



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 05:41 AM JST

PDB ID : 8K82
EMDB ID : EMD-36945
Title : Cryo-EM structure of the yeast 80S ribosome with tigecycline, Not5 and P-site tRNA
Authors : Buschauer, R.; Beckmann, R.; Cheng, J.
Deposited on : 2023-07-28
Resolution : 3.00 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:

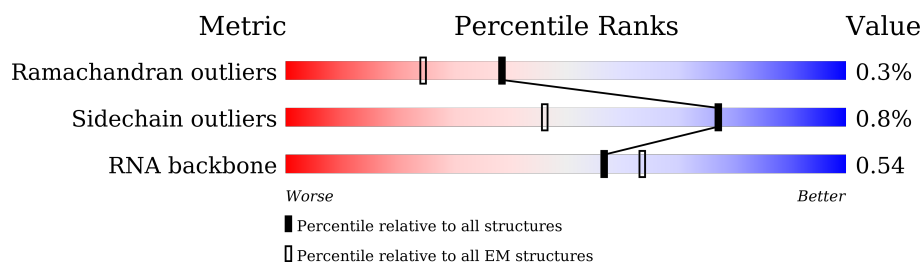
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 3.00 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.





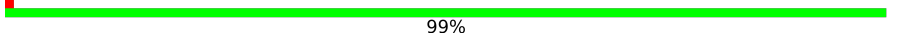














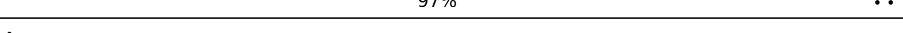
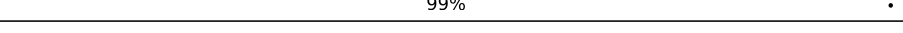

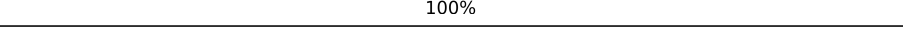
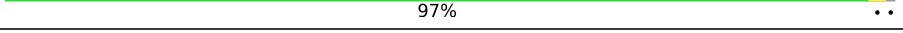
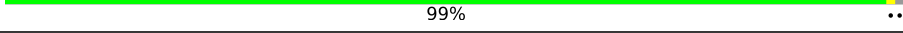
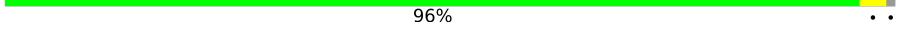

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	C2	1800	 70% 26% . .
2	C7	3	 100%
3	C5	75	 76% 19% 5%
4	C1	3396	 74% 19% . 6%
5	C4	121	 88% 12%
6	C3	158	 82% 18% .
7	SA	252	 81% . 18%
8	SB	255	 84% . 15%

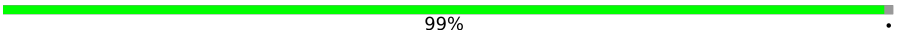
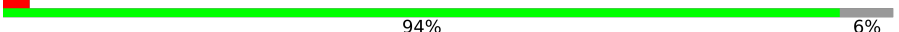
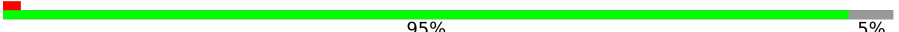


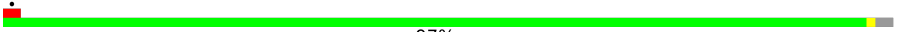






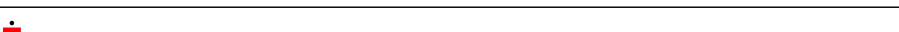

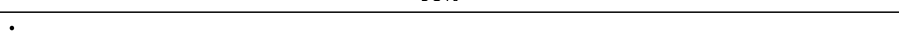
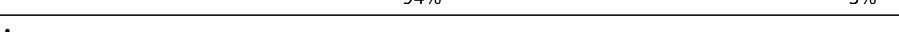
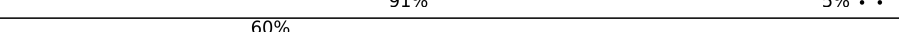

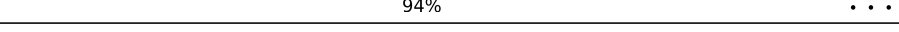
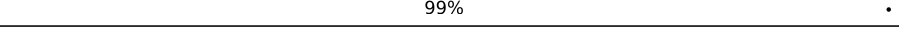
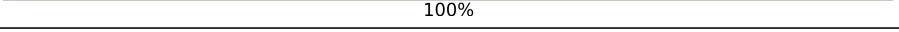
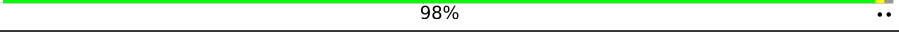
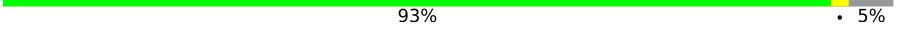
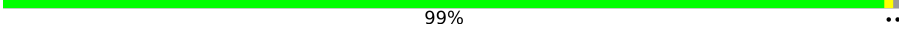

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Mol	Chain	Length	Quality of chain
9	SC	254	
10	SD	240	
11	SE	261	
12	SF	225	
13	SG	236	
14	SH	190	
15	SI	200	
16	SJ	197	
17	SK	105	
18	SL	156	
19	SM	143	
20	SN	151	
21	SO	137	
22	SP	142	
23	SQ	143	
24	SR	136	
25	SS	146	
26	ST	144	
27	SU	121	
28	SV	87	
29	SW	130	
30	SX	145	
31	SY	135	
32	SZ	108	
33	Sa	119	

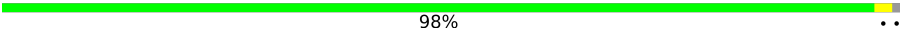

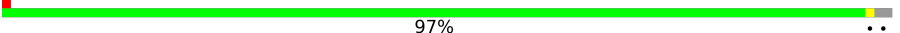


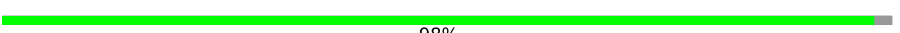
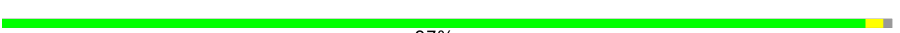








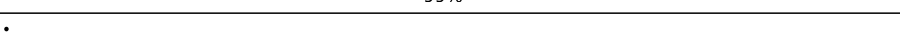
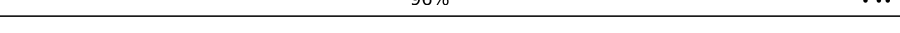
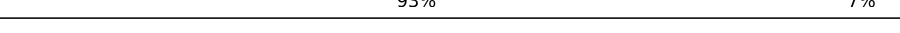
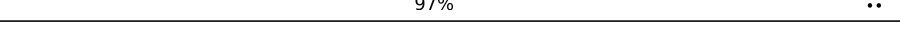
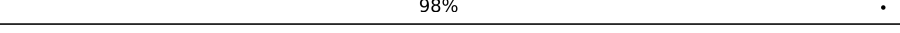

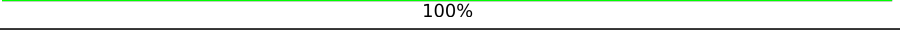
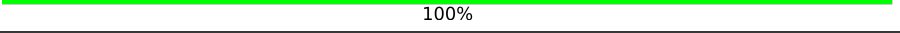
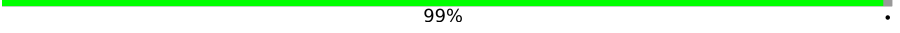
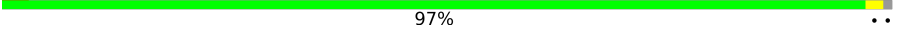
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Mol	Chain	Length	Quality of chain
34	Sb	82	 99%
35	Sc	67	 94% 6%
36	Sd	56	 95% 5%
37	Se	63	 10% 92% 5%
38	Sf	152	 19% 78%
39	Sg	319	 97% ..
40	LA	254	 99% .
41	LB	387	 99% .
42	LC	362	 99% .
43	LD	297	 98% ..
44	LE	176	 88% 11%
45	LF	244	 91% 9%
46	LG	256	 89% 10%
47	LH	191	 98% ..
48	LI	221	 94% 5%
49	LJ	174	 91% 5% ..
50	LK	165	 60% 91% ..
51	LL	199	 94% ..
52	LM	138	 99% .
53	LN	204	 100%
54	LO	199	 98% ..
55	LP	184	 93% 5%
56	LQ	186	 99% ..
57	LR	189	 92% 8%
58	LS	172	 99% .

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Mol	Chain	Length	Quality of chain
59	LT	160	 98%
60	LU	121	 81% 19%
61	LV	137	 97%
62	LW	155	 41% 59%
63	LX	142	 83% 15%
64	LY	127	 98%
65	LZ	136	 97%
66	La	149	 96%
67	Lb	59	 97%
68	Lc	105	 95% 5%
69	Ld	113	 96%
70	Le	130	 98%
71	Lf	107	 99%
72	Lg	121	 89% 7%
73	Lh	120	 99%
74	Li	100	 96%
75	Lj	88	 93% 7%
76	Lk	78	 97%
77	Ll	51	 98%
78	Lm	128	 41% 59%
79	L2	25	 32% 100%
79	Ln	25	 100%
80	Lo	106	 99%
81	Lp	92	 97%
82	L1	217	 60% 94% 6%

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Mol	Chain	Length	Quality of chain
83	P0	312	
84	CN	560	

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 205122 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C2	1771	Total	C	N	O	P	0	0
			37739	16872	6683	12413	1771		

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C7	3	Total	C	N	O	P	0	0
			65	29	12	21	3		

- Molecule 3 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C5	75	Total	C	N	O	P	0	0
			1624	728	298	523	75		

- Molecule 4 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C1	3204	Total	C	N	O	P	0	0
			68535	30613	12358	22360	3204		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C4	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 6 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C3	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 7 is a protein called Small ribosomal subunit protein uS2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SA	206	Total	C	N	O	S	0	0
			1583	1017	281	283	2		

- Molecule 8 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SB	216	Total	C	N	O	S	0	0
			1722	1091	312	315	4		

- Molecule 9 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SC	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 10 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SD	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 11 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SE	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 12 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SF	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 13 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SG	218	Total	C	N	O	S	0	0
			1755	1102	337	313	3		

- Molecule 14 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	SH	185	Total	C	N	O		
			1486	954	266	266	0	0

