83 (86%)	12 (12%)	1 (1%)	13	46
10	SL	151/153 (99%)	135 (89%)	15 (10%)	1 (1%)	19	53
11	SP	125/127 (98%)	111 (89%)	14 (11%)	0	100	100
12	SQ	144/146 (99%)	127 (88%)	15 (10%)	2 (1%)	9	40
13	SR	132/134 (98%)	119 (90%)	12 (9%)	1 (1%)	16	51
14	SS	143/145 (99%)	127 (89%)	16 (11%)	0	100	100
15	ST	141/143 (99%)	130 (92%)	10 (7%)	1 (1%)	19	53
16	SU	102/104 (98%)	93 (91%)	9 (9%)	0	100	100
17	SV	80/82 (98%)	72 (90%)	8 (10%)	0	100	100
18	SX	139/141 (99%)	126 (91%)	13 (9%)	0	100	100
19	Sa	100/102 (98%)	88 (88%)	11 (11%)	1 (1%)	13	46
20	Sc	62/64 (97%)	51 (82%)	11 (18%)	0	100	100
21	Sd	53/55 (96%)	44 (83%)	9 (17%)	0	100	100
22	Sg	310/312 (99%)	255 (82%)	55 (18%)	0	100	100
23	SC	219/220 (100%)	201 (92%)	17 (8%)	1 (0%)	25	59
24	SG	235/237 (99%)	212 (90%)	23 (10%)	0	100	100
25	SJ	184/185 (100%)	168 (91%)	15 (8%)	1 (0%)	25	59
26	SM	116/118 (98%)	102 (88%)	14 (12%)	0	100	100
27	SN	148/150 (99%)	145 (98%)	3 (2%)	0	100	100
28	SO	135/137 (98%)	117 (87%)	18 (13%)	0	100	100
29	SW	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
30	SY	130/131 (99%)	119 (92%)	10 (8%)	1 (1%)	16	51
31	SZ	71/73 (97%)	58 (82%)	13 (18%)	0	100	100
32	Sb	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
33	Se	55/57 (96%)	48 (87%)	7 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	Sf	65/67 (97%)	52 (80%)	13 (20%)	0	100	100
35	A	250/252 (99%)	222 (89%)	27 (11%)	1 (0%)	30	64
36	B	395/397 (100%)	355 (90%)	37 (9%)	3 (1%)	16	51
37	C	361/363 (99%)	326 (90%)	31 (9%)	4 (1%)	12	45
40	F	292/294 (99%)	257 (88%)	32 (11%)	3 (1%)	13	46
41	G	232/247 (94%)	194 (84%)	38 (16%)	0	100	100
42	H	223/225 (99%)	209 (94%)	13 (6%)	1 (0%)	30	64
43	I	232/234 (99%)	212 (91%)	20 (9%)	0	100	100
44	J	189/191 (99%)	170 (90%)	19 (10%)	0	100	100
45	K	204/211 (97%)	179 (88%)	24 (12%)	1 (0%)	25	59
46	L	167/169 (99%)	150 (90%)	16 (10%)	1 (1%)	22	56
47	M	203/205 (99%)	168 (83%)	31 (15%)	4 (2%)	6	33
48	N	137/139 (99%)	126 (92%)	11 (8%)	0	100	100
49	O	201/203 (99%)	181 (90%)	20 (10%)	0	100	100
50	P	193/195 (99%)	186 (96%)	6 (3%)	1 (0%)	25	59
51	Q	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
52	R	185/187 (99%)	171 (92%)	14 (8%)	0	100	100
53	S	179/181 (99%)	171 (96%)	8 (4%)	0	100	100
54	T	173/175 (99%)	158 (91%)	15 (9%)	0	100	100
55	U	155/157 (99%)	136 (88%)	17 (11%)	2 (1%)	10	41
56	V	97/99 (98%)	89 (92%)	8 (8%)	0	100	100
57	W	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
58	X	59/61 (97%)	55 (93%)	4 (7%)	0	100	100
59	Y	115/117 (98%)	107 (93%)	8 (7%)	0	100	100
60	Z	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
61	a	132/134 (98%)	118 (89%)	14 (11%)	0	100	100
62	b	145/147 (99%)	125 (86%)	19 (13%)	1 (1%)	19	53
63	c	94/121 (78%)	83 (88%)	11 (12%)	0	100	100
64	d	101/103 (98%)	86 (85%)	15 (15%)	0	100	100
65	e	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
66	f	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	g	107/109 (98%)	98 (92%)	9 (8%)	0	100	100
68	h	112/114 (98%)	101 (90%)	10 (9%)	1 (1%)	14	49
69	i	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16	51
70	j	95/97 (98%)	88 (93%)	6 (6%)	1 (1%)	12	45
71	k	82/84 (98%)	75 (92%)	7 (8%)	0	100	100
72	l	67/69 (97%)	62 (92%)	5 (8%)	0	100	100
73	m	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
74	n	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
75	o	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
76	p	103/105 (98%)	93 (90%)	9 (9%)	1 (1%)	13	46
77	q	89/91 (98%)	83 (93%)	6 (7%)	0	100	100
78	r	120/122 (98%)	105 (88%)	12 (10%)	3 (2%)	4	29
All	All	11195/11390 (98%)	10073 (90%)	1081 (10%)	41 (0%)	32	64

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	SK	63	ALA
10	SL	23	VAL
13	SR	129	LYS
15	ST	41	LYS
23	SC	78	LEU
55	U	19	PHE
62	b	95	THR
66	f	7	LEU
12	SQ	117	ARG
19	Sa	47	ALA
37	C	69	THR
40	F	10	LYS
47	M	64	VAL
68	h	47	GLY
70	j	35	LYS
2	SA	12	GLU
40	F	8	LYS
40	F	260	GLU
45	K	11	TYR
69	i	88	THR
78	r	23	GLN

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Mol	Chain	Res	Type
35	A	251	THR
36	B	4	ARG
36	B	299	ILE
42	H	223	LYS
55	U	53	PRO
76	p	104	ILE
12	SQ	116	ASP
37	C	56	GLU
37	C	303	ARG
47	M	63	THR
78	r	21	ASN
78	r	22	LYS
36	B	3	HIS
46	L	171	ASP
25	SJ	123	ILE
30	SY	95	GLY
37	C	70	GLY
47	M	153	PRO
50	P	185	VAL
47	M	47	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	SA	183/183 (100%)	178 (97%)	5 (3%)	40	65
3	SB	195/195 (100%)	192 (98%)	3 (2%)	60	77
4	SD	189/189 (100%)	188 (100%)	1 (0%)	86	93
5	SE	222/222 (100%)	218 (98%)	4 (2%)	54	74
6	SF	159/159 (100%)	154 (97%)	5 (3%)	35	63
7	SH	166/169 (98%)	163 (98%)	3 (2%)	54	74
8	SI	177/177 (100%)	172 (97%)	5 (3%)	38	65
9	SK	89/89 (100%)	85 (96%)	4 (4%)	23	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	SL	137/137 (100%)	132 (96%)	5 (4%)	30	59
11	SP	113/113 (100%)	109 (96%)	4 (4%)	31	59
12	SQ	121/121 (100%)	120 (99%)	1 (1%)	79	88
13	SR	121/121 (100%)	118 (98%)	3 (2%)	42	67
14	SS	126/126 (100%)	125 (99%)	1 (1%)	79	88
15	ST	113/113 (100%)	110 (97%)	3 (3%)	40	65
16	SU	94/94 (100%)	90 (96%)	4 (4%)	25	54
17	SV	66/66 (100%)	63 (96%)	3 (4%)	23	53
18	SX	113/113 (100%)	110 (97%)	3 (3%)	40	65
19	Sa	89/89 (100%)	87 (98%)	2 (2%)	47	70
20	Sc	57/57 (100%)	57 (100%)	0	100	100
21	Sd	48/48 (100%)	44 (92%)	4 (8%)	9	32
22	Sg	271/271 (100%)	268 (99%)	3 (1%)	70	83
23	SC	187/186 (100%)	186 (100%)	1 (0%)	86	93
24	SG	207/207 (100%)	201 (97%)	6 (3%)	37	64
25	SJ	162/161 (101%)	155 (96%)	7 (4%)	25	54
26	SM	98/100 (98%)	95 (97%)	3 (3%)	35	63
27	SN	130/130 (100%)	128 (98%)	2 (2%)	60	77
28	SO	107/107 (100%)	107 (100%)	0	100	100
29	SW	112/112 (100%)	108 (96%)	4 (4%)	30	59
30	SY	114/113 (101%)	110 (96%)	4 (4%)	31	59
31	SZ	64/64 (100%)	61 (95%)	3 (5%)	22	51
32	Sb	74/74 (100%)	74 (100%)	0	100	100
33	Se	46/46 (100%)	46 (100%)	0	100	100
34	Sf	60/60 (100%)	57 (95%)	3 (5%)	20	49
35	A	194/194 (100%)	189 (97%)	5 (3%)	41	66
36	B	345/345 (100%)	332 (96%)	13 (4%)	28	57
37	C	302/302 (100%)	293 (97%)	9 (3%)	36	63
40	F	248/248 (100%)	242 (98%)	6 (2%)	44	68
41	G	209/220 (95%)	203 (97%)	6 (3%)	37	64
42	H	194/194 (100%)	188 (97%)	6 (3%)	35	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	I	199/199 (100%)	199 (100%)	0	100	100
44	J	170/170 (100%)	165 (97%)	5 (3%)	37	64
45	K	178/179 (99%)	173 (97%)	5 (3%)	38	65
46	L	142/142 (100%)	140 (99%)	2 (1%)	62	79
47	M	171/171 (100%)	165 (96%)	6 (4%)	31	59
48	N	118/118 (100%)	115 (98%)	3 (2%)	42	67
49	O	171/171 (100%)	166 (97%)	5 (3%)	37	64
50	P	168/168 (100%)	160 (95%)	8 (5%)	21	50
51	Q	134/134 (100%)	131 (98%)	3 (2%)	47	70
52	R	164/164 (100%)	154 (94%)	10 (6%)	15	43
53	S	160/160 (100%)	157 (98%)	3 (2%)	52	73
54	T	156/156 (100%)	152 (97%)	4 (3%)	41	66
55	U	138/138 (100%)	132 (96%)	6 (4%)	25	54
56	V	89/89 (100%)	83 (93%)	6 (7%)	13	40
57	W	100/100 (100%)	100 (100%)	0	100	100
58	X	53/53 (100%)	52 (98%)	1 (2%)	52	73
59	Y	105/105 (100%)	101 (96%)	4 (4%)	28	57
60	Z	124/124 (100%)	122 (98%)	2 (2%)	58	76
61	a	117/117 (100%)	114 (97%)	3 (3%)	41	66
62	b	120/120 (100%)	114 (95%)	6 (5%)	20	49
63	c	82/101 (81%)	80 (98%)	2 (2%)	44	68
64	d	88/88 (100%)	85 (97%)	3 (3%)	32	60
65	e	97/97 (100%)	95 (98%)	2 (2%)	48	71
66	f	115/115 (100%)	114 (99%)	1 (1%)	75	86
67	g	88/88 (100%)	84 (96%)	4 (4%)	23	53
68	h	98/98 (100%)	96 (98%)	2 (2%)	50	72
69	i	109/109 (100%)	106 (97%)	3 (3%)	38	65
70	j	83/83 (100%)	82 (99%)	1 (1%)	67	82
71	k	71/71 (100%)	70 (99%)	1 (1%)	62	79
72	l	64/64 (100%)	62 (97%)	2 (3%)	35	63
73	m	47/47 (100%)	46 (98%)	1 (2%)	48	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	n	46/46 (100%)	45 (98%)	1 (2%)	47	70
75	o	24/24 (100%)	23 (96%)	1 (4%)	25	54
76	p	93/93 (100%)	88 (95%)	5 (5%)	18	46
77	q	74/74 (100%)	73 (99%)	1 (1%)	62	79
78	r	106/106 (100%)	104 (98%)	2 (2%)	52	73
All	All	9764/9797 (100%)	9506 (97%)	258 (3%)	42	66

All (258) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SA	29	ASN
2	SA	50	ASN
2	SA	82	THR
2	SA	89	LYS
2	SA	220	LYS
3	SB	186	ASN
3	SB	187	LYS
3	SB	188	LEU
4	SD	76	ARG
5	SE	7	LYS
5	SE	49	ARG
5	SE	198	ARG
5	SE	254	LYS
6	SF	60	ARG
6	SF	77	MET
6	SF	83	ASN
6	SF	88	MET
6	SF	130	ARG
7	SH	15	LYS
7	SH	57	ARG
7	SH	166	VAL
8	SI	47	ARG
8	SI	60	LEU
8	SI	124	LYS
8	SI	128	LYS
8	SI	144	LYS
9	SK	40	VAL
9	SK	46	MET
9	SK	55	ARG
9	SK	58	VAL

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Mol	Chain	Res	Type
10	SL	21	LYS
10	SL	32	LYS
10	SL	65	ASN
10	SL	69	ARG
10	SL	147	LYS
11	SP	13	ARG
11	SP	15	PHE
11	SP	79	HIS
11	SP	89	MET
12	SQ	125	ARG
13	SR	3	ARG
13	SR	74	GLN
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	9	VAL
17	SV	21	ASN
17	SV	27	LYS
18	SX	8	ARG
18	SX	18	ARG
18	SX	61	GLN
19	Sa	28	ARG
19	Sa	51	ARG
21	Sd	19	ARG
21	Sd	22	ARG
21	Sd	26	ASN
21	Sd	40	ARG
22	Sg	30	MET
22	Sg	162	ASN
22	Sg	280	LYS
23	SC	103	LYS
24	SG	98	ARG
24	SG	119	LYS
24	SG	132	ARG
24	SG	163	ASN
24	SG	217	MET

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Mol	Chain	Res	Type
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	46	THR
27	SN	133	ARG
29	SW	57	ARG
29	SW	68	ARG
29	SW	93	LEU
29	SW	103	VAL
30	SY	2	ASN
30	SY	10	ARG
30	SY	94	HIS
30	SY	118	ARG
31	SZ	43	LYS
31	SZ	62	VAL
31	SZ	66	LYS
34	Sf	89	LYS
34	Sf	91	ASN
34	Sf	96	LYS
35	A	64	ARG
35	A	68	ARG
35	A	140	ASN
35	A	193	ARG
35	A	250	LYS
36	B	39	LYS
36	B	67	VAL
36	B	85	VAL
36	B	121	ASN
36	B	144	LYS
36	B	213	GLN
36	B	258	HIS
36	B	271	GLN
36	B	294	LYS
36	B	295	ASP

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Mol	Chain	Res	Type
36	B	301	ASN
36	B	378	ARG
36	B	396	ARG
37	C	38	ASN
37	C	97	ARG
37	C	150	LEU
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	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	125	LEU
41	G	176	THR
41	G	279	ASN
42	H	24	ASN
42	H	41	MET
42	H	106	ARG
42	H	126	ASN
42	H	179	LEU
42	H	245	ARG
44	J	42	ASN
44	J	63	ASN
44	J	103	VAL
44	J	108	ASN
44	J	116	ASN
45	K	3	ARG
45	K	69	ARG
45	K	87	ILE
45	K	146	GLU
45	K	169	LYS
46	L	35	ARG
46	L	54	ARG

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Mol	Chain	Res	Type
47	M	21	ARG
47	M	102	ARG
47	M	144	LEU
47	M	157	VAL
47	M	165	LYS
47	M	169	ILE
48	N	5	ARG
48	N	31	ILE
48	N	119	ARG
49	O	63	ARG
49	O	64	ILE
49	O	93	LYS
49	O	133	ILE
49	O	183	THR
50	P	63	ASN
50	P	94	ARG
50	P	101	ARG
50	P	140	ARG
50	P	169	ARG
50	P	178	ARG
50	P	185	VAL
50	P	188	LYS
51	Q	24	VAL
51	Q	127	ARG
51	Q	146	ILE
52	R	4	ASP
52	R	5	ILE
52	R	14	ARG
52	R	28	LEU
52	R	37	ARG
52	R	63	LEU
52	R	91	ARG
52	R	138	LEU
52	R	163	THR
52	R	168	ARG
53	S	98	ARG
53	S	152	LYS
53	S	162	ARG
54	T	15	ARG
54	T	68	PHE
54	T	158	VAL
54	T	162	GLN

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Mol	Chain	Res	Type
55	U	9	ARG
55	U	12	ARG
55	U	21	LYS
55	U	68	THR
55	U	117	LYS
55	U	143	THR
56	V	20	LYS
56	V	52	LYS
56	V	67	LYS
56	V	69	LYS
56	V	101	ARG
56	V	112	LEU
58	X	43	LYS
59	Y	48	ARG
59	Y	96	LEU
59	Y	129	ARG
59	Y	152	LYS
60	Z	55	VAL
60	Z	59	ARG
61	a	13	VAL
61	a	17	ARG
61	a	98	LYS
62	b	10	LYS
62	b	44	ASN
62	b	63	LEU
62	b	87	ARG
62	b	94	LYS
62	b	105	ARG
63	c	41	ARG
63	c	65	MET
64	d	35	LEU
64	d	68	LYS
64	d	77	ASN
65	e	93	ASN
65	e	109	VAL
66	f	33	ARG
67	g	33	VAL
67	g	59	THR
67	g	63	LYS
67	g	109	ARG
68	h	4	ARG
68	h	54	ARG

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Mol	Chain	Res	Type
69	i	20	GLN
69	i	92	ARG
69	i	109	ARG
70	j	68	ARG
71	k	79	ARG
72	l	9	LYS
72	l	17	ARG
73	m	11	ARG
74	n	112	LYS
75	o	9	ARG
76	p	23	VAL
76	p	27	LYS
76	p	69	ARG
76	p	81	ARG
76	p	93	LEU
77	q	84	ARG
78	r	41	ASN
78	r	83	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (131) such sidechains are listed below:

Mol	Chain	Res	Type
2	SA	50	ASN
3	SB	40	ASN
3	SB	75	GLN
3	SB	186	ASN
3	SB	202	GLN
6	SF	118	ASN
7	SH	39	GLN
7	SH	168	HIS
8	SI	138	ASN
8	SI	181	GLN
9	SK	61	GLN
10	SL	18	GLN
10	SL	65	ASN
10	SL	83	GLN
11	SP	104	GLN
12	SQ	24	HIS
13	SR	83	ASN
13	SR	127	ASN
15	ST	128	GLN
16	SU	100	GLN

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Mol	Chain	Res	Type
17	SV	21	ASN
17	SV	35	ASN
18	SX	61	GLN
19	Sa	72	HIS
19	Sa	86	ASN
21	Sd	26	ASN
22	Sg	4	GLN
22	Sg	14	HIS
22	Sg	20	GLN
22	Sg	117	ASN
22	Sg	162	ASN
23	SC	235	ASN
23	SC	267	GLN
24	SG	13	GLN
24	SG	59	GLN
24	SG	110	ASN
24	SG	163	ASN
24	SG	197	GLN
25	SJ	124	HIS
25	SJ	177	ASN
27	SN	5	HIS
28	SO	79	GLN
29	SW	16	ASN
29	SW	92	ASN
29	SW	113	HIS
30	SY	2	ASN
30	SY	124	ASN
34	Sf	91	ASN
35	A	50	HIS
35	A	83	HIS
35	A	95	GLN
35	A	97	ASN
35	A	132	ASN
35	A	140	ASN
35	A	209	HIS
36	B	55	HIS
36	B	121	ASN
36	B	204	GLN
36	B	258	HIS
36	B	301	ASN
36	B	322	HIS
37	C	94	ASN

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Mol	Chain	Res	Type
37	C	236	ASN
37	C	278	ASN
37	C	338	ASN
37	C	347	HIS
40	F	122	GLN
40	F	191	ASN
41	G	190	HIS
41	G	191	GLN
41	G	279	ASN
42	H	24	ASN
42	H	80	ASN
42	H	126	ASN
42	H	131	ASN
42	H	226	HIS
43	I	225	ASN
44	J	42	ASN
44	J	63	ASN
44	J	78	GLN
44	J	108	ASN
44	J	116	ASN
45	K	86	HIS
45	K	213	HIS
46	L	71	HIS
46	L	112	HIS
46	L	155	HIS
47	M	87	HIS
48	N	20	HIS
48	N	44	GLN
48	N	48	GLN
48	N	70	GLN
49	O	87	HIS
49	O	199	GLN
50	P	14	HIS
50	P	63	ASN
50	P	173	GLN
51	Q	40	HIS
51	Q	80	GLN
52	R	160	HIS
53	S	39	GLN
53	S	58	HIS
53	S	130	ASN
54	T	162	GLN

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Mol	Chain	Res	Type
54	T	163	HIS
55	U	49	GLN
57	W	101	ASN
58	X	50	ASN
59	Y	111	GLN
60	Z	20	ASN
60	Z	61	HIS
60	Z	72	GLN
62	b	25	HIS
63	c	6	ASN
63	c	19	ASN
64	d	77	ASN
65	e	79	ASN
65	e	93	ASN
66	f	43	ASN
66	f	107	ASN
70	j	26	HIS
70	j	92	ASN
71	k	66	HIS
73	m	43	HIS
74	n	90	ASN
76	p	18	HIS
76	p	19	GLN
77	q	56	HIS
78	r	6	GLN
78	r	41	ASN
78	r	45	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1690/1714 (98%)	565 (33%)	31 (1%)
38	D	156/157 (99%)	38 (24%)	0
39	E	118/121 (97%)	19 (16%)	0
79	t	3590/3607 (99%)	878 (24%)	0
80	u	74/76 (97%)	28 (37%)	0
81	v	71/76 (93%)	28 (39%)	0
82	w	9/10 (90%)	2 (22%)	0
All	All	5708/5761 (99%)	1558 (27%)	31 (0%)

All (1558) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	2	A
1	S2	9	U
1	S2	10	G
1	S2	11	A
1	S2	16	G
1	S2	17	C
1	S2	24	C
1	S2	25	A
1	S2	33	G
1	S2	36	U
1	S2	37	C
1	S2	38	A
1	S2	39	A
1	S2	41	G
1	S2	42	A
1	S2	43	U
1	S2	44	U
1	S2	46	A
1	S2	49	C
1	S2	54	A
1	S2	55	U
1	S2	56	G
1	S2	58	C
1	S2	60	A
1	S2	61	A
1	S2	64	A
1	S2	65	C
1	S2	66	G
1	S2	67	C
1	S2	68	A
1	S2	69	C
1	S2	70	G
1	S2	72	C
1	S2	73	C
1	S2	74	G
1	S2	76	U
1	S2	79	A
1	S2	80	G
1	S2	103	A
1	S2	112	U
1	S2	113	G
1	S2	115	U
1	S2	116	OMU

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Mol	Chain	Res	Type
1	S2	119	PSU
1	S2	121	OMU
1	S2	125	C
1	S2	126	G
1	S2	130	G
1	S2	139	C
1	S2	140	C
1	S2	142	C
1	S2	143	U
1	S2	147	A
1	S2	155	G
1	S2	159	A2M
1	S2	161	U
1	S2	162	C
1	S2	163	U
1	S2	168	C
1	S2	170	A
1	S2	173	A
1	S2	176	U
1	S2	182	C
1	S2	183	G
1	S2	189	U
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	210	U
1	S2	215	G
1	S2	289	G
1	S2	293	C
1	S2	294	U

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Mol	Chain	Res	Type
1	S2	295	C
1	S2	302	A
1	S2	305	U
1	S2	308	G
1	S2	310	C
1	S2	311	C
1	S2	312	G
1	S2	313	A
1	S2	316	G
1	S2	318	A
1	S2	323	C
1	S2	324	C
1	S2	325	C
1	S2	326	C
1	S2	328	U
1	S2	329	G
1	S2	332	G
1	S2	333	G
1	S2	338	G
1	S2	340	C
1	S2	347	G
1	S2	351	G
1	S2	360	A
1	S2	363	A
1	S2	364	A
1	S2	367	U
1	S2	368	U
1	S2	369	C
1	S2	370	G
1	S2	373	G
1	S2	377	G
1	S2	379	C
1	S2	382	C
1	S2	385	G
1	S2	386	C
1	S2	387	C
1	S2	407	G
1	S2	408	A
1	S2	409	C
1	S2	413	G
1	S2	417	C
1	S2	418	A

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Mol	Chain	Res	Type
1	S2	419	G
1	S2	429	C
1	S2	436	G
1	S2	438	G
1	S2	446	G
1	S2	447	A
1	S2	448	A
1	S2	449	A
1	S2	450	C
1	S2	452	G
1	S2	464	A
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	496	C
1	S2	502	C
1	S2	507	G
1	S2	516	A
1	S2	528	A
1	S2	531	A
1	S2	532	C
1	S2	535	G
1	S2	537	C
1	S2	538	U
1	S2	540	U
1	S2	541	U
1	S2	542	U
1	S2	543	C
1	S2	544	G
1	S2	545	A
1	S2	546	G
1	S2	547	G
1	S2	548	C

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Mol	Chain	Res	Type
1	S2	549	C
1	S2	553	U
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	578	C
1	S2	579	C
1	S2	583	C
1	S2	587	A
1	S2	588	G
1	S2	589	G
1	S2	590	A
1	S2	591	U
1	S2	594	A
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	632	C
1	S2	634	A
1	S2	643	A
1	S2	655	A
1	S2	660	C
1	S2	662	G
1	S2	663	C
1	S2	664	A
1	S2	668	A2M
1	S2	669	A

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Mol	Chain	Res	Type
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	689	U
1	S2	690	G
1	S2	691	G
1	S2	692	G
1	S2	693	A
1	S2	695	C
1	S2	696	G
1	S2	697	G
1	S2	731	G
1	S2	732	U
1	S2	733	C
1	S2	734	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	750	C
1	S2	751	G
1	S2	752	G
1	S2	753	C
1	S2	788	G
1	S2	789	G
1	S2	790	C
1	S2	791	C
1	S2	792	C
1	S2	794	A
1	S2	797	C
1	S2	799	U
1	S2	804	U
1	S2	810	A
1	S2	811	A
1	S2	815	U
1	S2	821	G
1	S2	822	PSU

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Mol	Chain	Res	Type
1	S2	823	PSU
1	S2	830	A
1	S2	831	G
1	S2	834	C
1	S2	835	C
1	S2	836	G
1	S2	837	A
1	S2	838	G
1	S2	839	C
1	S2	841	G
1	S2	842	C
1	S2	847	A
1	S2	856	C
1	S2	858	A
1	S2	859	G
1	S2	861	A
1	S2	865	A
1	S2	866	U
1	S2	867	G
1	S2	868	G
1	S2	871	U
1	S2	873	G
1	S2	878	G
1	S2	883	U
1	S2	885	U
1	S2	886	A
1	S2	887	U
1	S2	889	U
1	S2	890	U
1	S2	891	G
1	S2	893	U
1	S2	894	G
1	S2	896	U
1	S2	897	U
1	S2	898	U
1	S2	899	U
1	S2	900	C
1	S2	902	G
1	S2	903	A
1	S2	906	U
1	S2	913	A
1	S2	914	U

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Mol	Chain	Res	Type
1	S2	917	U
1	S2	920	A
1	S2	922	A
1	S2	932	G
1	S2	933	G
1	S2	936	G
1	S2	966	U
1	S2	969	U
1	S2	970	G
1	S2	971	G
1	S2	973	C
1	S2	988	C
1	S2	989	C
1	S2	990	A
1	S2	992	A
1	S2	996	A
1	S2	999	G
1	S2	1001	A
1	S2	1002	U
1	S2	1003	U
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	1033	G
1	S2	1049	A
1	S2	1055	A
1	S2	1060	A
1	S2	1061	U
1	S2	1062	A
1	S2	1064	C
1	S2	1083	A
1	S2	1085	C
1	S2	1088	U
1	S2	1089	G
1	S2	1109	C

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Mol	Chain	Res	Type
1	S2	1114	U
1	S2	1115	U
1	S2	1116	C
1	S2	1117	C
1	S2	1119	A
1	S2	1121	G
1	S2	1123	C
1	S2	1133	A
1	S2	1135	C
1	S2	1138	C
1	S2	1144	A
1	S2	1145	A
1	S2	1146	C
1	S2	1149	A
1	S2	1154	U
1	S2	1155	U
1	S2	1158	G
1	S2	1159	G
1	S2	1166	G
1	S2	1195	A
1	S2	1197	G
1	S2	1207	G
1	S2	1208	A
1	S2	1215	C
1	S2	1217	A
1	S2	1220	A
1	S2	1221	G
1	S2	1224	G
1	S2	1233	G
1	S2	1242	U
1	S2	1244	U
1	S2	1246	A
1	S2	1251	A
1	S2	1253	A
1	S2	1256	G
1	S2	1257	G
1	S2	1259	A
1	S2	1260	A
1	S2	1262	C
1	S2	1265	A
1	S2	1269	G
1	S2	1273	C

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Mol	Chain	Res	Type
1	S2	1274	G
1	S2	1275	G
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
1	S2	1300	U
1	S2	1301	A
1	S2	1302	G
1	S2	1303	C
1	S2	1312	G
1	S2	1313	A
1	S2	1322	G
1	S2	1323	U
1	S2	1328	G
1	S2	1330	G
1	S2	1331	C
1	S2	1333	U
1	S2	1340	U
1	S2	1341	C
1	S2	1348	G
1	S2	1354	G
1	S2	1355	C
1	S2	1364	U
1	S2	1371	U
1	S2	1372	U
1	S2	1373	C
1	S2	1375	G
1	S2	1376	A
1	S2	1378	A
1	S2	1382	A
1	S2	1396	A
1	S2	1397	U
1	S2	1402	A
1	S2	1403	C
1	S2	1404	U
1	S2	1420	G

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Mol	Chain	Res	Type
1	S2	1421	A
1	S2	1422	G
1	S2	1423	C
1	S2	1424	G
1	S2	1433	C
1	S2	1434	C
1	S2	1435	C
1	S2	1436	C
1	S2	1437	C
1	S2	1438	A
1	S2	1442	U
1	S2	1446	A
1	S2	1447	G
1	S2	1454	A
1	S2	1458	G
1	S2	1462	U
1	S2	1463	U
1	S2	1464	C
1	S2	1466	G
1	S2	1470	C
1	S2	1477	U
1	S2	1478	U
1	S2	1480	A
1	S2	1482	C
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	1505	U
1	S2	1507	G
1	S2	1508	A
1	S2	1509	U
1	S2	1519	U
1	S2	1520	G
1	S2	1521	C
1	S2	1523	C
1	S2	1531	A
1	S2	1533	A
1	S2	1534	C

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Mol	Chain	Res	Type
1	S2	1535	U
1	S2	1536	G
1	S2	1543	U
1	S2	1544	C
1	S2	1545	A
1	S2	1548	G
1	S2	1552	G
1	S2	1553	C
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	1573	G
1	S2	1578	U
1	S2	1579	A
1	S2	1580	A
1	S2	1581	C
1	S2	1585	U
1	S2	1586	U
1	S2	1588	A
1	S2	1594	A
1	S2	1598	G
1	S2	1599	U
1	S2	1600	G
1	S2	1601	A
1	S2	1606	G
1	S2	1621	U
1	S2	1623	A
1	S2	1634	A
1	S2	1638	G
1	S2	1639	G
1	S2	1647	A
1	S2	1648	G
1	S2	1654	G
1	S2	1661	A
1	S2	1662	U
1	S2	1663	A
1	S2	1665	G
1	S2	1671	G

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Mol	Chain	Res	Type
1	S2	1675	A
1	S2	1676	U
1	S2	1680	G
1	S2	1682	C
1	S2	1683	C
1	S2	1686	G
1	S2	1688	C
1	S2	1693	G
1	S2	1695	A
1	S2	1698	C
1	S2	1699	A
1	S2	1702	G
1	S2	1703	OMC
1	S2	1720	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	1749	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	1789	G
1	S2	1797	U
1	S2	1800	A
1	S2	1803	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

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Mol	Chain	Res	Type
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	1841	C
1	S2	1849	G
1	S2	1852	C
1	S2	1861	G
1	S2	1862	G
1	S2	1863	A
1	S2	1864	U
1	S2	1865	C
1	S2	1869	A
38	D	13	G
38	D	23	C
38	D	32	C
38	D	34	U
38	D	35	C
38	D	37	A
38	D	59	A
38	D	63	U
38	D	72	A
38	D	80	A
38	D	81	C
38	D	83	C
38	D	84	A
38	D	85	U
38	D	87	G
38	D	94	G
38	D	95	A
38	D	101	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

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Mol	Chain	Res	Type
38	D	116	C
38	D	120	G
38	D	121	G
38	D	122	G
38	D	123	U
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
38	D	150	C
39	E	7	G
39	E	14	C
39	E	22	A
39	E	23	A
39	E	25	G
39	E	27	G
39	E	38	U
39	E	48	G
39	E	53	U
39	E	54	A
39	E	63	C
39	E	64	G
39	E	74	A
39	E	76	U
39	E	88	A
39	E	97	G
39	E	98	G
39	E	103	A
39	E	110	G
79	t	9	C
79	t	17	A
79	t	18	C
79	t	21	G
79	t	25	A
79	t	30	C
79	t	32	G
79	t	39	A
79	t	42	A

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Mol	Chain	Res	Type
79	t	48	G
79	t	49	U
79	t	59	A
79	t	64	A
79	t	65	A
79	t	71	C
79	t	72	C
79	t	73	A
79	t	74	G
79	t	91	G
79	t	93	G
79	t	98	A
79	t	101	A
79	t	108	A
79	t	110	C
79	t	112	C
79	t	116	G
79	t	119	G
79	t	120	A
79	t	121	A
79	t	131	C
79	t	132	G
79	t	134	G
79	t	135	G
79	t	137	G
79	t	138	C
79	t	143	G
79	t	144	A
79	t	148	G
79	t	149	U
79	t	156	C
79	t	157	G
79	t	158	G
79	t	169	C
79	t	173	G
79	t	181	U
79	t	182	C
79	t	183	G
79	t	184	U
79	t	185	G
79	t	196	G
79	t	197	U

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Mol	Chain	Res	Type
79	t	205	A
79	t	206	U
79	t	212	C
79	t	213	C
79	t	214	C
79	t	215	A
79	t	221	U
79	t	226	G
79	t	227	G
79	t	228	U
79	t	229	G
79	t	230	U
79	t	233	G
79	t	234	G
79	t	235	C
79	t	236	C
79	t	237	G
79	t	242	C
79	t	250	G
79	t	251	G
79	t	252	C
79	t	253	G
79	t	260	C
79	t	261	G
79	t	272	G
79	t	274	G
79	t	289	A
79	t	291	U
79	t	300	A
79	t	309	G
79	t	310	U
79	t	311	A
79	t	323	A
79	t	334	C
79	t	338	A
79	t	339	C
79	t	341	A
79	t	343	A
79	t	346	G
79	t	348	U
79	t	357	A
79	t	367	G

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Mol	Chain	Res	Type
79	t	370	A
79	t	375	U
79	t	377	A
79	t	381	G
79	t	404	A
79	t	405	G
79	t	406	G
79	t	407	G
79	t	408	C
79	t	409	G
79	t	425	G
79	t	426	U
79	t	434	U
79	t	437	G
79	t	443	C
79	t	444	G
79	t	446	A
79	t	447	G
79	t	448	U
79	t	449	C
79	t	451	G
79	t	456	G
79	t	458	G
79	t	463	C
79	t	465	A
79	t	473	G
79	t	474	C
79	t	479	C
79	t	481	G
79	t	482	G
79	t	483	C
79	t	486	U
79	t	487	G
79	t	489	C
79	t	492	C
79	t	493	G
79	t	494	G
79	t	495	C
79	t	497	C
79	t	498	G
79	t	504	U
79	t	507	U

Continued on next page...