- Molecule 15 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SI	188	Total	C	N	O	S		
			1489	925	298	264	2	0	0

- Molecule 16 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SJ	185	Total	C	N	O	S		
			1494	943	289	261	1	0	0

- Molecule 17 is a protein called Small ribosomal subunit protein eS10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SK	92	Total	C	N	O	S		
			741	478	121	140	2	0	0

- Molecule 18 is a protein called Small ribosomal subunit protein uS17A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SL	146	Total	C	N	O	S		
			1168	747	221	197	3	0	0

- Molecule 19 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SM	124	Total	C	N	O	S		
			890	560	156	172	2	0	0

- Molecule 20 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SN	150	Total	C	N	O	S		
			1192	759	224	207	2	0	0

- Molecule 21 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SO	128	Total	C	N	O	S	0	0
			949	582	188	176	3		

- Molecule 22 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SP	119	Total	C	N	O	S	0	0
			939	595	176	161	7		

- Molecule 23 is a protein called Small ribosomal subunit protein uS9A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SQ	141	Total	C	N	O	S	0	0
			1105	708	203	194			

- Molecule 24 is a protein called Small ribosomal subunit protein eS17A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SR	115	Total	C	N	O	S	0	0
			896	557	172	165	2		

- Molecule 25 is a protein called Small ribosomal subunit protein uS13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SS	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 26 is a protein called Small ribosomal subunit protein eS19A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	ST	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 27 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SU	101	Total	C	N	O	S	0	0
			805	512	145	147	1		

- Molecule 28 is a protein called Small ribosomal subunit protein eS21A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SV	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 29 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 30 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SX	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 31 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SY	134	Total	C	N	O		0	0
			1073	676	208	189			

- Molecule 32 is a protein called Small ribosomal subunit protein eS25A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SZ	69	Total	C	N	O		0	0
			558	357	103	98			

- Molecule 33 is a protein called Small ribosomal subunit protein eS26B.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sa	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 34 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Sb	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 35 is a protein called Small ribosomal subunit protein eS28A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Sc	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 36 is a protein called Small ribosomal subunit protein uS14A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Sd	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 37 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Se	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 38 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Sf	33	Total	C	N	O	S	0	0
			248	153	46	45	4		

- Molecule 39 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Sg	313	Total	C	N	O	S	0	0
			2403	1521	411	463	8		

- Molecule 40 is a protein called Large ribosomal subunit protein uL2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LA	252	Total	C	N	O	S	0	0
			1912	1190	388	333	1		

- Molecule 41 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LB	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 42 is a protein called Large ribosomal subunit protein uL4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LC	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 43 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LD	294	Total	C	N	O	S	0	0
			2359	1489	412	456	2		

- Molecule 44 is a protein called Large ribosomal subunit protein eL6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LE	157	Total	C	N	O	S	0	0
			1248	806	224	217	1		

- Molecule 45 is a protein called Large ribosomal subunit protein uL30A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LF	223	Total	C	N	O	S	0	0
			1791	1155	325	310	1		

- Molecule 46 is a protein called Large ribosomal subunit protein eL8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LG	231	Total	C	N	O	S	0	0
			1763	1130	316	314	3		

- Molecule 47 is a protein called Large ribosomal subunit protein uL6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LH	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		

- Molecule 48 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LI	209	Total	C	N	O	S	0	0
			1696	1077	321	293	5		

- Molecule 49 is a protein called Large ribosomal subunit protein uL5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	LJ	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 50 is a protein called Large ribosomal subunit protein uL11A.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	LK	158	Total	C	N	O	0	0
			778	461	158	159		

- Molecule 51 is a protein called Large ribosomal subunit protein eL13A.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	LL	194	Total	C	N	O	0	0
			1548	965	316	267		

- Molecule 52 is a protein called Large ribosomal subunit protein eL14A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LM	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 53 is a protein called Large ribosomal subunit protein eL15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	LN	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 54 is a protein called Large ribosomal subunit protein uL13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	LO	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 55 is a protein called Large ribosomal subunit protein uL22A.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	LP	175	Total	C	N	O	0	0
			1378	856	273	249		

- Molecule 56 is a protein called Large ribosomal subunit protein eL18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LQ	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 57 is a protein called Large ribosomal subunit protein eL19A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	LR	174	Total	C	N	O	S	0	0
			1365	843	286	236			

- Molecule 58 is a protein called Large ribosomal subunit protein eL20A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LS	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 59 is a protein called Large ribosomal subunit protein eL21A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	LT	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 60 is a protein called Large ribosomal subunit protein eL22A.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	LU	98	Total	C	N	O	S	0	0
			778	505	127	146			

- Molecule 61 is a protein called Large ribosomal subunit protein uL14A.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	LV	134	Total	C	N	O	S	0	0
			993	623	187	176	7		

- Molecule 62 is a protein called Large ribosomal subunit protein eL24A.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LW	63	Total	C	N	O	S	0	0
			521	336	102	82	1		

- Molecule 63 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	LX	120	Total	C	N	O	S	0	0
			959	617	168	172	2		

- Molecule 64 is a protein called Large ribosomal subunit protein uL24A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	LY	124	Total	C	N	O		0	0
			976	614	190	172			

- Molecule 65 is a protein called Large ribosomal subunit protein eL27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	LZ	135	Total	C	N	O		0	0
			1092	710	202	180			

- Molecule 66 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	La	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 67 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Lb	58	Total	C	N	O		0	0
			462	289	100	73			

- Molecule 68 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Lc	100	Total	C	N	O	S	0	0
			767	492	128	146	1		

- Molecule 69 is a protein called Large ribosomal subunit protein eL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ld	109	Total	C	N	O	S	0	0
			883	559	167	156	1		

- Molecule 70 is a protein called Large ribosomal subunit protein eL32.

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

- Molecule 71 is a protein called Large ribosomal subunit protein eL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Lf	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 72 is a protein called Large ribosomal subunit protein eL34A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Lg	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 73 is a protein called Large ribosomal subunit protein uL29A.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Lh	119	Total	C	N	O	S	0	0
			965	612	185	167	1		

- Molecule 74 is a protein called Large ribosomal subunit protein eL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Li	99	Total	C	N	O	S	0	0
			770	481	156	131	2		

- Molecule 75 is a protein called Large ribosomal subunit protein eL37A.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Lj	82	Total	C	N	O	S	0	0
			650	396	142	107	5		

- Molecule 76 is a protein called Large ribosomal subunit protein eL38.

Mol	Chain	Residues	Atoms				AltConf	Trace
76	Lk	77	Total	C	N	O	0	0
			608	388	114	106		

- Molecule 77 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	L1	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 78 is a protein called Ubiquitin-ribosomal protein eL40A fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Lm	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 79 is a protein called Large ribosomal subunit protein eL41A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Ln	25	Total	C	N	O	S	0	0
			233	142	63	27	1		
79	L2	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 80 is a protein called Large ribosomal subunit protein eL42A.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Lo	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 81 is a protein called Large ribosomal subunit protein eL43A.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Lp	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 82 is a protein called Large ribosomal subunit protein uL1A.

Mol	Chain	Residues	Atoms				AltConf	Trace
82	L1	204	Total	C	N	O	0	0
			1010	602	204	204		

- Molecule 83 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms				AltConf	Trace
83	P0	203	Total	C	N	O	0	0
			998	592	203	203		

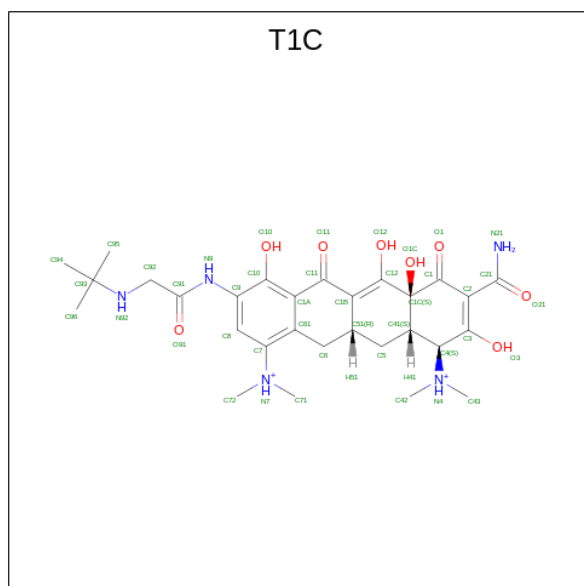
- Molecule 84 is a protein called General negative regulator of transcription subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	CN	112	Total	C	N	O	S	0	0
			940	585	170	182	3		

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

Mol	Chain	Residues	Atoms		AltConf
85	C2	89	Total	Mg	0
			89	89	
85	C5	3	Total	Mg	0
			3	3	
85	C1	222	Total	Mg	0
			222	222	
85	C4	1	Total	Mg	0
			1	1	
85	C3	1	Total	Mg	0
			1	1	

- Molecule 86 is TIGECYCLINE (three-letter code: T1C) (formula: C₂₉H₄₁N₅O₈) (labeled as "Ligand of Interest" by depositor).



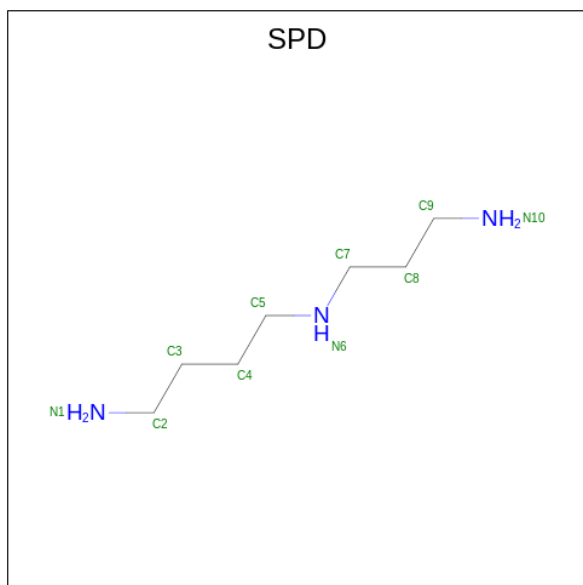
Mol	Chain	Residues	Atoms				AltConf
86	C2	1	Total	C	N	O	0
			42	29	5	8	
86	C1	1	Total	C	N	O	0
			42	29	5	8	
86	C1	1	Total	C	N	O	0
			42	29	5	8	

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Mol	Chain	Residues	Atoms				AltConf
86	C1	1	Total	C	N	O	0
			42	29	5	8	
86	C1	1	Total	C	N	O	0
			42	29	5	8	
86	C1	1	Total	C	N	O	0
			42	29	5	8	

- Molecule 87 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
87	C1	1	Total	C	N	0
			10	7	3	

- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
88	Sa	1	Total	Zn	0
			1	1	
88	Sb	1	Total	Zn	0
			1	1	
88	Sd	1	Total	Zn	0
			1	1	
88	Sf	1	Total	Zn	0
			1	1	
88	Lg	1	Total	Zn	0
			1	1	

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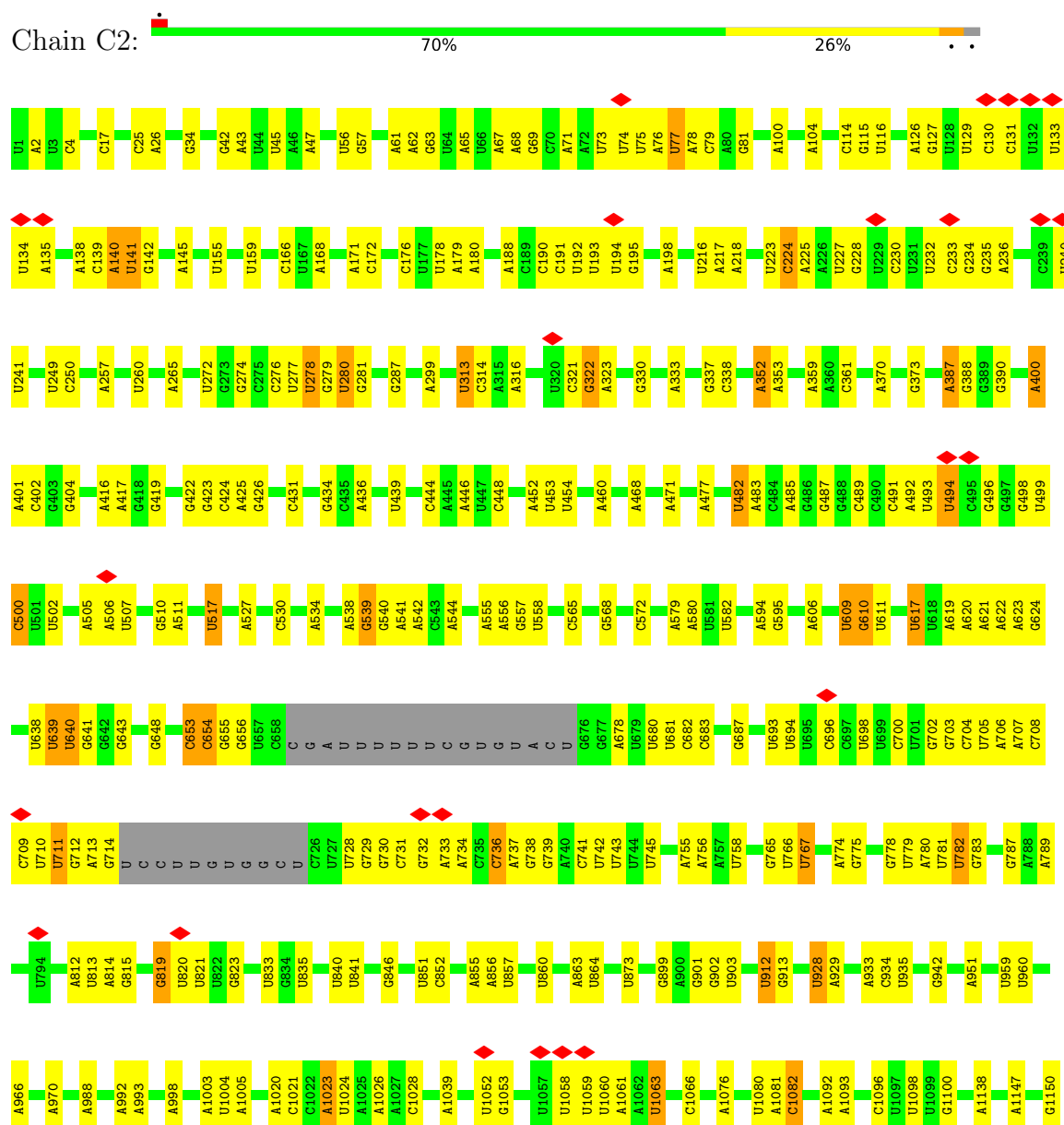
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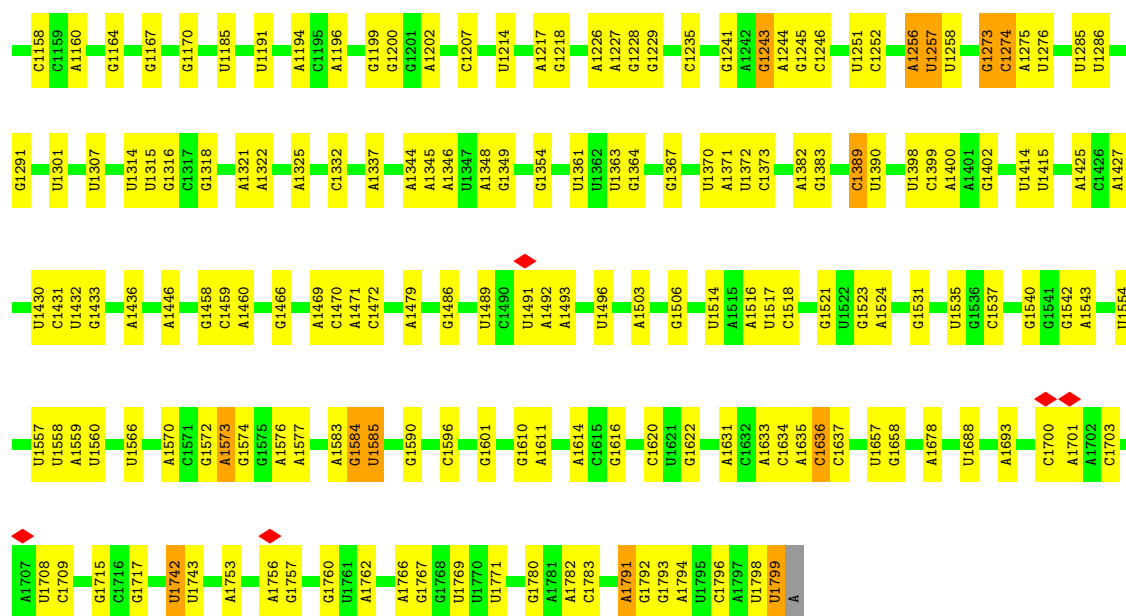
Mol	Chain	Residues	Atoms		AltConf
88	Lj	1	Total 1	Zn 1	0
88	Lm	1	Total 1	Zn 1	0
88	Lo	1	Total 1	Zn 1	0
88	Lp	1	Total 1	Zn 1	0

3 Residue-property plots

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

• Molecule 1: 18S rRNA



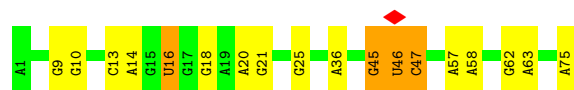
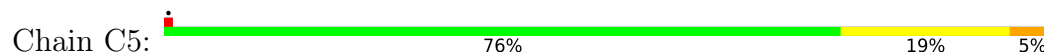


• Molecule 2: mRNA

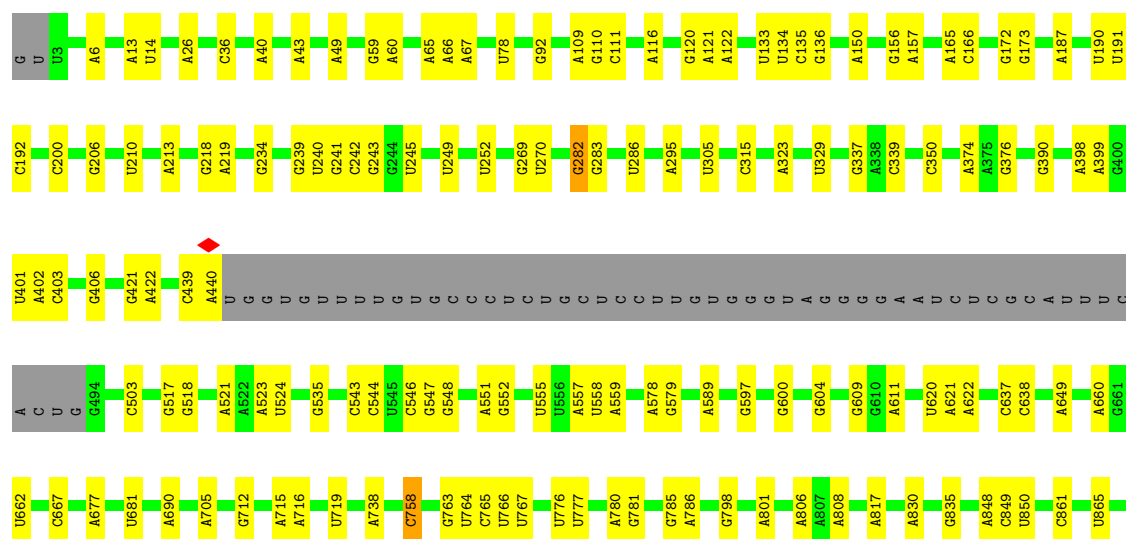
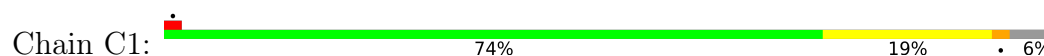


There are no outlier residues recorded for this chain.