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Mol	Chain	Res	Type
79	t	508	U
79	t	509	C
79	t	511	C
79	t	512	G
79	t	514	C
79	t	516	C
79	t	633	U
79	t	634	C
79	t	635	G
79	t	636	G
79	t	641	G
79	t	645	C
79	t	647	U
79	t	648	C
79	t	649	C
79	t	650	C
79	t	654	G
79	t	658	G
79	t	661	G
79	t	662	A
79	t	663	C
79	t	674	C
79	t	675	G
79	t	676	G
79	t	677	G
79	t	678	C
79	t	679	G
79	t	680	C
79	t	690	C
79	t	693	U
79	t	695	C
79	t	698	C
79	t	703	C
79	t	709	C
79	t	719	U
79	t	720	G
79	t	721	G
79	t	724	A
79	t	728	C
79	t	737	A
79	t	738	A
79	t	739	G

Continued on next page...

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Mol	Chain	Res	Type
79	t	899	G
79	t	902	A
79	t	904	A
79	t	905	G
79	t	906	C
79	t	907	C
79	t	914	G
79	t	917	G
79	t	919	A
79	t	920	G
79	t	921	C
79	t	922	A
79	t	923	C
79	t	924	U
79	t	925	C
79	t	926	G
79	t	927	C
79	t	929	G
79	t	933	C
79	t	944	G
79	t	947	A
79	t	948	G
79	t	949	C
79	t	950	G
79	t	952	G
79	t	953	A
79	t	954	C
79	t	957	G
79	t	958	U
79	t	959	C
79	t	976	U
79	t	1051	G
79	t	1055	C
79	t	1061	A
79	t	1065	C
79	t	1070	A
79	t	1083	U
79	t	1086	C
79	t	1087	C
79	t	1149	G
79	t	1150	C
79	t	1152	G

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Mol	Chain	Res	Type
79	t	1156	G
79	t	1162	U
79	t	1165	C
79	t	1167	A
79	t	1174	C
79	t	1176	C
79	t	1179	G
79	t	1192	U
79	t	1193	C
79	t	1196	G
79	t	1197	C
79	t	1198	C
79	t	1199	C
79	t	1201	G
79	t	1220	C
79	t	1221	A
79	t	1222	C
79	t	1223	G
79	t	1224	C
79	t	1225	G
79	t	1226	C
79	t	1228	C
79	t	1234	C
79	t	1236	G
79	t	1238	A
79	t	1240	G
79	t	1248	G
79	t	1249	G
79	t	1250	C
79	t	1251	G
79	t	1253	A
79	t	1258	G
79	t	1259	C
79	t	1268	U
79	t	1269	C
79	t	1271	G
79	t	1273	G
79	t	1277	A
79	t	1279	G
79	t	1285	U
79	t	1286	A
79	t	1301	C

Continued on next page...

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Mol	Chain	Res	Type
79	t	1309	A
79	t	1322	U
79	t	1336	G
79	t	1337	A
79	t	1341	G
79	t	1342	G
79	t	1348	C
79	t	1350	C
79	t	1351	A
79	t	1353	G
79	t	1360	G
79	t	1361	C
79	t	1362	C
79	t	1364	U
79	t	1370	A
79	t	1380	A
79	t	1381	A
79	t	1389	G
79	t	1390	C
79	t	1391	G
79	t	1392	C
79	t	1393	U
79	t	1394	C
79	t	1395	G
79	t	1401	C
79	t	1403	A
79	t	1404	G
79	t	1420	C
79	t	1421	U
79	t	1423	U
79	t	1424	C
79	t	1425	C
79	t	1426	A
79	t	1430	C
79	t	1431	G
79	t	1439	G
79	t	1463	C
79	t	1464	G
79	t	1465	C
79	t	1466	G
79	t	1467	C
79	t	1468	C

Continued on next page...

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Mol	Chain	Res	Type
79	t	1473	A
79	t	1474	G
79	t	1480	G
79	t	1484	G
79	t	1485	A
79	t	1498	G
79	t	1500	A
79	t	1507	A
79	t	1516	A
79	t	1517	C
79	t	1525	G
79	t	1531	G
79	t	1542	A
79	t	1545	A
79	t	1548	C
79	t	1560	U
79	t	1564	U
79	t	1573	U
79	t	1578	U
79	t	1583	A
79	t	1587	G
79	t	1595	A
79	t	1606	G
79	t	1607	G
79	t	1613	A
79	t	1614	A
79	t	1615	G
79	t	1616	A
79	t	1622	C
79	t	1623	G
79	t	1624	A
79	t	1636	G
79	t	1643	C
79	t	1652	G
79	t	1658	C
79	t	1659	U
79	t	1660	C
79	t	1663	G
79	t	1673	G
79	t	1679	G
79	t	1680	C
79	t	1700	C

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Mol	Chain	Res	Type
79	t	1701	A
79	t	1702	C
79	t	1711	A
79	t	1716	G
79	t	1723	G
79	t	1728	A
79	t	1742	G
79	t	1746	G
79	t	1747	A
79	t	1748	A
79	t	1750	C
79	t	1751	G
79	t	1769	A
79	t	1776	A
79	t	1786	A
79	t	1788	G
79	t	1794	C
79	t	1797	G
79	t	1801	G
79	t	1803	G
79	t	1804	U
79	t	1814	G
79	t	1816	G
79	t	1818	A
79	t	1823	G
79	t	1836	G
79	t	1840	C
79	t	1844	U
79	t	1850	G
79	t	1862	C
79	t	1863	U
79	t	1872	A
79	t	1873	A
79	t	1881	C
79	t	1887	U
79	t	1891	G
79	t	1896	C
79	t	1900	G
79	t	1902	C
79	t	1903	G
79	t	1906	G
79	t	1910	A

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Mol	Chain	Res	Type
79	t	1912	C
79	t	1913	A
79	t	1916	C
79	t	1920	A
79	t	1921	G
79	t	1928	U
79	t	1929	G
79	t	1932	G
79	t	1933	G
79	t	1938	U
79	t	1940	U
79	t	1941	A
79	t	1942	G
79	t	1943	A
79	t	1952	C
79	t	1956	G
79	t	1961	U
79	t	1963	G
79	t	1964	A
79	t	1968	C
79	t	1972	A
79	t	1973	U
79	t	1978	U
79	t	1979	A
79	t	1980	A
79	t	1983	A
79	t	1984	G
79	t	1991	A
79	t	1994	A
79	t	2003	C
79	t	2007	A
79	t	2011	A
79	t	2021	A
79	t	2025	U
79	t	2027	G
79	t	2029	U
79	t	2036	G
79	t	2037	G
79	t	2043	C
79	t	2051	U
79	t	2065	C
79	t	2069	G

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Mol	Chain	Res	Type
79	t	2070	U
79	t	2072	G
79	t	2073	A
79	t	2075	A
79	t	2077	U
79	t	2078	G
79	t	2081	C
79	t	2082	G
79	t	2087	C
79	t	2088	G
79	t	2090	C
79	t	2091	G
79	t	2092	G
79	t	2231	G
79	t	2232	A
79	t	2233	G
79	t	2234	C
79	t	2235	C
79	t	2236	C
79	t	2237	C
79	t	2241	G
79	t	2242	A
79	t	2245	C
79	t	2246	U
79	t	2247	A
79	t	2264	A
79	t	2265	G
79	t	2268	C
79	t	2278	G
79	t	2279	A
79	t	2280	G
79	t	2282	C
79	t	2285	G
79	t	2292	A
79	t	2295	G
79	t	2321	G
79	t	2323	U
79	t	2325	C
79	t	2327	G
79	t	2330	C
79	t	2340	G
79	t	2343	G

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Mol	Chain	Res	Type
79	t	2358	A
79	t	2374	A
79	t	2375	A
79	t	2391	A
79	t	2396	A
79	t	2400	G
79	t	2401	C
79	t	2404	U
79	t	2405	U
79	t	2416	C
79	t	2421	G
79	t	2426	U
79	t	2429	G
79	t	2431	G
79	t	2432	A
79	t	2442	G
79	t	2446	U
79	t	2447	U
79	t	2449	C
79	t	2458	G
79	t	2467	C
79	t	2468	C
79	t	2469	U
79	t	2473	U
79	t	2482	G
79	t	2483	C
79	t	2484	C
79	t	2485	G
79	t	2490	A
79	t	2492	A
79	t	2499	C
79	t	2523	G
79	t	2524	U
79	t	2525	G
79	t	2526	G
79	t	2532	A
79	t	2533	U
79	t	2544	A
79	t	2562	C
79	t	2565	G
79	t	2566	A
79	t	2568	C

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Mol	Chain	Res	Type
79	t	2580	A
79	t	2585	G
79	t	2606	C
79	t	2617	G
79	t	2618	U
79	t	2632	C
79	t	2640	U
79	t	2648	C
79	t	2652	G
79	t	2665	G
79	t	2666	U
79	t	2673	G
79	t	2675	A
79	t	2687	U
79	t	2689	C
79	t	2690	G
79	t	2691	G
79	t	2698	C
79	t	2700	G
79	t	2705	G
79	t	2714	G
79	t	2719	U
79	t	2722	A
79	t	2723	A
79	t	2726	U
79	t	2733	G
79	t	2737	G
79	t	2741	G
79	t	2745	A
79	t	2748	U
79	t	2766	A
79	t	2767	U
79	t	2768	A
79	t	2769	U
79	t	2773	C
79	t	2775	G
79	t	2776	C
79	t	2778	G
79	t	2785	A
79	t	2793	C
79	t	2798	U
79	t	2805	U

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Mol	Chain	Res	Type
79	t	2806	G
79	t	2809	G
79	t	2814	A
79	t	2817	G
79	t	2821	G
79	t	2824	A
79	t	2834	G
79	t	2835	C
79	t	2855	G
79	t	2858	A
79	t	2860	A
79	t	2863	G
79	t	2871	C
79	t	2879	U
79	t	2881	G
79	t	3570	A
79	t	3571	G
79	t	3572	C
79	t	3573	C
79	t	3577	U
79	t	3587	U
79	t	3589	C
79	t	3591	G
79	t	3596	G
79	t	3597	G
79	t	3606	A
79	t	3612	U
79	t	3615	U
79	t	3616	U
79	t	3617	A
79	t	3619	A
79	t	3624	A
79	t	3633	A
79	t	3635	G
79	t	3644	C
79	t	3651	U
79	t	3661	U
79	t	3662	G
79	t	3663	A
79	t	3667	C
79	t	3683	A
79	t	3700	U

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Mol	Chain	Res	Type
79	t	3707	A
79	t	3719	A
79	t	3722	G
79	t	3724	G
79	t	3725	G
79	t	3728	G
79	t	3730	A
79	t	3731	A
79	t	3733	U
79	t	3742	C
79	t	3744	U
79	t	3745	A
79	t	3748	G
79	t	3751	G
79	t	3754	A
79	t	3755	A
79	t	3759	C
79	t	3781	C
79	t	3782	G
79	t	3783	C
79	t	3784	A
79	t	3785	U
79	t	3788	A
79	t	3789	U
79	t	3790	G
79	t	3795	A
79	t	3798	G
79	t	3799	A
79	t	3809	U
79	t	3810	G
79	t	3811	U
79	t	3822	U
79	t	3838	A
79	t	3847	A
79	t	3848	A
79	t	3849	C
79	t	3850	G
79	t	3851	G
79	t	3852	G
79	t	3860	G
79	t	3863	U
79	t	3865	A

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Mol	Chain	Res	Type
79	t	3866	G
79	t	3868	G
79	t	3869	G
79	t	3872	A
79	t	3876	A
79	t	3877	A
79	t	3878	G
79	t	3879	A
79	t	3880	C
79	t	3886	U
79	t	3887	G
79	t	3894	A
79	t	3909	G
79	t	3917	G
79	t	3918	A
79	t	4046	G
79	t	4054	G
79	t	4062	G
79	t	4064	G
79	t	4065	G
79	t	4069	G
79	t	4070	C
79	t	4071	C
79	t	4072	C
79	t	4074	A
79	t	4079	C
79	t	4080	U
79	t	4083	C
79	t	4084	G
79	t	4086	U
79	t	4088	C
79	t	4096	A
79	t	4101	C
79	t	4106	C
79	t	4107	C
79	t	4108	G
79	t	4109	G
79	t	4110	C
79	t	4111	C
79	t	4119	A
79	t	4124	C
79	t	4125	U

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Mol	Chain	Res	Type
79	t	4126	C
79	t	4130	G
79	t	4132	A
79	t	4139	C
79	t	4145	G
79	t	4146	G
79	t	4153	G
79	t	4158	G
79	t	4165	A
79	t	4167	A
79	t	4174	A
79	t	4176	A
79	t	4187	G
79	t	4190	G
79	t	4191	U
79	t	4195	A
79	t	4205	C
79	t	4211	G
79	t	4213	A
79	t	4216	G
79	t	4217	A
79	t	4228	G
79	t	4230	A
79	t	4234	G
79	t	4235	A
79	t	4242	A
79	t	4243	A
79	t	4253	G
79	t	4266	A
79	t	4267	G
79	t	4276	C
79	t	4291	G
79	t	4292	G
79	t	4294	C
79	t	4300	G
79	t	4301	A
79	t	4311	C
79	t	4316	U
79	t	4322	U
79	t	4326	G
79	t	4333	G
79	t	4334	U

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Mol	Chain	Res	Type
79	t	4338	A
79	t	4339	G
79	t	4340	A
79	t	4341	A
79	t	4343	A
79	t	4344	G
79	t	4349	C
79	t	4353	G
79	t	4356	A
79	t	4358	A
79	t	4360	C
79	t	4367	G
79	t	4384	A
79	t	4388	C
79	t	4402	G
79	t	4406	C
79	t	4414	U
79	t	4426	A
79	t	4428	C
79	t	4437	G
79	t	4453	G
79	t	4455	U
79	t	4460	U
79	t	4462	U
79	t	4464	C
79	t	4472	A
79	t	4474	U
79	t	4475	A
79	t	4480	A
79	t	4485	A
79	t	4486	G
79	t	4490	G
79	t	4501	U
79	t	4510	A
79	t	4511	G
79	t	4517	U
79	t	4522	C
79	t	4529	G
79	t	4531	U
79	t	4537	G
79	t	4551	A
79	t	4552	A

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Mol	Chain	Res	Type
79	t	4561	A
79	t	4562	G
79	t	4570	G
79	t	4578	A
79	t	4595	G
79	t	4598	U
79	t	4599	G
79	t	4601	G
79	t	4614	G
79	t	4618	A
79	t	4619	U
79	t	4632	C
79	t	4640	G
79	t	4656	G
79	t	4657	C
79	t	4662	A
79	t	4671	U
79	t	4682	C
79	t	4683	G
79	t	4684	G
79	t	4686	A
79	t	4692	C
79	t	4693	G
79	t	4694	G
79	t	4695	C
79	t	4696	A
79	t	4697	G
79	t	4703	C
79	t	4704	G
79	t	4706	A
79	t	4714	U
79	t	4715	U
79	t	4716	G
79	t	4718	C
79	t	4720	U
79	t	4722	G
79	t	4726	A
79	t	4732	U
79	t	4736	C
79	t	4737	G
79	t	4817	G
79	t	4824	C

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Mol	Chain	Res	Type
79	t	4827	U
79	t	4828	G
79	t	4830	G
79	t	4831	G
79	t	4832	A
79	t	4833	G
79	t	4834	U
79	t	4838	C
79	t	4840	U
79	t	4841	C
79	t	4847	G
79	t	4852	A
79	t	4853	C
79	t	4854	G
79	t	4855	G
79	t	4856	G
79	t	4858	C
79	t	4859	G
79	t	4864	C
79	t	4865	G
79	t	4866	G
79	t	4867	A
79	t	4868	A
79	t	4870	G
79	t	4871	G
79	t	4872	C
79	t	4882	C
79	t	4883	U
79	t	4884	C
79	t	4885	G
79	t	4886	C
79	t	4892	A
79	t	4894	G
79	t	4895	C
79	t	4896	A
79	t	4898	C
79	t	4901	A
79	t	4902	C
79	t	4903	G
79	t	4909	G
79	t	4914	A
79	t	4921	G

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Mol	Chain	Res	Type
79	t	4924	A
79	t	4933	G
79	t	4934	U
79	t	4936	G
79	t	4943	U
79	t	4946	U
79	t	4947	U
79	t	4949	U
79	t	4950	G
79	t	4957	G
79	t	4971	C
79	t	4972	A
79	t	4975	G
79	t	4981	C
79	t	4982	C
79	t	4984	U
79	t	4985	C
79	t	4986	G
79	t	4999	G
79	t	5007	G
79	t	5008	C
79	t	5011	U
79	t	5012	C
79	t	5013	G
79	t	5015	C
79	t	5016	A
79	t	5020	G
79	t	5024	U
79	t	5028	C
80	u	4	C
80	u	7	A
80	u	8	U
80	u	11	C
80	u	17	C
80	u	18	G
80	u	19	G
80	u	20	U
80	u	21	A
80	u	22	G
80	u	23	A
80	u	25	C
80	u	38	A

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Mol	Chain	Res	Type
80	u	46	G
80	u	47	U
80	u	48	C
80	u	52	G
80	u	56	C
80	u	59	U
80	u	60	U
80	u	61	C
80	u	62	C
80	u	64	A
80	u	69	G
80	u	71	G
80	u	72	C
80	u	74	C
80	u	76	A
81	v	2	G
81	v	8	U
81	v	10	G
81	v	15	G
81	v	16	A
81	v	17	A
81	v	19	G
81	v	20	U
81	v	21	A
81	v	30	G
81	v	46	G
81	v	47	U
81	v	48	C
81	v	49	C
81	v	51	U
81	v	54	U
81	v	55	U
81	v	56	C
81	v	57	G
81	v	58	A
81	v	61	C
81	v	62	C
81	v	69	G
81	v	70	G
81	v	71	G
81	v	72	C
81	v	75	C

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Mol	Chain	Res	Type
81	v	76	A
82	w	17	G
82	w	21	G

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	42	A
1	S2	53	C
1	S2	60	A
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	386	C
1	S2	417	C
1	S2	445	A
1	S2	536	A
1	S2	559	G
1	S2	563	G
1	S2	670	A
1	S2	814	5MU
1	S2	872	A
1	S2	1261	C
1	S2	1375	G
1	S2	1396	A
1	S2	1567	G
1	S2	1572	C
1	S2	1600	G
1	S2	1661	A
1	S2	1681	U
1	S2	1802	C
1	S2	1813	A
1	S2	1814	G
1	S2	1815	A
1	S2	1828	C

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

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	B8Q	S2	1219	1	18,22,23	4.74	7 (38%)	21,32,35	1.90	5 (23%)
1	UR3	S2	1830	1	19,22,23	2.79	7 (36%)	26,32,35	3.04	9 (34%)
1	A2M	S2	1678	1	18,25,26	4.29	5 (27%)	20,36,39	3.50	6 (30%)
1	4AC	S2	1842	1	21,24,25	3.23	9 (42%)	28,34,37	1.12	3 (10%)
1	PSU	S2	822	1	18,21,22	4.38	8 (44%)	21,30,33	1.92	4 (19%)
1	A2M	S2	1031	1	18,25,26	4.19	5 (27%)	20,36,39	3.68	5 (25%)
1	A2M	S2	27	1	18,25,26	4.17	5 (27%)	20,36,39	3.57	6 (30%)
1	OMC	S2	174	1	19,22,23	3.53	8 (42%)	25,31,34	0.92	1 (4%)
1	4AC	S2	1337	1	21,24,25	3.28	9 (42%)	28,34,37	1.25	3 (10%)
1	5MU	S2	814	1	19,22,23	7.59	8 (42%)	27,32,35	3.61	11 (40%)
1	PSU	S2	823	1	18,21,22	4.49	8 (44%)	21,30,33	2.18	4 (19%)
1	OMC	S2	1710	1	19,22,23	3.58	8 (42%)	25,31,34	0.65	0
1	MA6	S2	1850	1	19,26,27	1.67	2 (10%)	18,38,41	3.89	4 (22%)
1	PSU	S2	612	1	18,21,22	4.25	8 (44%)	21,30,33	2.22	6 (28%)
1	OMG	S2	683	1	19,26,27	2.37	8 (42%)	21,38,41	1.47	5 (23%)
1	B8N	S2	1248	1	25,29,30	3.15	7 (28%)	28,42,45	2.12	7 (25%)
1	A2M	S2	668	1	18,25,26	4.07	5 (27%)	20,36,39	3.84	8 (40%)
1	OMG	S2	509	1	19,26,27	2.37	8 (42%)	21,38,41	1.47	4 (19%)
1	OMC	S2	1703	1	19,22,23	3.48	8 (42%)	25,31,34	0.61	0
1	PSU	S2	1081	1	18,21,22	4.30	8 (44%)	21,30,33	1.95	4 (19%)
1	OMC	S2	517	1	19,22,23	3.39	8 (42%)	25,31,34	0.86	1 (4%)
1	6MZ	S2	1832	1	17,25,26	1.60	4 (23%)	15,36,39	2.26	4 (26%)
1	E3C	S2	568	1	19,23,24	3.59	7 (36%)	21,33,36	2.64	6 (28%)
1	PSU	S2	119	1	18,21,22	4.45	7 (38%)	21,30,33	2.10	5 (23%)
1	OMU	S2	121	1	19,22,23	3.08	7 (36%)	25,31,34	2.00	6 (24%)
1	A2M	S2	166	1	18,25,26	4.28	6 (33%)	20,36,39	3.80	5 (25%)
1	OMU	S2	116	1	19,22,23	3.16	6 (31%)	25,31,34	1.81	4 (16%)
1	PSU	S2	1243	1	18,21,22	4.39	7 (38%)	21,30,33	1.96	4 (19%)
1	OMG	S2	644	1	19,26,27	2.44	8 (42%)	21,38,41	1.50	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	S2	159	1	18,25,26	4.34	5 (27%)	20,36,39	3.63	10 (50%)
1	5MC	S2	1374	1	19,22,23	3.64	8 (42%)	26,32,35	1.05	2 (7%)
1	M7A	S2	1806	1	19,25,26	1.67	2 (10%)	25,37,40	3.74	8 (32%)
1	MA6	S2	1851	1	19,26,27	1.63	2 (10%)	18,38,41	3.88	4 (22%)
1	A2M	S2	484	1	18,25,26	4.16	6 (33%)	20,36,39	3.66	6 (30%)

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	B8Q	S2	1219	1	-	0/7/42/43	0/2/2/2
1	UR3	S2	1830	1	-	4/7/25/26	0/2/2/2
1	A2M	S2	1678	1	-	0/5/27/28	0/3/3/3
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
1	PSU	S2	822	1	-	4/7/25/26	0/2/2/2
1	A2M	S2	1031	1	-	1/5/27/28	0/3/3/3
1	A2M	S2	27	1	-	1/5/27/28	0/3/3/3
1	OMC	S2	174	1	-	1/9/27/28	0/2/2/2
1	4AC	S2	1337	1	-	0/11/29/30	0/2/2/2
1	5MU	S2	814	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	823	1	-	3/7/25/26	0/2/2/2
1	OMC	S2	1710	1	-	0/9/27/28	0/2/2/2
1	MA6	S2	1850	1	-	4/7/29/30	0/3/3/3
1	PSU	S2	612	1	-	2/7/25/26	0/2/2/2
1	OMG	S2	683	1	-	2/5/27/28	0/3/3/3
1	B8N	S2	1248	1	-	4/16/34/35	0/2/2/2
1	A2M	S2	668	1	-	2/5/27/28	0/3/3/3
1	OMG	S2	509	1	-	1/5/27/28	0/3/3/3
1	OMC	S2	1703	1	-	2/9/27/28	0/2/2/2
1	PSU	S2	1081	1	-	2/7/25/26	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
1	6MZ	S2	1832	1	-	2/5/27/28	0/3/3/3
1	E3C	S2	568	1	-	4/9/44/45	0/2/2/2
1	PSU	S2	119	1	-	2/7/25/26	0/2/2/2
1	OMU	S2	121	1	-	3/9/27/28	0/2/2/2
1	A2M	S2	166	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	S2	116	1	-	2/9/27/28	0/2/2/2
1	PSU	S2	1243	1	-	2/7/25/26	0/2/2/2
1	OMG	S2	644	1	-	1/5/27/28	0/3/3/3
1	A2M	S2	159	1	-	3/5/27/28	0/3/3/3
1	5MC	S2	1374	1	-	0/7/25/26	0/2/2/2
1	M7A	S2	1806	1	-	3/7/37/38	0/3/3/3
1	MA6	S2	1851	1	-	4/7/29/30	0/3/3/3
1	A2M	S2	484	1	-	0/5/27/28	0/3/3/3