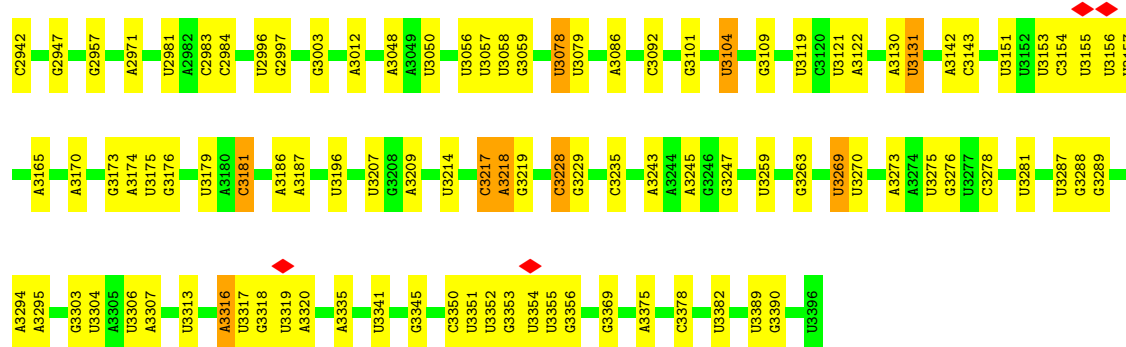
• Molecule 3: tRNA



• Molecule 4: 23S rRNA

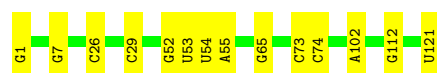






- Molecule 5: 5S rRNA

Chain C4: 88% 12%



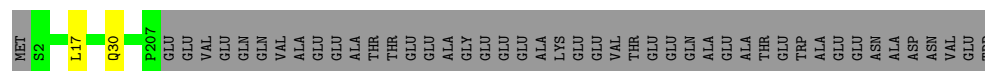
- Molecule 6: 5.8S rRNA

Chain C3: 82% 18%



- Molecule 7: Small ribosomal subunit protein uS2A

Chain SA: 81% 18%



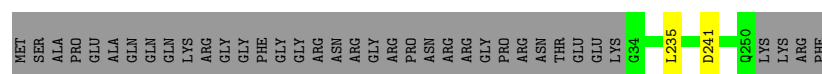
- Molecule 8: 40S ribosomal protein S1-A

Chain SB: 84% 15%



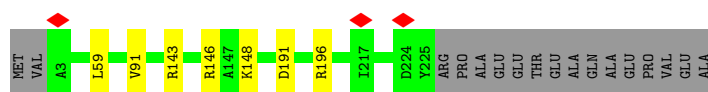
- Molecule 9: 40S ribosomal protein S2

Chain SC: 85% 15%

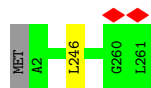


- Molecule 10: Small ribosomal subunit protein uS3

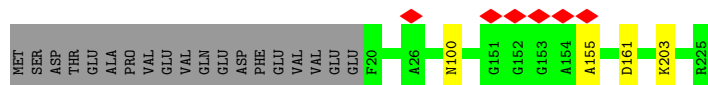
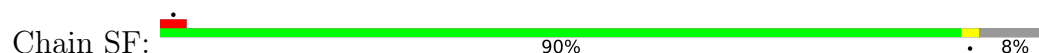
Chain SD: 90% 7%



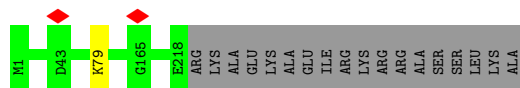
- Molecule 11: 40S ribosomal protein S4-A



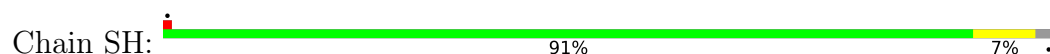
- Molecule 12: Small ribosomal subunit protein uS7



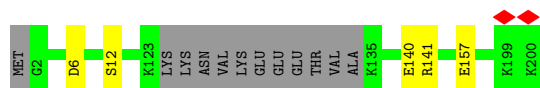
- Molecule 13: 40S ribosomal protein S6-A



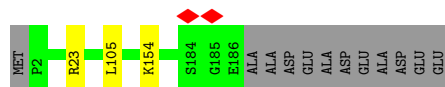
- Molecule 14: 40S ribosomal protein S7-A



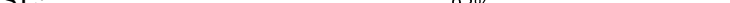
- Molecule 15: 40S ribosomal protein S8-A

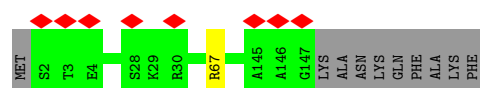


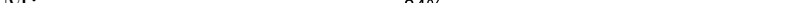
- Molecule 16: 40S ribosomal protein S9-A

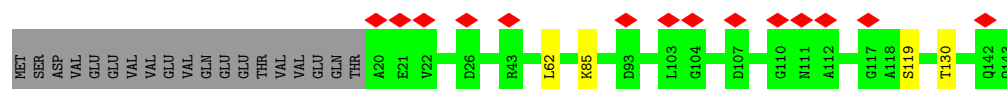


- Molecule 17: Small ribosomal subunit protein eS10A

- Chain SL:  5% 93% 6%



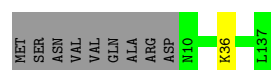
- Chain SM: 




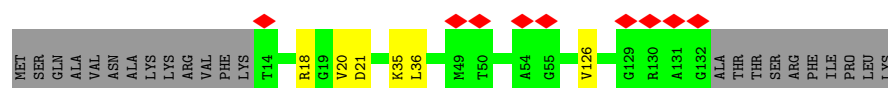
- Chain SN: 99%



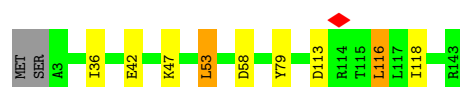
- Chain SO:  93% 7%




- Chain SP: 

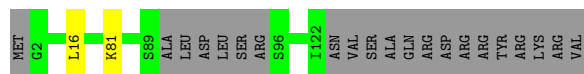


- Chain SQ: 



- Molecule 24: Small ribosomal subunit protein eS17A

Chain SR:  83% 15%



- Molecule 25: Small ribosomal subunit protein uS13A

Chain SS:  97%




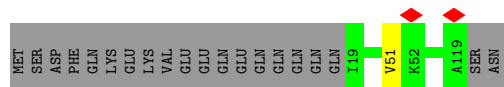
- Molecule 26: Small ribosomal subunit protein eS19A

Chain ST:  99%



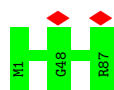
- Molecule 27: Small ribosomal subunit protein uS10

Chain SU:  83% 17%



- Molecule 28: Small ribosomal subunit protein eS21A

Chain SV:  100%



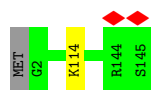
- Molecule 29: 40S ribosomal protein S22-A

Chain SW:  97%



- Molecule 30: 40S ribosomal protein S23-A

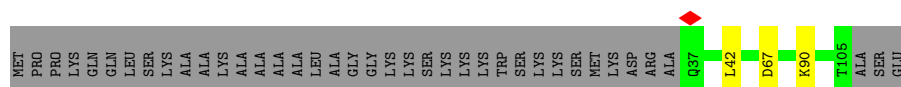
Chain SX:  99%



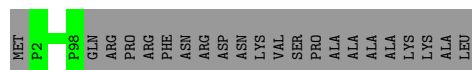
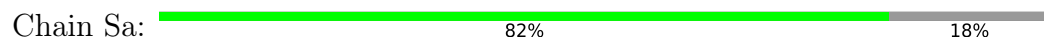
- Molecule 31: 40S ribosomal protein S24-A



- Molecule 32: Small ribosomal subunit protein eS25A



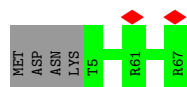
- Molecule 33: Small ribosomal subunit protein eS26B



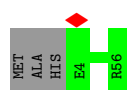
- Molecule 34: 40S ribosomal protein S27-A



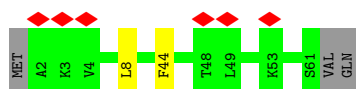
- Molecule 35: Small ribosomal subunit protein eS28A



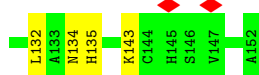
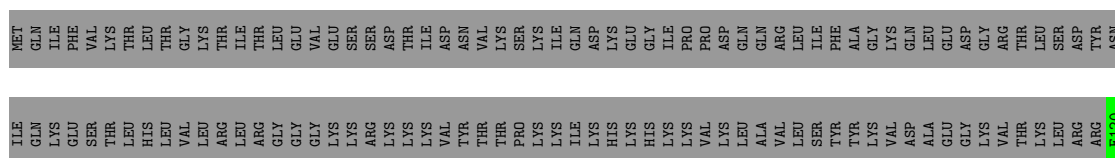
- Molecule 36: Small ribosomal subunit protein uS14A



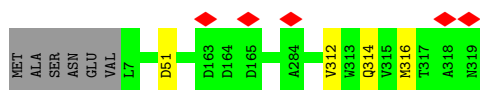
- Molecule 37: 40S ribosomal protein S30-A



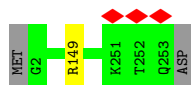
- Chain Sf:  19% 78%



- Chain Sg: 97%



- Chain LA: 99%



- Chain LB: 99%

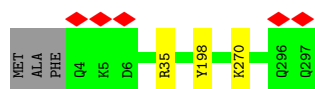


- Chain LC: 99%




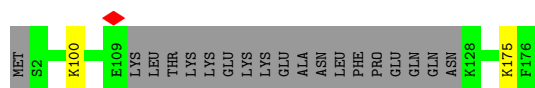
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Chain LD:  98%



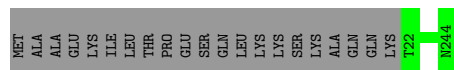
- Molecule 44: Large ribosomal subunit protein eL6A

Chain LE:  88%



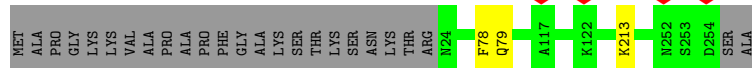
- Molecule 45: Large ribosomal subunit protein uL30A

Chain LF:  91%



- Molecule 46: Large ribosomal subunit protein eL8A

Chain LG:  89%



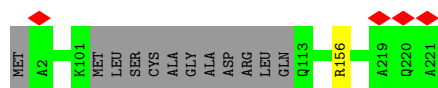
- Molecule 47: Large ribosomal subunit protein uL6A

Chain LH:  98%




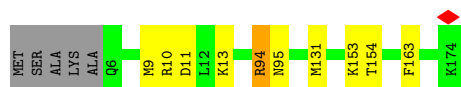
- Molecule 48: Large ribosomal subunit protein uL16