All (224) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	814	5MU	C4-C5	22.49	1.81	1.44
1	S2	814	5MU	C6-N1	16.54	1.66	1.38
1	S2	159	A2M	O4'-C1'	11.96	1.56	1.40
1	S2	823	PSU	C6-C5	11.93	1.48	1.35
1	S2	166	A2M	O4'-C1'	11.89	1.56	1.40
1	S2	814	5MU	C6-C5	-11.89	1.15	1.34
1	S2	1243	PSU	C6-C5	11.78	1.48	1.35
1	S2	1678	A2M	O4'-C1'	11.43	1.55	1.40
1	S2	1219	B8Q	C4-N3	11.32	1.65	1.48
1	S2	27	A2M	O4'-C1'	11.29	1.55	1.40
1	S2	1031	A2M	O4'-C1'	11.26	1.55	1.40
1	S2	822	PSU	C6-C5	11.14	1.47	1.35
1	S2	1081	PSU	C6-C5	11.12	1.47	1.35
1	S2	119	PSU	C6-C5	11.08	1.47	1.35
1	S2	814	5MU	C4-N3	-11.03	1.18	1.38
1	S2	1219	B8Q	C6-C5	10.97	1.56	1.33
1	S2	484	A2M	O4'-C1'	10.95	1.55	1.40
1	S2	612	PSU	C6-C5	10.74	1.47	1.35
1	S2	668	A2M	O4'-C1'	10.58	1.54	1.40
1	S2	1678	A2M	C3'-C4'	-10.42	1.26	1.53
1	S2	1031	A2M	C3'-C4'	-10.27	1.26	1.53
1	S2	27	A2M	C3'-C4'	-10.22	1.27	1.53
1	S2	668	A2M	C3'-C4'	-10.18	1.27	1.53
1	S2	484	A2M	C3'-C4'	-10.05	1.27	1.53
1	S2	166	A2M	C3'-C4'	-10.01	1.27	1.53
1	S2	159	A2M	C3'-C4'	-10.01	1.27	1.53
1	S2	119	PSU	C2-N1	9.95	1.49	1.36
1	S2	822	PSU	C2-N1	9.29	1.48	1.36
1	S2	1219	B8Q	C2-N1	9.25	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	612	PSU	C2-N1	9.21	1.48	1.36
1	S2	1081	PSU	C2-N1	9.06	1.48	1.36
1	S2	1243	PSU	C2-N1	9.05	1.48	1.36
1	S2	1374	5MC	C6-C5	9.01	1.49	1.34
1	S2	823	PSU	C2-N1	8.97	1.48	1.36
1	S2	1703	OMC	C4-N4	8.44	1.54	1.33
1	S2	1710	OMC	C4-N4	8.41	1.54	1.33
1	S2	174	OMC	C4-N4	8.35	1.54	1.33
1	S2	116	OMU	C2-N1	8.26	1.51	1.38
1	S2	517	OMC	C4-N4	8.19	1.53	1.33
1	S2	568	E3C	C2-N3	8.16	1.47	1.37
1	S2	1248	B8N	C4-N3	-8.10	1.26	1.40
1	S2	1830	UR3	C2-N1	8.08	1.49	1.38
1	S2	568	E3C	C6-C5	8.03	1.50	1.33
1	S2	121	OMU	C2-N1	7.99	1.51	1.38
1	S2	823	PSU	C2-N3	7.94	1.50	1.37
1	S2	568	E3C	C2-N1	7.88	1.49	1.38
1	S2	1842	4AC	C4-N3	7.83	1.45	1.32
1	S2	1337	4AC	C4-N3	7.39	1.45	1.32
1	S2	1248	B8N	C6-N1	7.39	1.54	1.36
1	S2	119	PSU	C2-N3	7.35	1.49	1.37
1	S2	1248	B8N	C4-C5	7.16	1.63	1.47
1	S2	822	PSU	C2-N3	6.96	1.48	1.37
1	S2	1243	PSU	C2-N3	6.93	1.48	1.37
1	S2	174	OMC	C2-N3	6.83	1.49	1.36
1	S2	1710	OMC	C2-N3	6.80	1.49	1.36
1	S2	612	PSU	C2-N3	6.78	1.48	1.37
1	S2	1703	OMC	C6-C5	6.63	1.50	1.35
1	S2	1710	OMC	C6-C5	6.59	1.50	1.35
1	S2	1703	OMC	C2-N3	6.57	1.49	1.36
1	S2	174	OMC	C6-C5	6.54	1.50	1.35
1	S2	116	OMU	C2-N3	6.53	1.49	1.38
1	S2	517	OMC	C6-C5	6.52	1.50	1.35
1	S2	1081	PSU	C2-N3	6.48	1.48	1.37
1	S2	121	OMU	C2-N3	6.43	1.49	1.38
1	S2	517	OMC	C2-N3	6.39	1.49	1.36
1	S2	1710	OMC	C4-N3	6.29	1.46	1.34
1	S2	1374	5MC	C4-N3	6.25	1.44	1.34
1	S2	1374	5MC	C5-C4	6.17	1.48	1.44
1	S2	116	OMU	C6-C5	6.13	1.49	1.35
1	S2	159	A2M	C3'-C2'	6.08	1.66	1.53
1	S2	1337	4AC	C6-C5	6.05	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1842	4AC	C2-N3	6.00	1.48	1.36
1	S2	121	OMU	C6-C5	5.93	1.48	1.35
1	S2	174	OMC	C4-N3	5.92	1.46	1.34
1	S2	1337	4AC	C2-N3	5.90	1.48	1.36
1	S2	1703	OMC	C4-N3	5.90	1.46	1.34
1	S2	484	A2M	C3'-C2'	5.75	1.65	1.53
1	S2	668	A2M	C3'-C2'	5.73	1.65	1.53
1	S2	1842	4AC	C6-C5	5.63	1.48	1.35
1	S2	1374	5MC	C2-N3	5.63	1.47	1.36
1	S2	1678	A2M	C3'-C2'	5.57	1.65	1.53
1	S2	1248	B8N	C2-N1	5.55	1.55	1.39
1	S2	517	OMC	C4-N3	5.48	1.45	1.34
1	S2	1031	A2M	C3'-C2'	5.46	1.64	1.53
1	S2	1219	B8Q	C2-N3	-5.41	1.25	1.35
1	S2	509	OMG	C2-N3	5.36	1.46	1.33
1	S2	166	A2M	C3'-C2'	5.35	1.64	1.53
1	S2	1830	UR3	C6-C5	5.35	1.47	1.35
1	S2	1081	PSU	O2-C2	-5.26	1.12	1.23
1	S2	1850	MA6	C6-C5	-5.22	1.36	1.44
1	S2	27	A2M	C3'-C2'	5.21	1.64	1.53
1	S2	568	E3C	C4-N3	5.18	1.56	1.48
1	S2	644	OMG	C2-N3	5.16	1.45	1.33
1	S2	612	PSU	O2-C2	-5.14	1.12	1.23
1	S2	814	5MU	C2-N3	5.10	1.46	1.38
1	S2	823	PSU	O2-C2	-5.01	1.12	1.23
1	S2	1081	PSU	O4-C4	-4.99	1.14	1.23
1	S2	166	A2M	O4'-C4'	4.97	1.56	1.45
1	S2	119	PSU	O4-C4	-4.95	1.14	1.23
1	S2	644	OMG	C4-N3	4.94	1.49	1.37
1	S2	509	OMG	C4-N3	4.94	1.49	1.37
1	S2	822	PSU	O2-C2	-4.92	1.12	1.23
1	S2	1243	PSU	O2-C2	-4.91	1.12	1.23
1	S2	159	A2M	O4'-C4'	4.91	1.55	1.45
1	S2	822	PSU	O4-C4	-4.87	1.14	1.23
1	S2	1806	M7A	C6-N6	4.87	1.46	1.34
1	S2	683	OMG	C2-N3	4.84	1.45	1.33
1	S2	116	OMU	C4-N3	4.83	1.46	1.38
1	S2	1830	UR3	C2-N3	4.81	1.48	1.39
1	S2	1248	B8N	C6-C5	4.80	1.41	1.35
1	S2	1851	MA6	C6-C5	-4.79	1.37	1.44
1	S2	119	PSU	O2-C2	-4.78	1.13	1.23
1	S2	1337	4AC	C7-N4	4.76	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	683	OMG	C4-N3	4.74	1.48	1.37
1	S2	612	PSU	O4-C4	-4.71	1.14	1.23
1	S2	1243	PSU	O4-C4	-4.69	1.14	1.23
1	S2	484	A2M	O4'-C4'	4.68	1.55	1.45
1	S2	683	OMG	C2-N2	4.68	1.45	1.34
1	S2	644	OMG	C2-N2	4.67	1.45	1.34
1	S2	1678	A2M	C6-N6	4.64	1.50	1.34
1	S2	1678	A2M	O4'-C4'	4.64	1.55	1.45
1	S2	1031	A2M	O4'-C4'	4.63	1.55	1.45
1	S2	1219	B8Q	C4-C5	-4.63	1.39	1.49
1	S2	27	A2M	O4'-C4'	4.55	1.55	1.45
1	S2	1337	4AC	C4-N4	4.46	1.46	1.39
1	S2	1842	4AC	C2-N1	4.45	1.49	1.40
1	S2	1842	4AC	C7-N4	4.45	1.46	1.37
1	S2	121	OMU	C4-N3	4.44	1.46	1.38
1	S2	174	OMC	C2-N1	4.37	1.49	1.40
1	S2	1374	5MC	C4-N4	4.29	1.45	1.34
1	S2	1832	6MZ	C6-C5	-4.27	1.38	1.44
1	S2	509	OMG	C2-N2	4.25	1.44	1.34
1	S2	668	A2M	O4'-C4'	4.23	1.54	1.45
1	S2	119	PSU	C6-N1	4.21	1.43	1.36
1	S2	1374	5MC	C6-N1	4.15	1.45	1.38
1	S2	1337	4AC	C2-N1	4.14	1.48	1.40
1	S2	1337	4AC	C5-C4	4.14	1.50	1.41
1	S2	1842	4AC	C4-N4	4.02	1.45	1.39
1	S2	822	PSU	C6-N1	4.01	1.42	1.36
1	S2	1710	OMC	C2-N1	3.96	1.48	1.40
1	S2	159	A2M	C6-N6	3.95	1.48	1.34
1	S2	27	A2M	C6-N6	3.95	1.48	1.34
1	S2	166	A2M	C6-N6	3.94	1.48	1.34
1	S2	1031	A2M	C6-N6	3.92	1.48	1.34
1	S2	668	A2M	C6-N6	3.91	1.48	1.34
1	S2	517	OMC	C2-N1	3.91	1.48	1.40
1	S2	484	A2M	C6-N6	3.91	1.48	1.34
1	S2	1806	M7A	C5-N7	3.90	1.48	1.39
1	S2	1243	PSU	C6-N1	3.88	1.42	1.36
1	S2	814	5MU	C2-N1	3.85	1.44	1.38
1	S2	1081	PSU	C6-N1	3.85	1.42	1.36
1	S2	612	PSU	C6-N1	3.85	1.42	1.36
1	S2	1710	OMC	C6-N1	3.84	1.47	1.38
1	S2	1374	5MC	C2-N1	3.80	1.48	1.40
1	S2	823	PSU	C6-N1	3.78	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1337	4AC	C6-N1	3.77	1.47	1.38
1	S2	1842	4AC	C5-C4	3.67	1.49	1.41
1	S2	1851	MA6	C6-N6	3.65	1.45	1.37
1	S2	1850	MA6	C6-N6	3.63	1.45	1.37
1	S2	1842	4AC	C6-N1	3.61	1.46	1.38
1	S2	174	OMC	C6-N1	3.58	1.46	1.38
1	S2	1703	OMC	C6-N1	3.57	1.46	1.38
1	S2	823	PSU	C4-N3	3.48	1.45	1.38
1	S2	1703	OMC	C2-N1	3.46	1.47	1.40
1	S2	823	PSU	O4-C4	-3.41	1.17	1.23
1	S2	683	OMG	C5-C4	-3.30	1.34	1.43
1	S2	517	OMC	C6-N1	3.28	1.45	1.38
1	S2	644	OMG	C6-N1	3.26	1.42	1.37
1	S2	1374	5MC	O2-C2	-3.17	1.17	1.23
1	S2	683	OMG	C6-N1	3.09	1.42	1.37
1	S2	568	E3C	C6-N1	3.02	1.45	1.38
1	S2	1219	B8Q	C31-N3	3.00	1.52	1.46
1	S2	1832	6MZ	C2-N3	2.96	1.36	1.32
1	S2	822	PSU	C4-N3	2.95	1.44	1.38
1	S2	1830	UR3	O2-C2	-2.92	1.17	1.22
1	S2	644	OMG	C5-C4	-2.91	1.35	1.43
1	S2	509	OMG	C5-C4	-2.89	1.35	1.43
1	S2	119	PSU	C4-N3	2.87	1.44	1.38
1	S2	1219	B8Q	C6-N1	-2.85	1.31	1.38
1	S2	509	OMG	C6-N1	2.85	1.42	1.37
1	S2	1243	PSU	C4-N3	2.85	1.44	1.38
1	S2	568	E3C	C31-N3	2.82	1.55	1.47
1	S2	644	OMG	C5-C6	2.80	1.53	1.47
1	S2	1081	PSU	O4'-C1'	-2.76	1.40	1.43
1	S2	612	PSU	C4-N3	2.75	1.44	1.38
1	S2	1830	UR3	C5-C4	2.75	1.50	1.43
1	S2	1830	UR3	C4-N3	2.72	1.46	1.40
1	S2	509	OMG	C5-C6	2.70	1.52	1.47
1	S2	116	OMU	C6-N1	2.67	1.44	1.38
1	S2	121	OMU	C6-N1	2.61	1.44	1.38
1	S2	1081	PSU	C4-N3	2.58	1.43	1.38
1	S2	823	PSU	O4'-C1'	-2.56	1.40	1.43
1	S2	568	E3C	C4-C5	-2.44	1.44	1.49
1	S2	517	OMC	O2-C2	-2.43	1.19	1.23
1	S2	1703	OMC	O2-C2	-2.43	1.19	1.23
1	S2	1710	OMC	O2-C2	-2.43	1.19	1.23
1	S2	814	5MU	O4-C4	-2.42	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1337	4AC	O2-C2	-2.39	1.19	1.23
1	S2	822	PSU	O4'-C1'	-2.39	1.40	1.43
1	S2	644	OMG	C2-N1	2.35	1.43	1.37
1	S2	1710	OMC	C5-C4	2.31	1.48	1.42
1	S2	683	OMG	C5-C6	2.30	1.52	1.47
1	S2	683	OMG	C2-N1	2.26	1.43	1.37
1	S2	509	OMG	C2-N1	2.26	1.43	1.37
1	S2	1830	UR3	C6-N1	2.25	1.43	1.38
1	S2	484	A2M	C2-N3	2.24	1.35	1.32
1	S2	166	A2M	C2-N3	2.22	1.35	1.32
1	S2	644	OMG	O6-C6	-2.19	1.18	1.23
1	S2	1248	B8N	O4-C4	-2.16	1.18	1.23
1	S2	683	OMG	O6-C6	-2.15	1.18	1.23
1	S2	814	5MU	O2-C2	-2.14	1.19	1.23
1	S2	1248	B8N	O4'-C1'	-2.13	1.40	1.43
1	S2	174	OMC	C5-C4	2.12	1.47	1.42
1	S2	174	OMC	O2-C2	-2.11	1.19	1.23
1	S2	1832	6MZ	C9-N6	2.11	1.48	1.45
1	S2	121	OMU	O4-C4	-2.10	1.20	1.24
1	S2	116	OMU	O4-C4	-2.10	1.20	1.24
1	S2	1842	4AC	O2-C2	-2.08	1.19	1.23
1	S2	1832	6MZ	C5-N7	-2.08	1.32	1.39
1	S2	509	OMG	O6-C6	-2.08	1.18	1.23
1	S2	121	OMU	C5-C4	2.07	1.48	1.43
1	S2	517	OMC	C5-C4	2.06	1.47	1.42
1	S2	1703	OMC	C5-C4	2.02	1.47	1.42
1	S2	612	PSU	O4'-C1'	-2.02	1.41	1.43

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1851	MA6	N1-C6-N6	-13.97	100.69	116.83
1	S2	1850	MA6	N1-C6-N6	-13.27	101.50	116.83
1	S2	1806	M7A	C5-C6-N6	11.08	142.57	123.75
1	S2	668	A2M	C1'-N9-C4	-10.11	108.88	126.64
1	S2	814	5MU	C5-C4-N3	9.88	123.91	115.32
1	S2	1806	M7A	N6-C6-N1	-9.59	97.03	118.38
1	S2	1031	A2M	C1'-N9-C4	-9.38	110.16	126.64
1	S2	166	A2M	C1'-N9-C4	-9.29	110.31	126.64
1	S2	484	A2M	C1'-N9-C4	-9.29	110.32	126.64
1	S2	1678	A2M	C5-C6-N6	8.94	133.93	120.31
1	S2	166	A2M	C5-C6-N6	8.77	133.67	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	668	A2M	C5-C6-N6	8.49	133.24	120.31
1	S2	814	5MU	C5-C6-N1	-8.41	114.18	123.31
1	S2	27	A2M	C5-C6-N6	8.31	132.97	120.31
1	S2	159	A2M	C5-C6-N6	8.31	132.97	120.31
1	S2	1031	A2M	C5-C6-N6	8.27	132.91	120.31
1	S2	27	A2M	C1'-N9-C4	-8.21	112.21	126.64
1	S2	484	A2M	C5-C6-N6	8.14	132.71	120.31
1	S2	1678	A2M	C1'-N9-C4	-8.07	112.46	126.64
1	S2	1830	UR3	C1'-N1-C2	8.03	130.18	117.04
1	S2	159	A2M	C1'-N9-C4	-7.70	113.12	126.64
1	S2	568	E3C	C1'-N1-C2	7.37	129.10	117.04
1	S2	814	5MU	C4-N3-C2	-7.30	117.77	127.34
1	S2	1806	M7A	N3-C4-N9	6.93	135.55	126.88
1	S2	1850	MA6	N3-C2-N1	-6.85	119.38	128.67
1	S2	1830	UR3	O2-C2-N3	-6.81	111.92	121.33
1	S2	1830	UR3	C6-N1-C2	-6.75	116.28	121.80
1	S2	484	A2M	N3-C2-N1	-6.70	119.58	128.67
1	S2	159	A2M	N3-C2-N1	-6.68	119.60	128.67
1	S2	1031	A2M	N3-C2-N1	-6.66	119.63	128.67
1	S2	27	A2M	N3-C2-N1	-6.46	119.90	128.67
1	S2	1832	6MZ	N3-C2-N1	-6.41	119.97	128.67
1	S2	166	A2M	C4'-O4'-C1'	-6.38	104.08	109.92
1	S2	668	A2M	N3-C2-N1	-6.37	120.03	128.67
1	S2	166	A2M	N3-C2-N1	-6.34	120.06	128.67
1	S2	1851	MA6	N3-C2-N1	-6.33	120.08	128.67
1	S2	121	OMU	C4-N3-C2	-5.94	119.23	126.61
1	S2	1248	B8N	C1'-C5-C4	5.83	126.45	117.61
1	S2	166	A2M	N6-C6-N1	-5.73	106.10	118.33
1	S2	159	A2M	N6-C6-N1	-5.61	106.35	118.33
1	S2	27	A2M	N6-C6-N1	-5.54	106.49	118.33
1	S2	1830	UR3	C4-N3-C2	-5.54	120.12	124.58
1	S2	668	A2M	N6-C6-N1	-5.54	106.50	118.33
1	S2	484	A2M	N6-C6-N1	-5.52	106.53	118.33
1	S2	1850	MA6	C1'-N9-C4	5.46	136.23	126.64
1	S2	1031	A2M	C4'-O4'-C1'	-5.39	104.99	109.92
1	S2	1806	M7A	N3-C2-N1	-5.38	120.44	128.58
1	S2	568	E3C	O2-C2-N3	-5.31	115.31	122.10
1	S2	823	PSU	C6-N1-C2	-5.30	117.77	122.69
1	S2	1678	A2M	N3-C2-N1	-5.28	121.50	128.67
1	S2	612	PSU	C4-N3-C2	-5.23	119.17	126.37
1	S2	116	OMU	C4-N3-C2	-5.20	120.15	126.61
1	S2	119	PSU	C4-N3-C2	-5.19	119.22	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	814	5MU	N3-C2-N1	5.13	121.57	114.89
1	S2	612	PSU	N1-C2-N3	5.09	120.54	115.17
1	S2	814	5MU	C5M-C5-C6	-5.02	116.06	122.85
1	S2	1678	A2M	C4'-O4'-C1'	-4.96	105.38	109.92
1	S2	823	PSU	O2-C2-N1	-4.96	117.67	122.79
1	S2	121	OMU	N3-C2-N1	4.95	121.33	114.89
1	S2	27	A2M	C4'-O4'-C1'	-4.94	105.40	109.92
1	S2	1678	A2M	N6-C6-N1	-4.92	107.82	118.33
1	S2	1219	B8Q	N3-C2-N1	4.92	124.02	117.16
1	S2	484	A2M	C4'-O4'-C1'	-4.92	105.42	109.92
1	S2	1031	A2M	N6-C6-N1	-4.91	107.84	118.33
1	S2	1081	PSU	C4-N3-C2	-4.74	119.84	126.37
1	S2	1248	B8N	C5-C4-N3	4.73	124.74	116.15
1	S2	1243	PSU	C4-N3-C2	-4.65	119.97	126.37
1	S2	1219	B8Q	C31-N3-C4	4.63	122.78	114.76
1	S2	119	PSU	N1-C2-N3	4.56	119.98	115.17
1	S2	822	PSU	C4-N3-C2	-4.53	120.13	126.37
1	S2	1243	PSU	N1-C2-N3	4.46	119.87	115.17
1	S2	1081	PSU	N1-C2-N3	4.46	119.87	115.17
1	S2	822	PSU	N1-C2-N3	4.43	119.84	115.17
1	S2	823	PSU	N1-C2-N3	4.42	119.83	115.17
1	S2	814	5MU	O4-C4-C5	-4.33	119.96	124.92
1	S2	814	5MU	C6-C5-C4	4.23	121.50	118.02
1	S2	568	E3C	C6-N1-C2	-4.22	118.35	121.80
1	S2	159	A2M	C4'-O4'-C1'	-4.14	106.14	109.92
1	S2	1851	MA6	C1'-N9-C4	4.07	133.78	126.64
1	S2	1248	B8N	C4-N3-C2	-4.06	120.62	125.62
1	S2	668	A2M	C4'-O4'-C1'	-4.03	106.23	109.92
1	S2	1850	MA6	C2-N1-C6	3.99	120.75	116.84
1	S2	1830	UR3	C3U-N3-C4	3.96	123.35	117.87
1	S2	568	E3C	C1'-N1-C6	-3.88	112.49	120.78
1	S2	1806	M7A	C4-N9-C1'	-3.85	117.65	126.63
1	S2	509	OMG	C2-N1-C6	-3.72	118.31	125.11
1	S2	568	E3C	C31-N3-C2	3.70	122.14	117.49
1	S2	612	PSU	C6-C5-C4	3.70	120.67	118.17
1	S2	1832	6MZ	C2-N1-C6	3.69	119.47	116.60
1	S2	116	OMU	C5-C4-N3	3.69	119.97	114.80
1	S2	1248	B8N	N3-C2-N1	3.67	121.20	116.72
1	S2	116	OMU	N3-C2-N1	3.65	119.64	114.89
1	S2	823	PSU	C4-N3-C2	-3.62	121.38	126.37
1	S2	1806	M7A	C71-N7-C5	-3.60	108.44	123.44
1	S2	1219	B8Q	O2-C2-N3	-3.58	117.92	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1851	MA6	C2-N1-C6	3.53	120.30	116.84
1	S2	1830	UR3	C1'-N1-C6	-3.51	113.28	120.78
1	S2	612	PSU	C6-N1-C2	-3.47	119.47	122.69
1	S2	1243	PSU	C6-N1-C2	-3.47	119.47	122.69
1	S2	814	5MU	C5M-C5-C4	3.42	122.43	118.78
1	S2	644	OMG	C5-C6-N1	3.41	120.58	114.07
1	S2	121	OMU	C5-C4-N3	3.39	119.55	114.80
1	S2	822	PSU	C6-N1-C2	-3.38	119.55	122.69
1	S2	119	PSU	C6-C5-C4	3.36	120.44	118.17
1	S2	1081	PSU	C6-N1-C2	-3.35	119.58	122.69
1	S2	509	OMG	C5-C6-N1	3.32	120.40	114.07
1	S2	568	E3C	C4-N3-C2	-3.29	116.08	122.00
1	S2	1337	4AC	C6-C5-C4	3.26	120.92	117.00
1	S2	668	A2M	O4'-C1'-N9	-3.24	104.45	108.75
1	S2	1806	M7A	C2-N3-C4	3.23	119.72	111.83
1	S2	644	OMG	C8-N7-C5	3.21	108.01	102.55
1	S2	116	OMU	O4-C4-C5	-3.16	119.71	125.16
1	S2	644	OMG	C2-N1-C6	-3.16	119.33	125.11
1	S2	1243	PSU	O2-C2-N1	-3.16	119.53	122.79
1	S2	119	PSU	C6-N1-C2	-3.16	119.76	122.69
1	S2	509	OMG	C8-N7-C5	3.12	107.86	102.55
1	S2	1374	5MC	C5-C6-N1	-3.09	119.95	123.31
1	S2	159	A2M	O2'-C2'-C1'	3.07	114.95	109.00
1	S2	683	OMG	C5-C6-N1	3.02	119.84	114.07
1	S2	1832	6MZ	C6-C5-C4	3.02	120.88	117.68
1	S2	822	PSU	O2-C2-N1	-3.01	119.68	122.79
1	S2	1248	B8N	C31-N3-C4	3.01	121.44	117.18
1	S2	683	OMG	C8-N7-C5	3.00	107.66	102.55
1	S2	1806	M7A	C5-C4-N3	-3.00	119.63	126.56
1	S2	1337	4AC	C5-C4-N3	-2.96	117.97	122.60
1	S2	668	A2M	C3'-C2'-C1'	2.94	108.43	102.81
1	S2	612	PSU	O2-C2-N1	-2.84	119.86	122.79
1	S2	119	PSU	O2-C2-N1	-2.79	119.91	122.79
1	S2	814	5MU	O3'-C3'-C2'	2.75	120.63	111.82
1	S2	668	A2M	C2'-C3'-C4'	2.74	107.88	101.99
1	S2	683	OMG	C2-N1-C6	-2.70	120.17	125.11
1	S2	683	OMG	O6-C6-C5	-2.67	119.04	124.32
1	S2	1248	B8N	O4-C4-N3	-2.61	115.75	119.99
1	S2	159	A2M	O4'-C1'-N9	-2.58	105.33	108.75
1	S2	121	OMU	O4-C4-C5	-2.55	120.76	125.16
1	S2	1842	4AC	C6-C5-C4	2.46	119.96	117.00
1	S2	517	OMC	O2-C2-N3	-2.45	118.47	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1081	PSU	C6-C5-C4	2.42	119.81	118.17
1	S2	121	OMU	C6-N1-C2	-2.41	118.06	121.00
1	S2	1374	5MC	CM5-C5-C6	-2.41	119.58	122.85
1	S2	1832	6MZ	C9-N6-C6	-2.40	120.63	122.85
1	S2	1842	4AC	C5-C4-N3	-2.38	118.88	122.60
1	S2	1219	B8Q	C31-N3-C2	2.35	121.40	117.70
1	S2	644	OMG	O6-C6-C5	-2.33	119.71	124.32
1	S2	1830	UR3	O4-C4-N3	2.31	122.47	119.66
1	S2	814	5MU	O2-C2-N1	-2.30	119.80	122.80
1	S2	509	OMG	O6-C6-C5	-2.28	119.79	124.32
1	S2	1830	UR3	C6-C5-C4	2.28	125.09	120.73
1	S2	1337	4AC	O7-C7-CM7	-2.22	118.10	122.05
1	S2	1842	4AC	O7-C7-CM7	-2.21	118.11	122.05
1	S2	159	A2M	C2'-C3'-C4'	2.21	106.75	101.99
1	S2	174	OMC	O2-C2-N3	-2.21	118.84	122.33
1	S2	159	A2M	C2'-C1'-N9	-2.21	107.65	112.56
1	S2	484	A2M	C3'-C2'-C1'	2.18	106.98	102.81
1	S2	121	OMU	O2-C2-N1	-2.17	119.97	122.80
1	S2	27	A2M	C3'-C2'-C1'	2.13	106.88	102.81
1	S2	612	PSU	O4'-C1'-C2'	2.12	108.09	105.15
1	S2	1678	A2M	C4-C5-N7	-2.12	107.09	109.34
1	S2	814	5MU	O4-C4-N3	-2.12	116.13	120.11
1	S2	1219	B8Q	O2-C2-N1	-2.12	118.06	122.78
1	S2	683	OMG	N1-C2-N3	-2.11	119.45	123.32
1	S2	159	A2M	C5'-C4'-C3'	-2.07	107.77	115.21
1	S2	1248	B8N	O4'-C1'-C2'	2.04	107.97	105.15
1	S2	1830	UR3	C3'-C2'-C1'	2.03	105.31	101.46