Chain LI:  94%

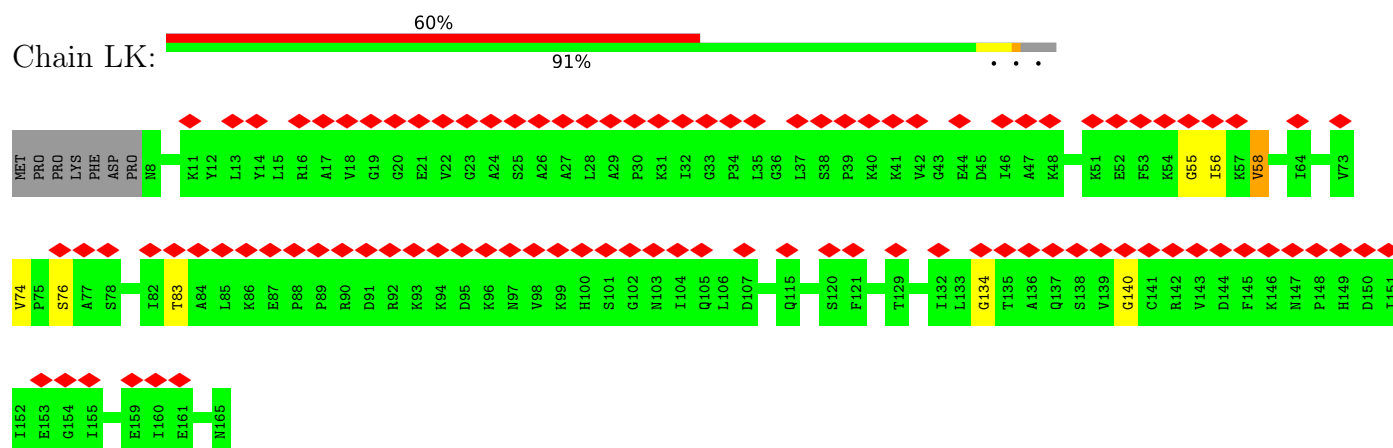


- Molecule 49: Large ribosomal subunit protein uL5A

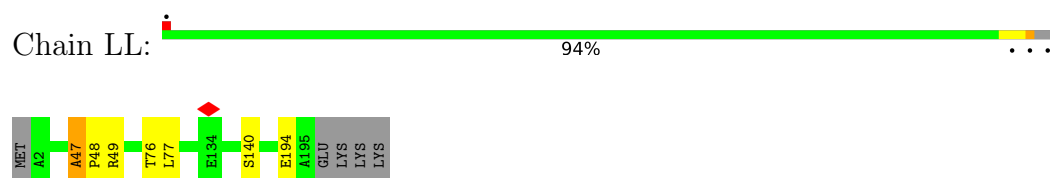
Chain LJ:  91%



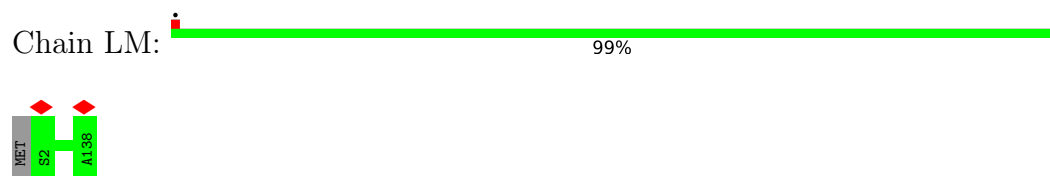
- Molecule 50: Large ribosomal subunit protein uL11A



- Molecule 51: Large ribosomal subunit protein eL13A



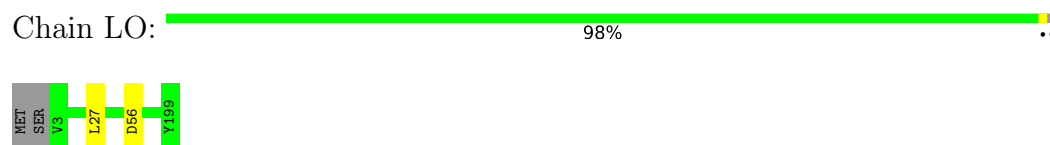
- Molecule 52: Large ribosomal subunit protein eL14A



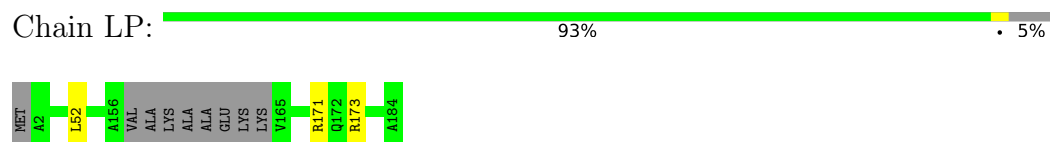
- Molecule 53: Large ribosomal subunit protein eL15A



- Molecule 54: Large ribosomal subunit protein uL13A

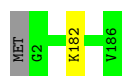


- Molecule 55: Large ribosomal subunit protein uL22A




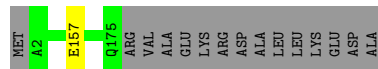
- Molecule 56: Large ribosomal subunit protein eL18A

Chain LQ:  99% ..



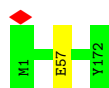
- Molecule 57: Large ribosomal subunit protein eL19A

Chain LR:  92% • 8%



- Molecule 58: Large ribosomal subunit protein eL20A

Chain LS:  99% •




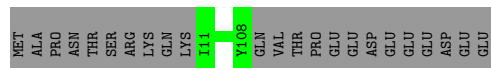
- Molecule 59: Large ribosomal subunit protein eL21A

Chain LT:  98% ..



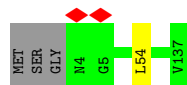
- Molecule 60: Large ribosomal subunit protein eL22A

Chain LU:  81% 19%



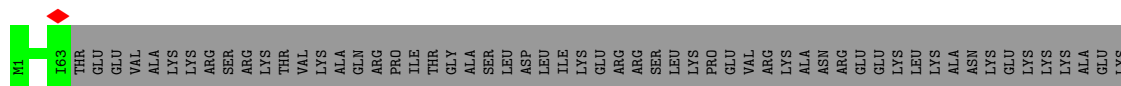
- Molecule 61: Large ribosomal subunit protein uL14A

Chain LV:  97% ..




- Molecule 62: Large ribosomal subunit protein eL24A

Chain LW:  41% 59%



ALA
ALA
ARG
LYS
LYS
GLU
LYS
LYS
ALA
SER
ALA
GLY
THR
GLN
SER
SER
LYS
PHE
SER
LYS
GLN
GLN
ALA
LYS
GLY
ALA
PHE
GLN
LYS
VAL
ALA
ALA
THR
SER
ARG

- Molecule 63: Large ribosomal subunit protein uL23

Chain LX: 

MET
ALA
PRO
SER
LYS
ALA
LYS
THR
ALA
LYS
LYS
VAL
VAL
LYS
THR
GLY
ASN
GLY
LYS
LYS
A23
E77
Q85
I142

- Molecule 64: Large ribosomal subunit protein uL24A

Chain LY: 

MET
A2
K125
LEU
GLU

- Molecule 65: Large ribosomal subunit protein eL27A

Chain LZ: 

MET
A2
K93
F101
E102
Q103
F136

- Molecule 66: Large ribosomal subunit protein uL15

Chain La: 

MET
P2
A17
G18
K47
Y48
A66
A149

- Molecule 67: Large ribosomal subunit protein eL29

Chain Lb: 

MET
A2
I21
K22
K59

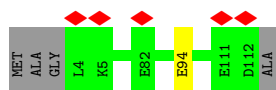
- Molecule 68: Large ribosomal subunit protein eL30

Chain Lc: 

MET
ALA
PRO
VAL
LYS
S6
Q7
E8
L104
A105

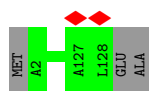
- Molecule 69: Large ribosomal subunit protein eL31A

Chain Ld: 



- Molecule 70: Large ribosomal subunit protein eL32

Chain Le: 98%



- Molecule 71: Large ribosomal subunit protein eL33A

Chain Lf: 99%



- Molecule 72: Large ribosomal subunit protein eL34A

Chain Lg: 89% 7%



- Molecule 73: Large ribosomal subunit protein uL29A

Chain Lh: 99%



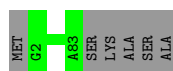
- Molecule 74: Large ribosomal subunit protein eL36A

Chain Li: 96%



- Molecule 75: Large ribosomal subunit protein eL37A

Chain Lj: 93% 7%



- Molecule 76: Large ribosomal subunit protein eL38

Chain Lk:  97% ..



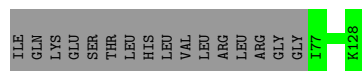
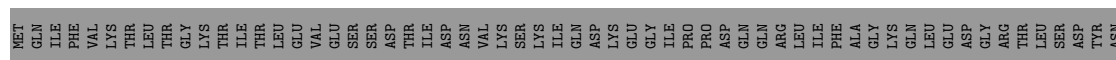
- Molecule 77: Large ribosomal subunit protein eL39

Chain Ll:  98% .



- Molecule 78: Ubiquitin-ribosomal protein eL40A fusion protein

Chain Lm:  41% 59%



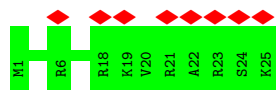
- Molecule 79: Large ribosomal subunit protein eL41A

Chain Ln:  100%



- Molecule 79: Large ribosomal subunit protein eL41A

Chain L2:  32% 100%



- Molecule 80: Large ribosomal subunit protein eL42A

Chain Lo:  99% .



- Molecule 81: Large ribosomal subunit protein eL43A

Chain Lp:  97% ..