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S2	27	A2M	C1'-C2'-O2'-CM'
1	S2	116	OMU	O4'-C4'-C5'-O5'
1	S2	121	OMU	C3'-C4'-C5'-O5'
1	S2	121	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	568	E3C	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	S2	668	A2M	O4'-C4'-C5'-O5'
1	S2	668	A2M	C3'-C4'-C5'-O5'
1	S2	822	PSU	C2'-C1'-C5-C4
1	S2	822	PSU	O4'-C4'-C5'-O5'
1	S2	1031	A2M	C1'-C2'-O2'-CM'
1	S2	1703	OMC	O4'-C4'-C5'-O5'
1	S2	1830	UR3	O4'-C4'-C5'-O5'
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	C5-C6-N6-C9
1	S2	1851	MA6	O4'-C4'-C5'-O5'
1	S2	1851	MA6	C5-C6-N6-C9
1	S2	116	OMU	C3'-C4'-C5'-O5'
1	S2	119	PSU	O4'-C4'-C5'-O5'
1	S2	568	E3C	C3'-C4'-C5'-O5'
1	S2	683	OMG	C3'-C4'-C5'-O5'
1	S2	822	PSU	C3'-C4'-C5'-O5'
1	S2	1850	MA6	C3'-C4'-C5'-O5'
1	S2	1851	MA6	C3'-C4'-C5'-O5'
1	S2	823	PSU	O4'-C4'-C5'-O5'
1	S2	1850	MA6	N1-C6-N6-C9
1	S2	1703	OMC	C3'-C4'-C5'-O5'
1	S2	823	PSU	C3'-C4'-C5'-O5'
1	S2	1248	B8N	O4'-C4'-C5'-O5'
1	S2	1830	UR3	C3'-C4'-C5'-O5'
1	S2	119	PSU	C3'-C4'-C5'-O5'
1	S2	159	A2M	C3'-C4'-C5'-O5'
1	S2	683	OMG	O4'-C4'-C5'-O5'
1	S2	1806	M7A	C3'-C4'-C5'-O5'
1	S2	1243	PSU	O4'-C4'-C5'-O5'
1	S2	1243	PSU	C3'-C4'-C5'-O5'
1	S2	1806	M7A	O4'-C4'-C5'-O5'
1	S2	1806	M7A	C2'-C1'-N9-C8
1	S2	1081	PSU	O4'-C4'-C5'-O5'
1	S2	174	OMC	C3'-C2'-O2'-CM2
1	S2	644	OMG	C4'-C5'-O5'-P
1	S2	612	PSU	O4'-C1'-C5-C4
1	S2	823	PSU	O4'-C1'-C5-C4
1	S2	1081	PSU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	S2	1248	B8N	C32-C33-C34-O35
1	S2	121	OMU	C4'-C5'-O5'-P
1	S2	1248	B8N	C32-C33-C34-O36
1	S2	1851	MA6	C4'-C5'-O5'-P
1	S2	612	PSU	O4'-C1'-C5-C6
1	S2	1248	B8N	C3'-C4'-C5'-O5'
1	S2	822	PSU	C2'-C1'-C5-C6

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	5110	-	32,35,35	1.68	5 (15%)	39,49,49	2.43	14 (35%)

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	5110	-	-	1/20/28/28	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	t	5110	MVM	C5-N1	5.94	1.45	1.37
86	t	5110	MVM	N5-N4	-3.74	1.31	1.37
86	t	5110	MVM	C6-N1	2.40	1.45	1.39
86	t	5110	MVM	C12-C5	2.26	1.53	1.50
86	t	5110	MVM	C7-C3	-2.01	1.48	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	t	5110	MVM	C15-N4-C22	-6.43	121.84	130.09
86	t	5110	MVM	C15-N4-N5	5.28	128.40	119.95
86	t	5110	MVM	C21-N7-C22	4.95	122.73	116.81
86	t	5110	MVM	C6-N1-C5	-4.82	117.17	122.94
86	t	5110	MVM	C1-C9-N1	-4.15	105.75	116.16
86	t	5110	MVM	N3-C6-N1	3.80	120.42	116.35
86	t	5110	MVM	C7-C3-C9	3.02	116.55	110.81
86	t	5110	MVM	N6-N5-N4	2.88	109.58	106.37
86	t	5110	MVM	C8-N3-C6	2.78	121.35	115.05
86	t	5110	MVM	C20-C21-N7	-2.75	119.92	123.97
86	t	5110	MVM	C3-C9-C1	-2.66	107.65	110.81
86	t	5110	MVM	C19-C18-N6	2.58	134.39	130.19
86	t	5110	MVM	C6-N1-C9	2.15	121.60	118.40
86	t	5110	MVM	C12-C5-N1	2.14	121.19	118.36

There are no chirality outliers.

All (1) torsion outliers are listed below:

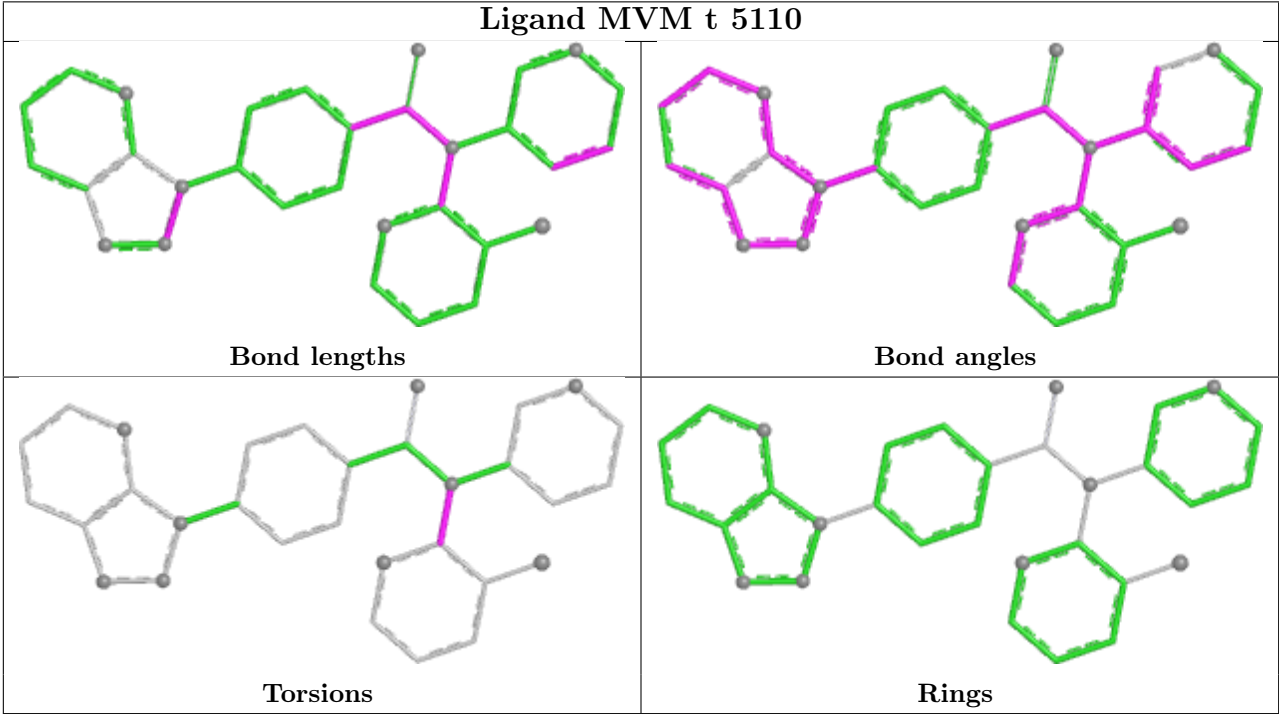
Mol	Chain	Res	Type	Atoms
86	t	5110	MVM	C2-C6-N1-C5

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
79	t	16
1	S2	5
81	v	4
63	c	1
80	u	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	25.98
1	t	750:G	O3'	890:C	P	20.40
1	t	3919:C	O3'	4035:G	P	18.39
1	t	517:C	O3'	629:G	P	17.30

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	t	1680:C	O3'	1699:C	P	16.29
1	t	4737:G	O3'	4815:C	P	15.93
1	S2	1752:C	O3'	1779:G	P	15.75
1	t	1089:A	O3'	1145:G	P	15.58
1	t	976:U	O3'	1047:G	P	15.45
1	t	1202:G	O3'	1216:G	P	15.13
1	t	2881:G	O3'	3569:C	P	14.86
1	t	2093:C	O3'	2228:C	P	14.28
1	t	1253:A	O3'	1256:G	P	13.38
1	S2	698:G	O3'	730:C	P	12.31
1	S2	739:C	O3'	746:C	P	11.72
1	c	119:CYS	C	120:ARG	N	7.10
1	S2	225:G	O3'	287:U	P	6.95
1	t	945:G	O3'	946:G	P	6.49
1	v	17:A	O3'	18:G	P	5.54
1	t	4734:C	O3'	4735:C	P	4.98
1	v	10:G	O3'	11:C	P	4.38
1	u	54:U	O3'	55:U	P	4.19
1	v	21:A	O3'	22:G	P	3.91
1	t	4817:G	O3'	4818:G	P	3.34
1	t	964:C	O3'	965:G	P	3.27
1	t	1938:U	O3'	1939:A	P	3.24
1	v	41:C	O3'	42:C	P	3.22

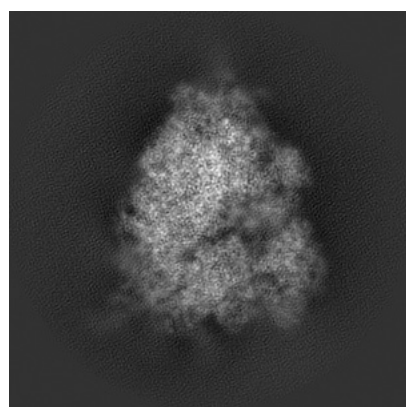
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0526. These allow visual inspection of the internal detail of the map and identification of artifacts.

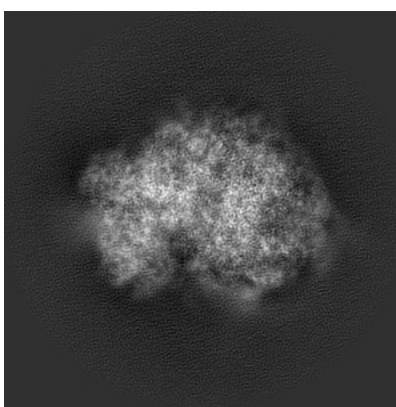
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

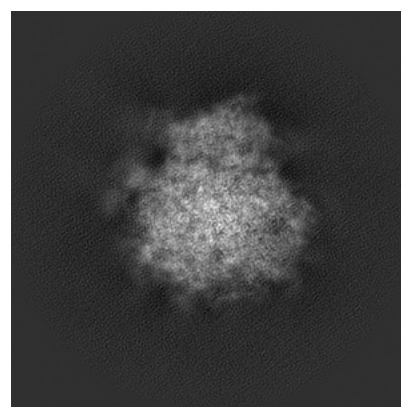
6.1.1 Primary map



X



Y

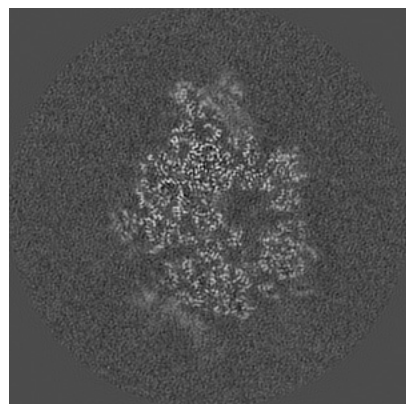


Z

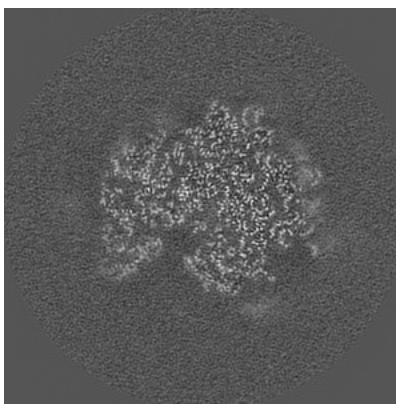
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

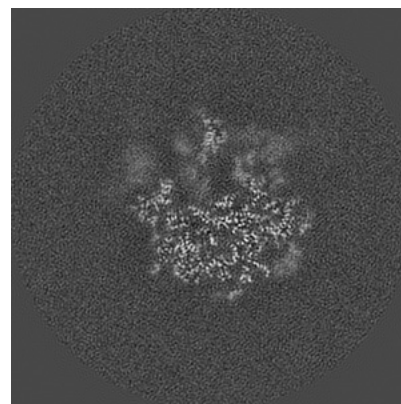
6.2.1 Primary map



X Index: 200



Y Index: 200

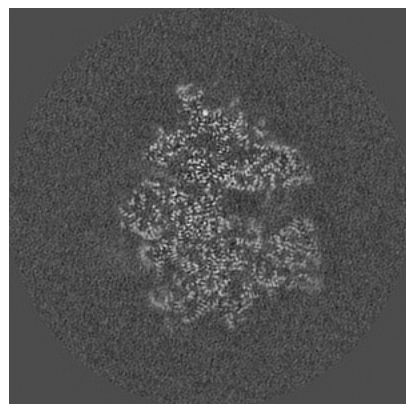


Z Index: 200

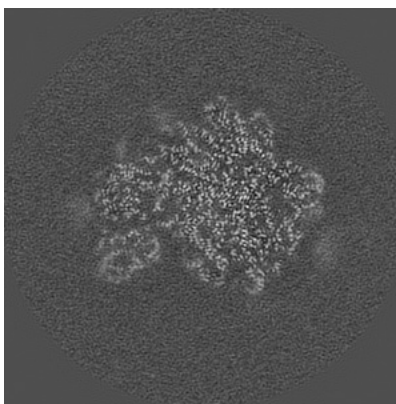
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

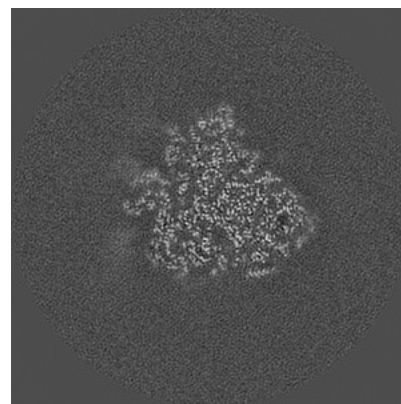
6.3.1 Primary map



X Index: 216



Y Index: 192

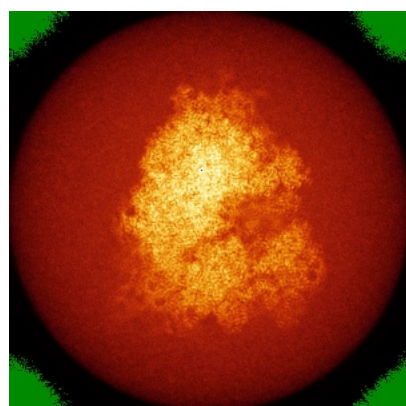


Z Index: 230

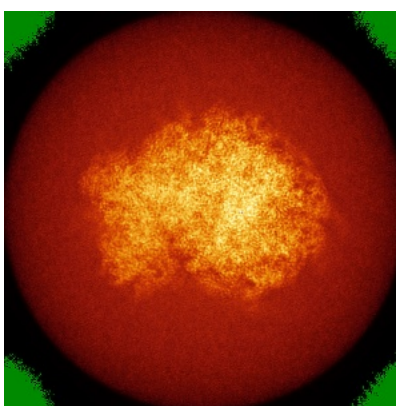
The images above show the largest variance slices of the map in three orthogonal directions.

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

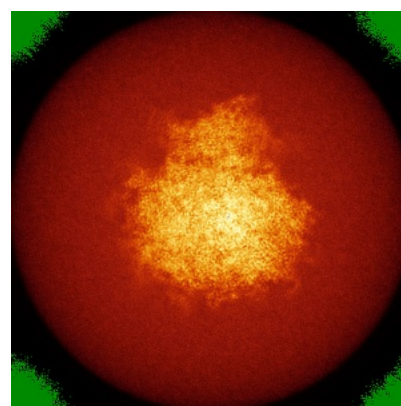
6.4.1 Primary map



X



Y

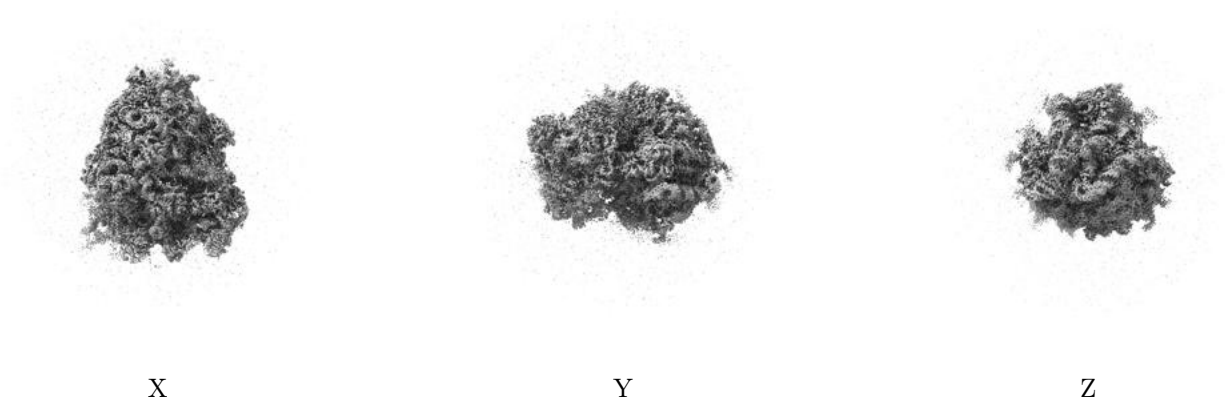


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

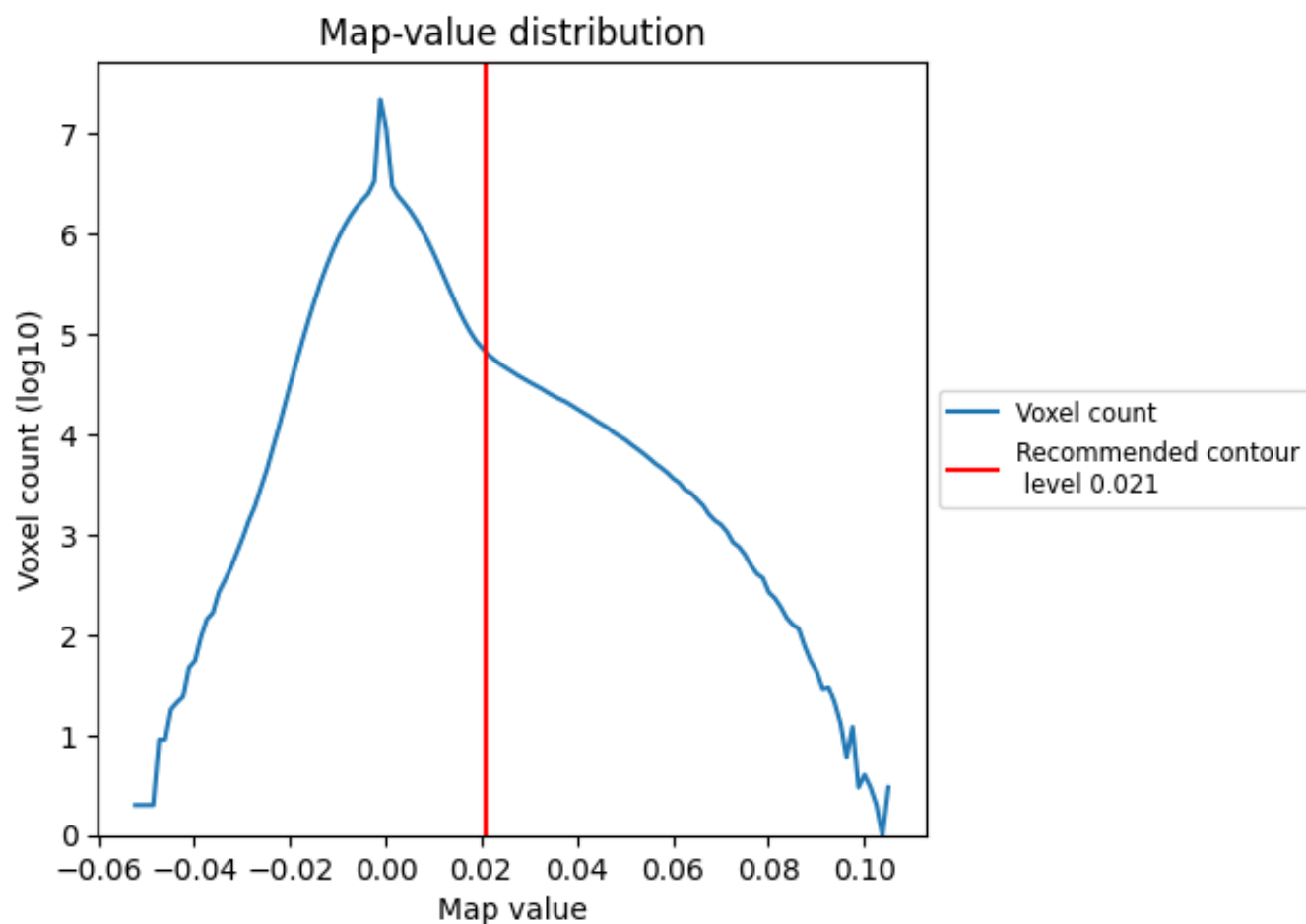
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

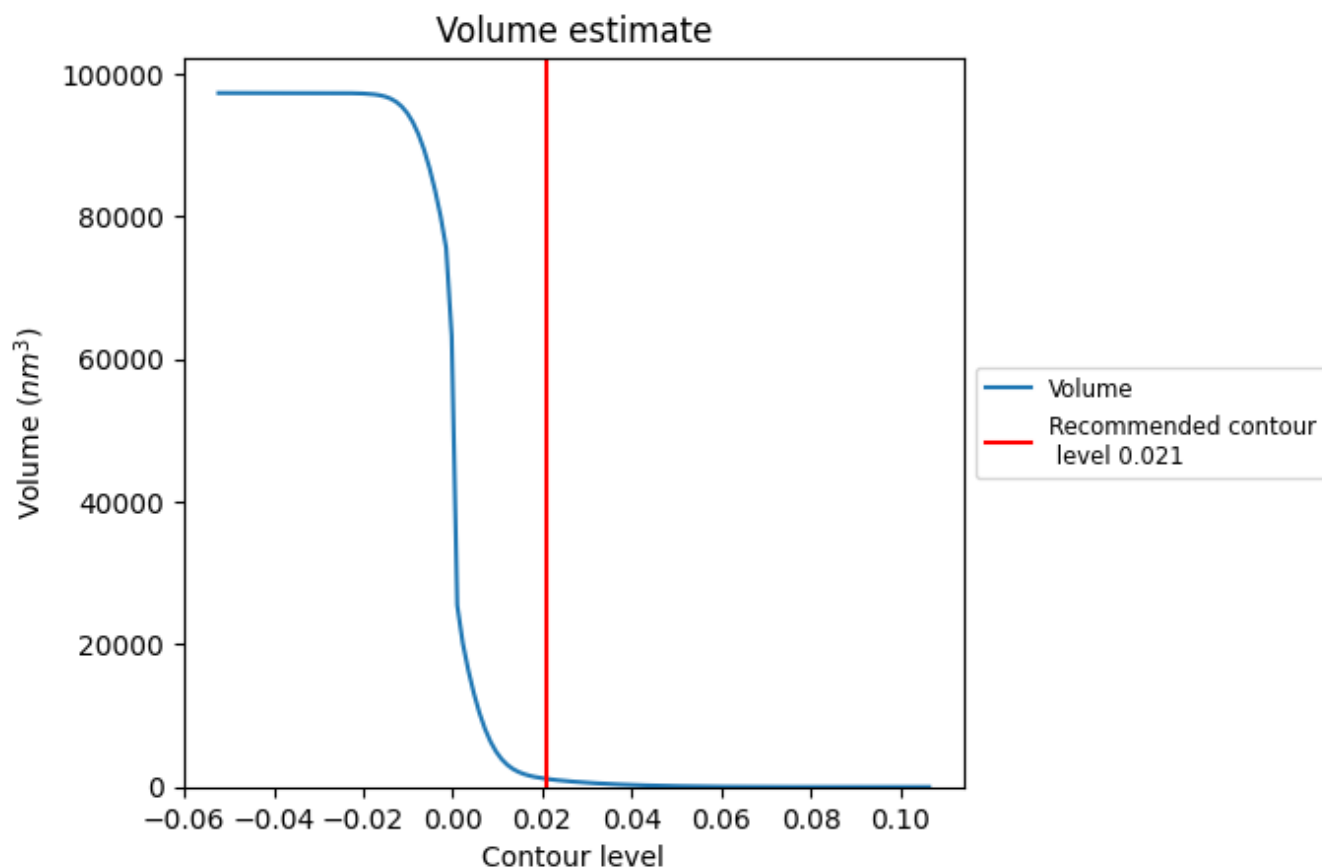
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

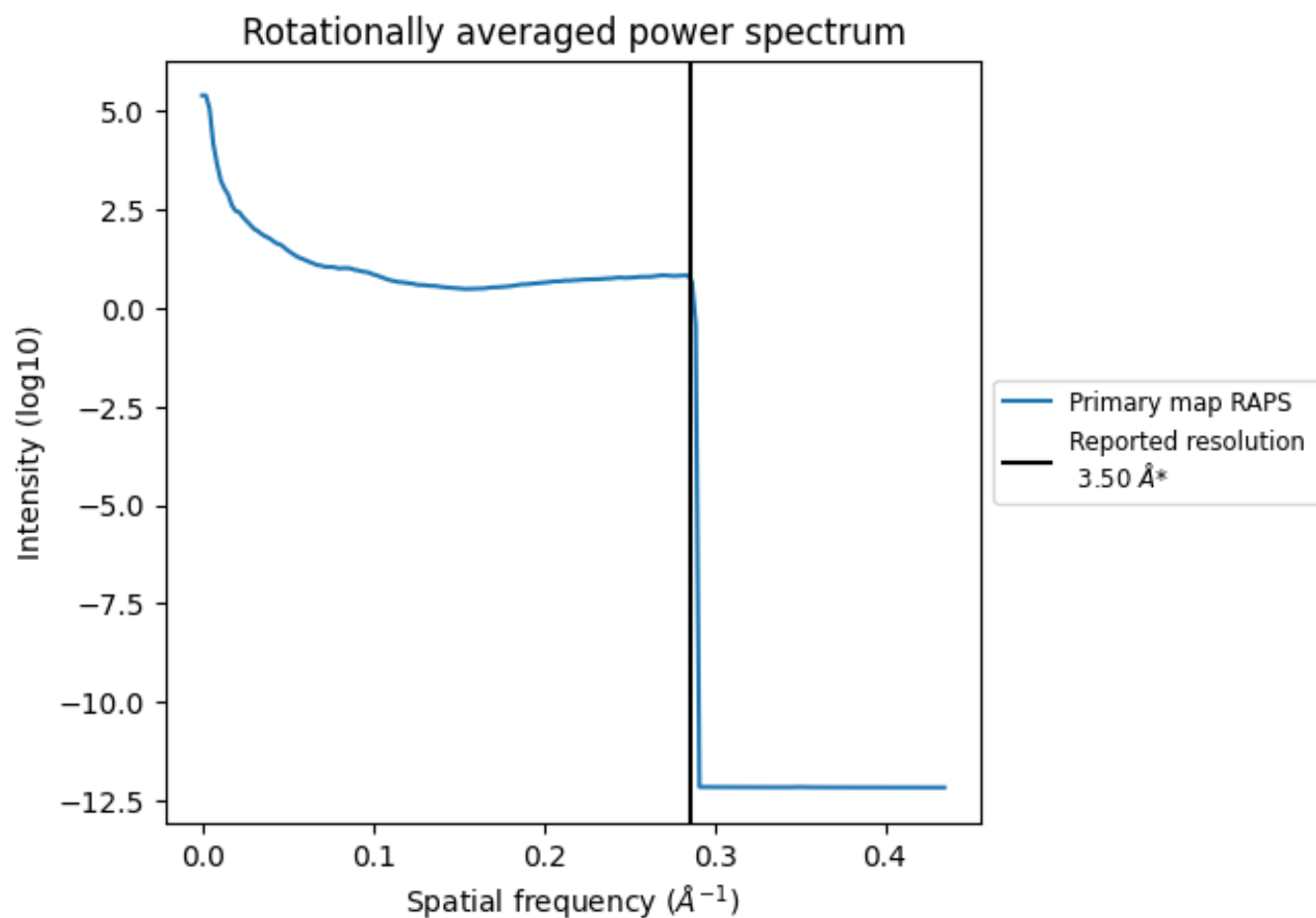
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1131 nm^3 ; this corresponds to an approximate mass of 1022 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