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	140917	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.362	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	406.56, 406.56, 406.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.847, 0.847, 0.847	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 7MG, T6A, ZN, 1MG, T1C, SPD, 1MA, 2MG, H2U, M2G, 5MC

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	C2	0.43	0/42211	0.95	122/65773 (0.2%)
2	C7	0.43	0/72	0.74	0/110
3	C5	0.36	0/1577	0.95	0/2457
4	C1	0.53	15/76717 (0.0%)	0.98	258/119611 (0.2%)
5	C4	0.39	0/2883	0.89	3/4491 (0.1%)
6	C3	0.51	0/3746	0.87	2/5832 (0.0%)
7	SA	0.34	0/1623	0.71	1/2222 (0.0%)
8	SB	0.31	0/1748	0.66	2/2352 (0.1%)
9	SC	0.35	0/1665	0.67	1/2263 (0.0%)
10	SD	0.35	0/1759	0.70	2/2368 (0.1%)
11	SE	0.39	0/2109	0.72	1/2839 (0.0%)
12	SF	0.32	0/1629	0.69	1/2202 (0.0%)
13	SG	0.28	0/1779	0.62	0/2379
14	SH	0.37	0/1511	0.74	2/2036 (0.1%)
15	SI	0.43	1/1514 (0.1%)	0.73	2/2021 (0.1%)
16	SJ	0.38	0/1519	0.70	0/2035
17	SK	0.44	0/757	0.73	0/1022
18	SL	0.36	0/1194	0.62	0/1610
19	SM	0.33	0/898	0.87	2/1220 (0.2%)
20	SN	0.32	0/1215	0.62	0/1638
21	SO	0.32	0/960	0.66	0/1290
22	SP	0.41	0/959	0.79	0/1288
23	SQ	0.44	0/1125	0.79	1/1510 (0.1%)
24	SR	0.36	0/904	0.73	1/1210 (0.1%)
25	SS	0.32	0/1211	0.76	0/1628
26	ST	0.35	0/1130	0.67	0/1517
27	SU	0.32	0/815	0.68	0/1102
28	SV	0.32	0/693	0.71	0/935
29	SW	0.35	0/1038	0.65	1/1395 (0.1%)
30	SX	0.32	0/1139	0.66	0/1518
31	SY	0.33	0/1087	0.74	1/1449 (0.1%)
32	SZ	0.37	0/566	0.83	2/761 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Sa	0.30	0/782	0.69	0/1047
34	Sb	0.28	0/620	0.65	0/838
35	Sc	0.33	0/499	0.75	0/670
36	Sd	0.37	0/452	0.68	0/600
37	Se	0.28	0/483	0.72	1/643 (0.2%)
38	Sf	0.43	0/253	0.71	0/340
39	Sg	0.32	0/2456	0.68	0/3343
40	LA	0.37	0/1946	0.68	1/2614 (0.0%)
41	LB	0.35	0/3146	0.61	0/4228
42	LC	0.35	0/2800	0.64	0/3790
43	LD	0.33	0/2408	0.61	1/3248 (0.0%)
44	LE	0.36	0/1269	0.70	1/1705 (0.1%)
45	LF	0.35	0/1828	0.59	0/2461
46	LG	0.36	0/1795	0.64	1/2429 (0.0%)
47	LH	0.32	0/1531	0.65	3/2062 (0.1%)
48	LI	0.36	0/1732	0.67	0/2323
49	LJ	0.39	0/1374	0.75	0/1842
50	LK	0.56	1/777 (0.1%)	0.81	0/1077
51	LL	0.35	0/1573	0.69	1/2113 (0.0%)
52	LM	0.35	0/1074	0.58	0/1446
53	LN	0.36	0/1757	0.66	0/2354
54	LO	0.35	0/1585	0.64	1/2128 (0.0%)
55	LP	0.37	0/1400	0.68	3/1882 (0.2%)
56	LQ	0.33	0/1465	0.63	0/1965
57	LR	0.36	1/1382 (0.1%)	0.64	2/1849 (0.1%)
58	LS	0.35	0/1481	0.60	0/1990
59	LT	0.39	1/1300 (0.1%)	0.62	0/1743
60	LU	0.32	0/794	0.56	0/1076
61	LV	0.36	0/1008	0.68	1/1356 (0.1%)
62	LW	0.32	0/533	0.64	0/707
63	LX	0.37	0/974	0.70	1/1314 (0.1%)
64	LY	0.31	0/987	0.62	0/1318
65	LZ	0.37	0/1118	0.69	1/1497 (0.1%)
66	La	0.35	0/1204	0.68	1/1612 (0.1%)
67	Lb	0.31	0/473	0.62	0/629
68	Lc	0.30	0/775	0.53	0/1040
69	Ld	0.45	1/897 (0.1%)	0.66	0/1205
70	Le	0.31	0/1041	0.64	0/1394
71	Lf	0.36	0/868	0.64	0/1168
72	Lg	0.46	0/890	0.72	0/1189
73	Lh	0.28	0/974	0.57	0/1297
74	Li	0.31	0/777	0.69	2/1033 (0.2%)
75	Lj	0.37	0/665	0.65	0/882

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Lk	0.30	0/614	0.77	0/822
77	Ll	0.33	0/443	0.72	0/588
78	Lm	0.31	0/423	0.65	0/562
79	L2	0.28	0/234	0.74	0/300
79	Ln	0.31	0/234	0.76	0/300
80	Lo	0.32	0/860	0.61	0/1136
81	Lp	0.39	0/701	0.70	0/934
82	L1	0.28	0/1009	0.66	0/1405
83	P0	0.40	0/997	0.81	2/1384 (0.1%)
84	CN	0.34	0/950	0.71	3/1260 (0.2%)
All	All	0.44	20/219364 (0.0%)	0.87	431/322222 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	SF	0	1
14	SH	0	1
16	SJ	0	1
19	SM	0	2
21	SO	0	1
23	SQ	0	1
25	SS	0	1
27	SU	0	1
31	SY	0	1
37	Se	0	1
42	LC	0	1
43	LD	0	1
46	LG	0	1
49	LJ	0	1
50	LK	0	5
51	LL	0	2
65	LZ	0	1
66	La	0	2
67	Lb	0	1
74	Li	0	1
81	Lp	0	1
82	L1	0	1
83	P0	0	3
All	All	0	32

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C1	1242	G	N9-C4	8.82	1.45	1.38
4	C1	1233	G	P-O5'	7.44	1.67	1.59
4	C1	1235	U	C2-O2	-7.41	1.15	1.22
4	C1	1242	G	C8-N7	-7.12	1.26	1.30
4	C1	1242	G	N7-C5	-7.12	1.34	1.39
15	SI	140	GLU	CD-OE1	-6.54	1.18	1.25
50	LK	58	VAL	C-N	6.36	1.48	1.34
4	C1	1258	U	C2-N3	-6.00	1.33	1.37
4	C1	1242	G	N9-C8	-5.97	1.33	1.37
69	Ld	94	GLU	CB-CG	-5.97	1.40	1.52
4	C1	1242	G	O3'-P	5.91	1.68	1.61
4	C1	1233	G	N9-C4	-5.91	1.33	1.38
4	C1	1237	G	N9-C4	5.73	1.42	1.38
4	C1	1258	U	O3'-P	5.59	1.67	1.61
4	C1	1234	G	N7-C5	-5.54	1.35	1.39
57	LR	157	GLU	CD-OE1	-5.49	1.19	1.25
4	C1	1233	G	C2-N3	-5.44	1.28	1.32
4	C1	1282	G	O3'-P	5.29	1.67	1.61
59	LT	118	GLU	CD-OE1	-5.23	1.19	1.25
4	C1	1243	G	P-O5'	5.22	1.65	1.59

All (431) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C1	1242	G	N3-C4-C5	-26.64	115.28	128.60
4	C1	1242	G	C2-N3-C4	24.41	124.10	111.90
4	C1	1241	U	O5'-P-OP1	-18.65	88.32	110.70
4	C1	1235	U	C5-C4-O4	17.42	136.35	125.90
4	C1	1242	G	C5-N7-C8	17.12	112.86	104.30
4	C1	1242	G	C4-C5-N7	-17.08	103.97	110.80
4	C1	1235	U	N3-C2-O2	-16.02	110.98	122.20
4	C1	1242	G	N3-C4-N9	15.46	135.27	126.00
4	C1	1235	U	C6-N1-C2	-14.82	112.11	121.00
4	C1	1235	U	N1-C2-N3	14.15	123.39	114.90
4	C1	1258	U	O5'-P-OP1	-12.89	94.10	105.70
4	C1	1242	G	C4-N9-C1'	12.07	142.19	126.50
4	C1	1240	A	N7-C8-N9	11.96	119.78	113.80
4	C1	1232	C	OP1-P-OP2	-11.80	101.90	119.60
4	C1	1242	G	N1-C6-O6	-11.61	112.94	119.90
4	C1	1237	G	N3-C2-N2	11.57	128.00	119.90
4	C1	1240	A	N1-C6-N6	11.34	125.40	118.60
4	C1	1233	G	N1-C6-O6	-11.24	113.16	119.90