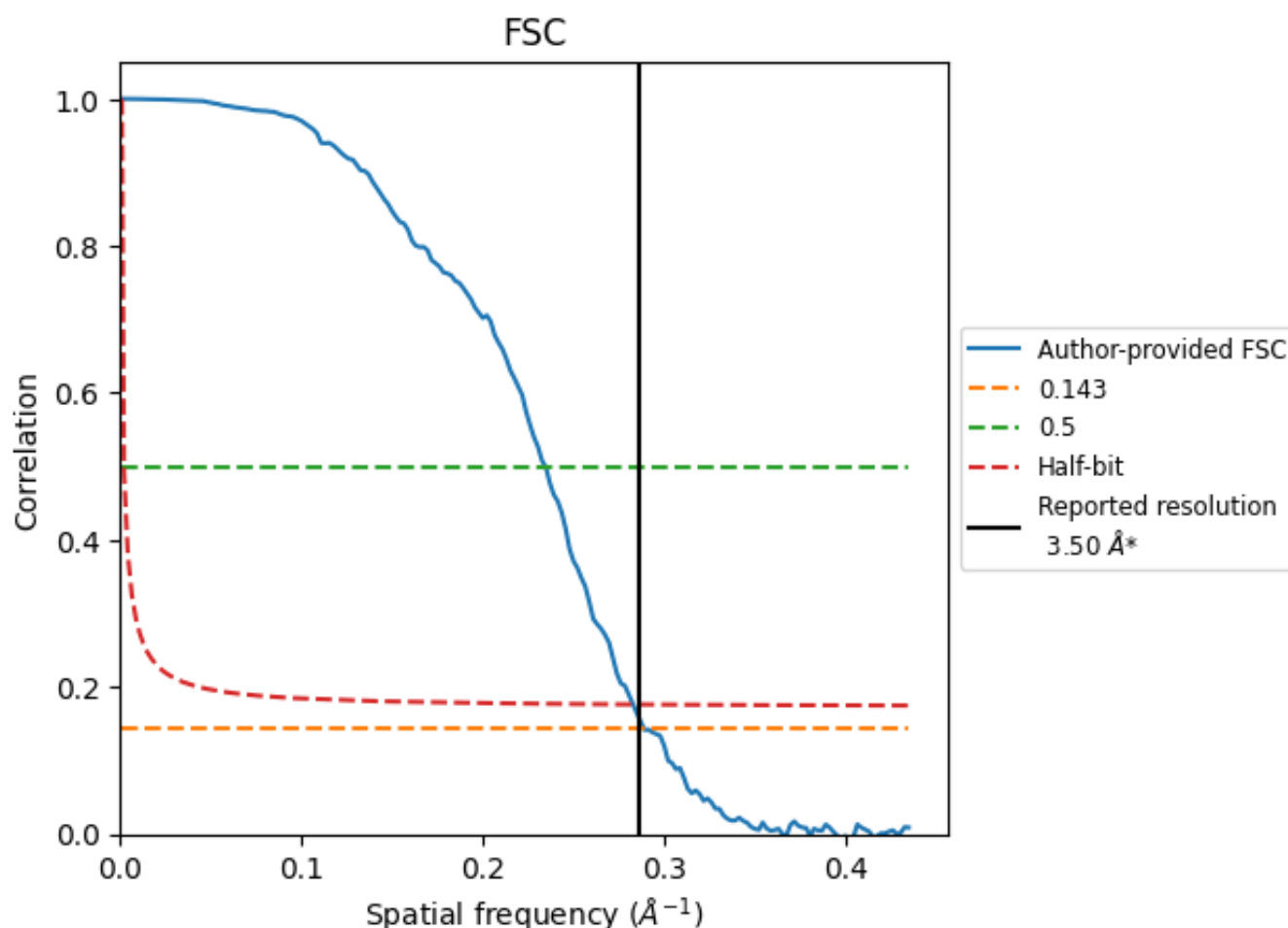


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

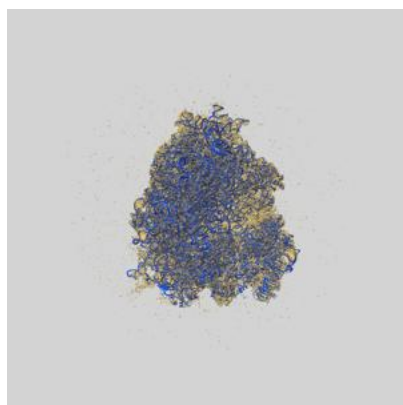
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.46	4.27	3.54
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

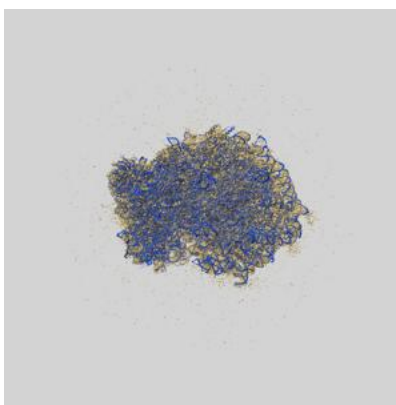
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0526 and PDB model 6OLI. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

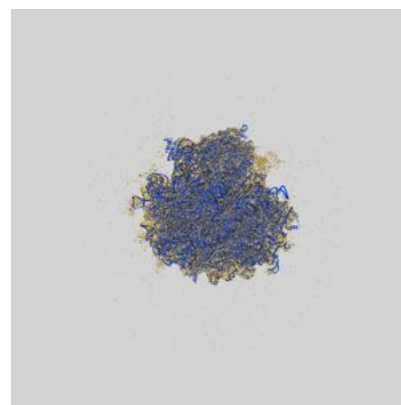
9.1 Map-model overlay [i](#)



X



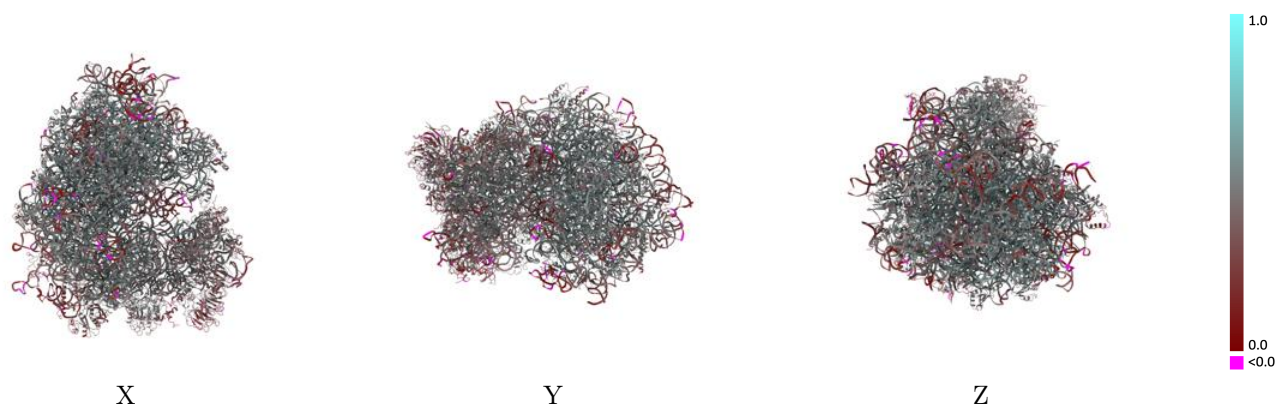
Y



Z

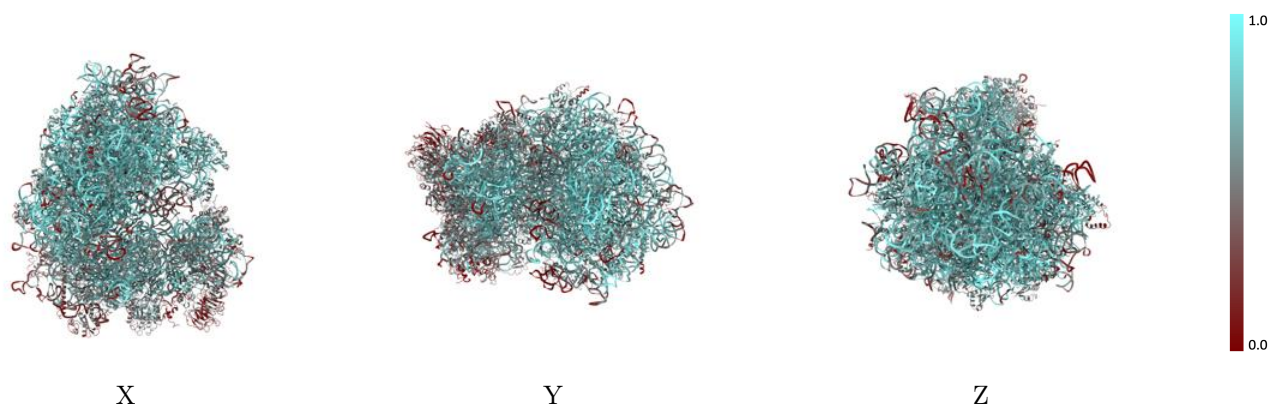
The images above show the 3D surface view of the map at the recommended contour level 0.021 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



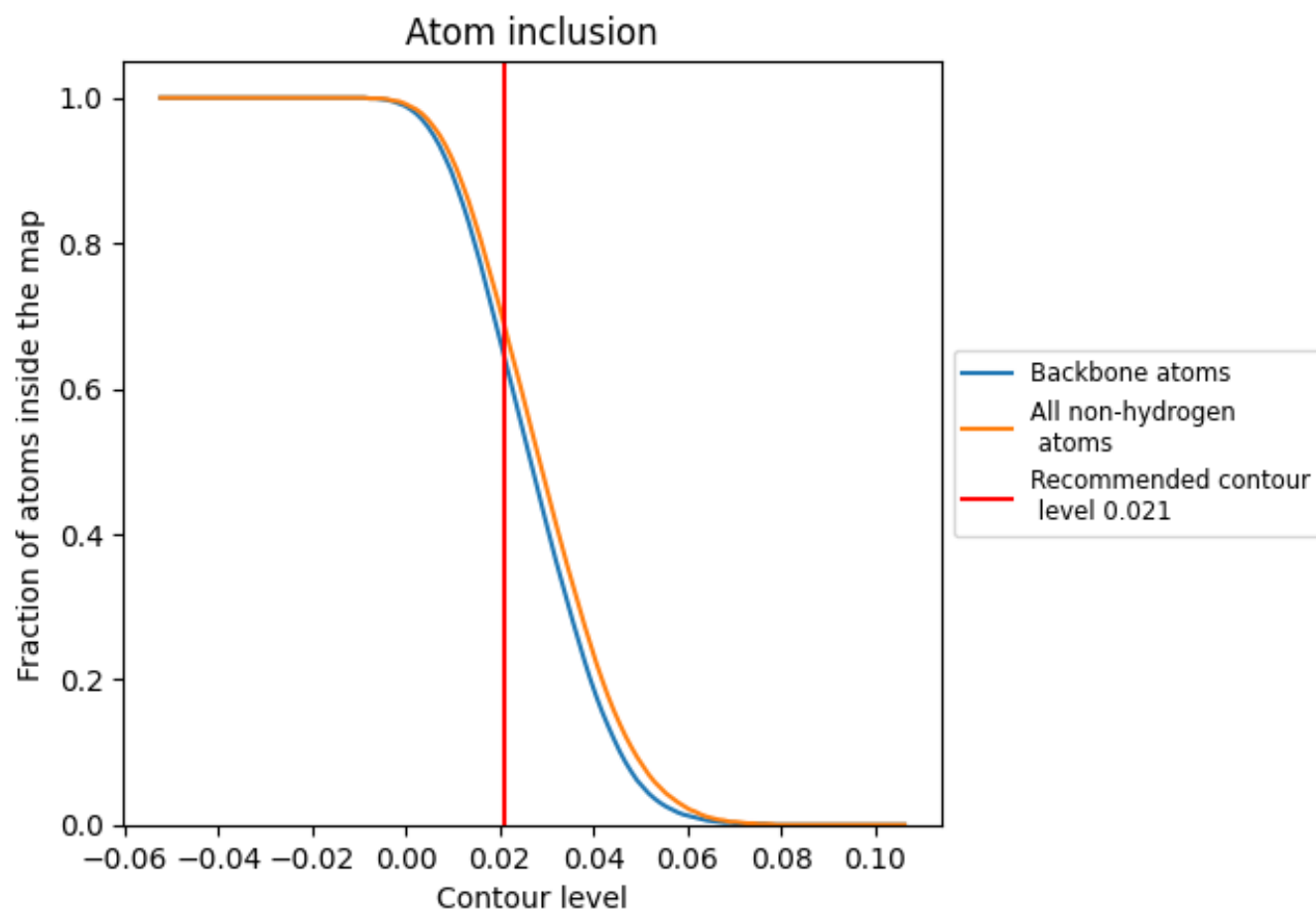
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.021).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 69% 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 (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6870	 0.4460
A	 0.7050	 0.5190
B	 0.6990	 0.4940
C	 0.7380	 0.5140
D	 0.8160	 0.4720
E	 0.9000	 0.5080
F	 0.6510	 0.4550
G	 0.6160	 0.4300
H	 0.7230	 0.5050
I	 0.5910	 0.4390
J	 0.6140	 0.4570
K	 0.6690	 0.4830
L	 0.6210	 0.4500
M	 0.6650	 0.4670
N	 0.6720	 0.4870
O	 0.7600	 0.5300
P	 0.7080	 0.5010
Q	 0.7410	 0.5120
R	 0.7090	 0.5040
S	 0.6140	 0.4470
S2	 0.7340	 0.4290
SA	 0.4960	 0.4220
SB	 0.5460	 0.4450
SC	 0.5710	 0.4530
SD	 0.4250	 0.3930
SE	 0.4950	 0.4090
SF	 0.4650	 0.3900
SG	 0.3580	 0.3210
SH	 0.3740	 0.3560
SI	 0.4570	 0.3860
SJ	 0.5280	 0.3850
SK	 0.3960	 0.3550
SL	 0.5350	 0.4160
SM	 0.0890	 0.1970
SN	 0.5730	 0.4500

















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Chain	Atom inclusion	Q-score
SO	 0.5630	 0.4530
SP	 0.5110	 0.4060
SQ	 0.4940	 0.4080
SR	 0.4050	 0.3720
SS	 0.5230	 0.3960
ST	 0.5300	 0.4170
SU	 0.3940	 0.3650
SV	 0.5250	 0.4280
SW	 0.6190	 0.4930
SX	 0.5890	 0.4600
SY	 0.4350	 0.3420
SZ	 0.4130	 0.3530
Sa	 0.6050	 0.4510
Sb	 0.4820	 0.4200
Sc	 0.3480	 0.3440
Sd	 0.6050	 0.4310
Se	 0.4530	 0.3850
Sf	 0.0810	 0.2030
Sg	 0.2720	 0.2970
T	 0.7280	 0.5090
U	 0.6790	 0.4890
V	 0.5590	 0.4190
W	 0.6740	 0.5070
X	 0.6970	 0.4850
Y	 0.6930	 0.5050
Z	 0.6960	 0.4900
a	 0.6450	 0.4660
b	 0.7440	 0.5230
c	 0.6150	 0.4490
d	 0.5820	 0.4390
e	 0.6950	 0.4720
f	 0.7520	 0.5240
g	 0.7540	 0.5210
h	 0.6810	 0.4820
i	 0.6800	 0.4830
j	 0.6500	 0.4650
k	 0.8050	 0.5360
l	 0.5460	 0.4340
m	 0.7230	 0.5010
n	 0.6930	 0.4800
o	 0.5640	 0.4820
p	 0.6660	 0.4870

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Chain	Atom inclusion	Q-score
q	 0.6820	 0.4990
r	 0.7620	 0.5120
t	 0.7940	 0.4590
u	 0.3360	 0.2860
v	 0.5480	 0.3300
w	 0.7650	 0.4830
y	 0.1290	 0.3260