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C1	1233	G	O5'-P-OP2	11.07	123.98	110.70
4	C1	1233	G	N3-C4-N9	-10.99	119.40	126.00
4	C1	1237	G	C4-N9-C1'	10.98	140.78	126.50
4	C1	1233	G	C4-N9-C1'	-10.92	112.30	126.50
4	C1	1243	G	N3-C4-N9	10.84	132.50	126.00
4	C1	1237	G	N1-C2-N2	-10.48	106.77	116.20
4	C1	1234	G	C8-N9-C4	-10.45	102.22	106.40
4	C1	1237	G	C8-N9-C1'	-10.39	113.49	127.00
4	C1	1234	G	N7-C8-N9	10.38	118.29	113.10
4	C1	1233	G	C6-C5-N7	10.34	136.60	130.40
4	C1	1238	C	N3-C4-N4	-10.28	110.81	118.00
4	C1	1238	C	C6-N1-C1'	10.23	133.08	120.80
4	C1	1237	G	N3-C4-N9	10.12	132.07	126.00
4	C1	3217	C	N1-C2-O2	10.09	124.96	118.90
4	C1	1258	U	N3-C4-O4	-10.09	112.34	119.40
4	C1	1232	C	OP2-P-O3'	-10.06	83.07	105.20
4	C1	1238	C	C2-N1-C1'	-10.05	107.75	118.80
4	C1	1233	G	C5-C6-O6	10.02	134.61	128.60
4	C1	1242	G	C8-N9-C4	-9.88	102.45	106.40
4	C1	1233	G	C8-N9-C1'	9.65	139.54	127.00
4	C1	1233	G	OP1-P-OP2	-9.58	105.23	119.60
4	C1	1235	U	N3-C4-O4	-9.51	112.74	119.40
4	C1	1240	A	C5-C6-N6	-9.49	116.11	123.70
1	C2	1389	C	C2-N1-C1'	9.16	128.87	118.80
4	C1	1242	G	C6-N1-C2	-9.08	119.65	125.10
4	C1	1238	C	C5-C4-N4	9.02	126.51	120.20
4	C1	1237	G	N9-C4-C5	-9.00	101.80	105.40
4	C1	1242	G	N9-C4-C5	9.00	109.00	105.40
4	C1	1240	A	C6-C5-N7	-8.99	126.01	132.30
4	C1	1242	G	C8-N9-C1'	-8.95	115.36	127.00
4	C1	3217	C	C2-N1-C1'	8.85	128.53	118.80
4	C1	1241	U	O4'-C1'-N1	8.85	115.28	108.20
4	C1	1234	G	OP1-P-OP2	-8.77	106.45	119.60
4	C1	1237	G	C6-C5-N7	-8.73	125.16	130.40
4	C1	1240	A	C5-N7-C8	-8.62	99.59	103.90
44	LE	175	LYS	CD-CE-NZ	-8.46	92.24	111.70
4	C1	1258	U	C5-C4-O4	8.45	130.97	125.90
4	C1	1238	C	N1-C2-N3	8.39	125.08	119.20
4	C1	1241	U	C5-C6-N1	8.39	126.90	122.70
4	C1	1242	G	C5-C6-N1	8.37	115.69	111.50
4	C1	3278	C	N1-C2-O2	8.33	123.90	118.90
4	C1	1242	G	P-O3'-C3'	8.28	129.63	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C1	406	G	O4'-C1'-N9	8.27	114.82	108.20
4	C1	1237	G	C4-C5-N7	8.22	114.09	110.80
4	C1	3181	C	N1-C2-O2	8.12	123.77	118.90
4	C1	3217	C	N3-C2-O2	-8.08	116.24	121.90
4	C1	1269	U	C2-N1-C1'	8.06	127.38	117.70
4	C1	1278	A	C8-N9-C4	-8.06	102.57	105.80
4	C1	1241	U	C6-N1-C1'	8.04	132.46	121.20
1	C2	500	C	N3-C2-O2	-8.04	116.27	121.90
4	C1	1233	G	N3-C4-C5	7.87	132.53	128.60
4	C1	1237	G	N3-C4-C5	-7.83	124.69	128.60
4	C1	922	U	C2-N1-C1'	7.73	126.98	117.70
4	C1	1235	U	C6-N1-C1'	7.71	132.00	121.20
1	C2	1082	C	C2-N1-C1'	7.64	127.20	118.80
4	C1	1258	U	N3-C2-O2	-7.63	116.86	122.20
4	C1	1234	G	C6-C5-N7	-7.62	125.83	130.40
4	C1	1240	A	C8-N9-C4	-7.62	102.75	105.80
4	C1	1269	U	N1-C2-O2	7.60	128.12	122.80
4	C1	1243	G	N3-C4-C5	-7.58	124.81	128.60
84	CN	34	THR	C-N-CA	7.57	140.63	121.70
4	C1	1242	G	C4-C5-C6	7.55	123.33	118.80
1	C2	653	C	N1-C2-O2	7.50	123.40	118.90
4	C1	1241	U	C6-N1-C2	-7.48	116.51	121.00
4	C1	3181	C	C2-N1-C1'	7.45	126.99	118.80
4	C1	2496	C	N3-C2-O2	-7.41	116.71	121.90
1	C2	656	G	N3-C4-N9	7.36	130.41	126.00
9	SC	241	ASP	CB-CG-OD1	7.34	124.91	118.30
4	C1	922	U	N1-C2-O2	7.34	127.94	122.80
4	C1	1239	C	N1-C1'-C2'	7.34	123.54	114.00
4	C1	1269	U	N3-C2-O2	-7.33	117.06	122.20
4	C1	1278	A	N7-C8-N9	7.28	117.44	113.80
1	C2	1243	G	C2-N3-C4	7.25	115.52	111.90
4	C1	3278	C	N3-C2-O2	-7.23	116.84	121.90
1	C2	1560	U	N3-C2-O2	-7.17	117.18	122.20
1	C2	1458	G	C4-N9-C1'	7.16	135.81	126.50
84	CN	35	ASP	CB-CG-OD1	7.13	124.72	118.30
1	C2	656	G	C4-N9-C1'	7.08	135.71	126.50
63	LX	77	GLU	OE1-CD-OE2	-7.08	114.80	123.30
19	SM	62	LEU	CB-CG-CD1	-7.08	98.97	111.00
4	C1	3278	C	C2-N1-C1'	7.06	126.56	118.80
4	C1	1238	C	C2-N3-C4	-7.03	116.38	119.90
4	C1	1258	U	N1-C2-N3	7.03	119.12	114.90
4	C1	1255	C	C6-N1-C2	-7.03	117.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C1	758	C	C2-N1-C1'	7.01	126.51	118.80
1	C2	959	U	C2-N1-C1'	7.00	126.10	117.70
4	C1	1243	G	C6-C5-N7	-6.99	126.21	130.40
4	C1	3058	U	C2-N1-C1'	6.93	126.02	117.70
1	C2	959	U	N1-C2-O2	6.93	127.65	122.80
4	C1	1273	A	O5'-P-OP1	6.92	119.01	110.70
4	C1	1243	G	N1-C2-N2	-6.92	109.97	116.20
4	C1	2541	U	P-O3'-C3'	6.89	127.97	119.70
4	C1	1283	C	N3-C2-O2	-6.88	117.08	121.90
4	C1	1243	G	N9-C4-C5	-6.83	102.67	105.40
4	C1	1238	C	N3-C2-O2	-6.77	117.16	121.90
1	C2	1243	G	N3-C4-C5	-6.76	125.22	128.60
1	C2	656	G	N3-C4-C5	-6.76	125.22	128.60
1	C2	959	U	N3-C2-O2	-6.75	117.47	122.20
19	SM	62	LEU	CA-CB-CG	6.75	130.82	115.30
1	C2	1560	U	C2-N1-C1'	6.74	125.79	117.70
4	C1	1240	A	C5'-C4'-O4'	6.71	117.15	109.10
4	C1	1358	C	C5-C6-N1	6.66	124.33	121.00
4	C1	1233	G	N9-C4-C5	6.66	108.06	105.40
4	C1	1496	C	C2-N1-C1'	6.62	126.08	118.80
1	C2	1307	U	C2-N1-C1'	6.61	125.63	117.70
32	SZ	67	ASP	CB-CG-OD1	6.59	124.23	118.30
4	C1	835	G	O4'-C1'-N9	6.58	113.46	108.20
4	C1	1815	U	P-O3'-C3'	6.55	127.56	119.70
4	C1	1240	A	C4-C5-N7	6.54	113.97	110.70
4	C1	1645	U	C2-N1-C1'	6.54	125.55	117.70
1	C2	322	G	C2'-C3'-O3'	6.54	124.16	113.70
1	C2	654	C	N1-C2-O2	6.52	122.81	118.90
1	C2	782	U	C2-N1-C1'	6.52	125.52	117.70
4	C1	1272	C	N1-C2-O2	6.52	122.81	118.90
4	C1	1238	C	C5-C6-N1	-6.51	117.75	121.00
4	C1	1232	C	C6-N1-C2	-6.50	117.70	120.30
4	C1	2237	C	N3-C2-O2	-6.48	117.36	121.90
1	C2	782	U	N1-C2-O2	6.47	127.33	122.80
4	C1	1235	U	O4'-C1'-N1	6.46	113.37	108.20
83	P0	53	MET	N-CA-CB	-6.46	98.98	110.60
4	C1	1243	G	OP1-P-OP2	-6.44	109.94	119.60
1	C2	1307	U	N1-C2-O2	6.44	127.31	122.80
4	C1	1241	U	OP1-P-OP2	6.43	129.24	119.60
4	C1	1256	G	C5-C6-O6	6.39	132.44	128.60
1	C2	1458	G	N3-C4-N9	6.38	129.83	126.00
4	C1	1349	G	C4-N9-C1'	6.37	134.78	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C1	1355	A	P-O3'-C3'	6.37	127.34	119.70
66	La	47	LYS	C-N-CA	6.36	137.61	121.70
4	C1	1238	C	N1-C1'-C2'	6.36	122.27	114.00
4	C1	1604	G	C4-N9-C1'	6.36	134.76	126.50
4	C1	1238	C	O4'-C1'-N1	6.35	113.28	108.20
4	C1	2489	C	N3-C2-O2	-6.34	117.46	121.90
1	C2	1560	U	N1-C2-O2	6.34	127.24	122.80
4	C1	2496	C	N1-C2-O2	6.32	122.69	118.90
4	C1	1233	G	N3-C2-N2	-6.32	115.48	119.90
1	C2	736	C	N1-C2-O2	6.31	122.69	118.90
1	C2	1389	C	C6-N1-C1'	-6.29	113.25	120.80
1	C2	711	U	P-O3'-C3'	6.29	127.25	119.70
4	C1	1258	U	C6-N1-C1'	6.29	130.00	121.20
4	C1	1307	G	C2'-C3'-O3'	6.26	123.72	113.70
4	C1	3057	U	N3-C2-O2	-6.26	117.82	122.20
40	LA	149	ARG	C-N-CA	6.25	137.32	121.70
4	C1	78	U	N3-C2-O2	-6.25	117.83	122.20
1	C2	1389	C	C5-C6-N1	6.24	124.12	121.00
4	C1	1234	G	C4-C5-C6	6.23	122.54	118.80
4	C1	1243	G	N3-C2-N2	6.22	124.26	119.90
4	C1	2112	U	P-O3'-C3'	6.22	127.16	119.70
1	C2	653	C	C6-N1-C2	-6.21	117.81	120.30
4	C1	1233	G	C4-C5-N7	-6.21	108.31	110.80
4	C1	2112	U	OP2-P-O3'	6.21	118.87	105.20
4	C1	2846	U	C2-N1-C1'	6.21	125.16	117.70
5	C4	1	G	C2-N3-C4	6.19	115.00	111.90
4	C1	1233	G	C4-C5-C6	-6.19	115.08	118.80
4	C1	3181	C	N3-C2-O2	-6.19	117.57	121.90
4	C1	3058	U	N1-C2-O2	6.18	127.13	122.80
1	C2	1256	A	P-O3'-C3'	6.18	127.11	119.70
4	C1	2537	U	P-O3'-C3'	6.17	127.11	119.70
1	C2	453	U	N1-C2-O2	6.17	127.12	122.80
4	C1	1235	U	N3-C4-C5	-6.16	110.90	114.60
4	C1	1234	G	C4-N9-C1'	6.16	134.50	126.50
4	C1	3057	U	N1-C2-O2	6.15	127.10	122.80
4	C1	1233	G	N7-C8-N9	-6.15	110.03	113.10
4	C1	1604	G	N3-C4-C5	-6.14	125.53	128.60
1	C2	654	C	C2-N1-C1'	6.14	125.56	118.80
4	C1	2505	U	C2'-C3'-O3'	6.14	123.53	113.70
1	C2	1389	C	C6-N1-C2	-6.14	117.84	120.30
1	C2	656	G	C8-N9-C1'	-6.14	119.02	127.00
10	SD	59	LEU	CA-CB-CG	6.13	129.41	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C2	1458	G	C8-N9-C1'	-6.13	119.03	127.00
4	C1	3217	C	C6-N1-C1'	-6.12	113.46	120.80
1	C2	77	U	P-O3'-C3'	6.10	127.02	119.70
4	C1	3214	U	C2-N1-C1'	6.10	125.02	117.70
1	C2	782	U	N3-C2-O2	-6.09	117.93	122.20
4	C1	3306	U	N3-C2-O2	-6.09	117.94	122.20
4	C1	1243	G	C8-N9-C1'	-6.09	119.08	127.00
4	C1	3235	C	C2-N1-C1'	6.09	125.50	118.80
4	C1	1258	U	C2-N1-C1'	-6.09	110.40	117.70
4	C1	3131	U	C2-N1-C1'	6.09	125.00	117.70
4	C1	1233	G	O5'-P-OP1	6.08	117.99	110.70
4	C1	1255	C	N3-C2-O2	-6.08	117.65	121.90
1	C2	1791	A	P-O3'-C3'	6.07	126.98	119.70
1	C2	1274	C	P-O3'-C3'	6.06	126.97	119.70
4	C1	2237	C	N1-C2-O2	6.05	122.53	118.90
1	C2	1799	U	N1-C2-O2	6.05	127.03	122.80
4	C1	3217	C	C6-N1-C2	-6.04	117.88	120.30
1	C2	224	C	N1-C2-O2	6.04	122.52	118.90
4	C1	1234	G	N3-C4-C5	-6.04	125.58	128.60
4	C1	2550	U	N3-C2-O2	-6.03	117.98	122.20
4	C1	1716	U	P-O3'-C3'	6.02	126.92	119.70
4	C1	1240	A	N3-C4-N9	6.02	132.21	127.40
1	C2	1257	U	C2-N1-C1'	6.01	124.92	117.70
1	C2	1458	G	N3-C4-C5	-6.00	125.60	128.60
6	C3	100	U	C2-N1-C1'	5.99	124.89	117.70
29	SW	93	LEU	CA-CB-CG	5.99	129.07	115.30
1	C2	639	U	P-O3'-C3'	5.97	126.87	119.70
4	C1	2873	U	N3-C2-O2	-5.97	118.02	122.20
4	C1	1349	G	N3-C4-C5	-5.95	125.62	128.60
1	C2	453	U	N3-C2-O2	-5.95	118.04	122.20
1	C2	819	G	P-O3'-C3'	5.94	126.83	119.70
4	C1	2550	U	C2-N1-C1'	5.94	124.82	117.70
4	C1	2652	U	N3-C2-O2	-5.93	118.05	122.20
4	C1	922	U	N3-C2-O2	-5.93	118.05	122.20
1	C2	352	A	P-O3'-C3'	5.93	126.81	119.70
1	C2	1307	U	N3-C2-O2	-5.92	118.05	122.20
4	C1	2405	C	C6-N1-C2	-5.90	117.94	120.30
4	C1	1556	C	N1-C2-O2	5.90	122.44	118.90
1	C2	653	C	N3-C2-O2	-5.89	117.78	121.90
1	C2	1258	U	N1-C2-O2	5.89	126.92	122.80
1	C2	1389	C	N1-C2-O2	5.87	122.42	118.90
4	C1	1604	G	N3-C4-N9	5.86	129.52	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C1	2726	C	C2-N1-C1'	5.86	125.25	118.80
61	LV	54	LEU	CB-CG-CD1	-5.84	101.07	111.00
4	C1	1645	U	N1-C2-O2	5.83	126.88	122.80
1	C2	928	U	P-O3'-C3'	5.83	126.70	119.70
4	C1	1064	A	P-O3'-C3'	5.83	126.70	119.70
1	C2	1596	C	C2-N1-C1'	5.82	125.20	118.80
1	C2	387	A	OP2-P-O3'	5.81	117.97	105.20
1	C2	482	U	N1-C2-O2	5.80	126.86	122.80
1	C2	1636	C	P-O3'-C3'	5.80	126.66	119.70
4	C1	192	C	C2-N1-C1'	5.80	125.19	118.80
31	SY	48	TYR	C-N-CA	5.80	136.21	121.70
8	SB	33	LYS	C-N-CA	5.80	136.20	121.70
4	C1	3048	A	O4'-C1'-N9	5.79	112.83	108.20
1	C2	959	U	C5-C6-N1	5.79	125.59	122.70
4	C1	1241	U	C2-N1-C1'	-5.77	110.77	117.70
4	C1	2405	C	N3-C2-O2	-5.77	117.86	121.90
1	C2	758	U	N1-C2-O2	5.75	126.82	122.80
4	C1	1645	U	N3-C2-O2	-5.74	118.18	122.20
4	C1	1240	A	C4-C5-C6	5.74	119.87	117.00
24	SR	16	LEU	CA-CB-CG	5.74	128.50	115.30
1	C2	1799	U	N3-C2-O2	-5.73	118.19	122.20
1	C2	758	U	N3-C2-O2	-5.73	118.19	122.20
4	C1	3058	U	N3-C2-O2	-5.72	118.19	122.20
1	C2	140	A	O5'-P-OP2	5.72	117.57	110.70
4	C1	2617	U	N3-C2-O2	-5.72	118.19	122.20
1	C2	1258	U	N3-C2-O2	-5.71	118.20	122.20
1	C2	617	U	C2-N1-C1'	5.71	124.55	117.70
4	C1	1097	G	P-O3'-C3'	5.71	126.55	119.70
4	C1	1263	A	C6-C5-N7	-5.70	128.31	132.30
1	C2	482	U	N3-C2-O2	-5.69	118.22	122.20
4	C1	524	U	N1-C2-O2	5.69	126.78	122.80
4	C1	3306	U	C2-N1-C1'	5.68	124.52	117.70
4	C1	1240	A	O3'-P-O5'	5.68	114.79	104.00
4	C1	2846	U	N3-C2-O2	-5.67	118.23	122.20
1	C2	1573	A	P-O3'-C3'	5.67	126.50	119.70
14	SH	158	ASP	CB-CG-OD1	5.66	123.40	118.30
4	C1	1240	A	O4'-C1'-N9	5.66	112.73	108.20
1	C2	1273	G	P-O3'-C3'	5.66	126.49	119.70
10	SD	191	ASP	CB-CG-OD1	5.64	123.38	118.30
1	C2	517	U	C2-N1-C1'	5.64	124.46	117.70
4	C1	1243	G	C4-C5-C6	5.63	122.18	118.80
4	C1	2206	G	O4'-C1'-N9	5.62	112.70	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C2	653	C	C5-C6-N1	5.62	123.81	121.00
4	C1	3057	U	C2-N1-C1'	5.62	124.44	117.70
4	C1	2638	C	N1-C2-O2	5.62	122.27	118.90
1	C2	610	G	C4-N9-C1'	5.62	133.80	126.50
4	C1	2489	C	N1-C2-O2	5.61	122.27	118.90
4	C1	1563	C	C6-N1-C1'	5.61	127.53	120.80
4	C1	1257	C	N1-C2-O2	5.61	122.26	118.90
1	C2	387	A	P-O3'-C3'	5.60	126.42	119.70
74	Li	64	SER	C-N-CA	-5.60	110.54	122.30
1	C2	1620	C	N1-C2-O2	5.58	122.25	118.90
4	C1	1241	U	N1-C2-O2	-5.56	118.91	122.80
4	C1	2204	C	C2-N1-C1'	5.55	124.91	118.80
47	LH	161	LEU	CA-CB-CG	5.54	128.04	115.30
4	C1	1447	G	C3'-C2'-C1'	-5.54	97.07	101.50
1	C2	1082	C	O4'-C1'-N1	5.53	112.63	108.20
1	C2	224	C	N3-C2-O2	-5.53	118.03	121.90
4	C1	1269	U	C6-N1-C1'	-5.52	113.47	121.20
1	C2	313	U	P-O3'-C3'	5.52	126.32	119.70
4	C1	2550	U	N1-C2-O2	5.51	126.66	122.80
1	C2	224	C	C2-N1-C1'	5.51	124.86	118.80
1	C2	654	C	C6-N1-C2	-5.51	118.09	120.30
1	C2	166	C	N1-C2-O2	5.50	122.20	118.90
4	C1	36	C	N1-C2-O2	5.50	122.20	118.90
1	C2	400	A	P-O3'-C3'	5.49	126.29	119.70
11	SE	246	LEU	CA-CB-CG	5.49	127.93	115.30
4	C1	1233	G	OP1-P-O3'	5.49	117.27	105.20
1	C2	1066	C	C2-N1-C1'	5.47	124.81	118.80
4	C1	1263	A	C4-N9-C1'	5.46	136.14	126.30
4	C1	2471	U	N1-C2-O2	5.46	126.62	122.80
83	P0	41	VAL	C-N-CA	-5.45	108.08	121.70
1	C2	453	U	C2-N1-C1'	5.45	124.23	117.70
4	C1	2235	C	C2-N1-C1'	5.44	124.79	118.80
4	C1	1358	C	C6-N1-C2	-5.44	118.12	120.30
4	C1	1272	C	N3-C2-O2	-5.44	118.09	121.90
4	C1	1229	G	C4'-C3'-C2'	-5.43	97.17	102.60
1	C2	1023	A	P-O3'-C3'	5.43	126.22	119.70
1	C2	864	U	C2-N1-C1'	5.43	124.21	117.70
4	C1	1263	A	C5'-C4'-C3'	-5.43	107.32	116.00
37	Se	8	LEU	CA-CB-CG	5.42	127.77	115.30
1	C2	653	C	C2-N1-C1'	5.42	124.76	118.80
74	Li	60	LEU	CB-CG-CD1	5.42	120.21	111.00
4	C1	3181	C	C6-N1-C1'	-5.42	114.30	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	LL	140	SER	C-N-CA	5.42	135.24	121.70
1	C2	1584	G	C4-N9-C1'	-5.41	119.46	126.50
4	C1	2495	C	N3-C2-O2	-5.41	118.11	121.90
4	C1	1115	G	C4-N9-C1'	5.41	133.53	126.50
4	C1	1246	G	O5'-P-OP2	-5.41	100.83	105.70
4	C1	1259	A	C3'-C2'-C1'	5.41	105.83	101.50
4	C1	2366	C	C2-N1-C1'	5.41	124.75	118.80
1	C2	1489	U	C2-N1-C1'	5.40	124.18	117.70
4	C1	1272	C	C6-N1-C2	-5.40	118.14	120.30
4	C1	1242	G	N3-C2-N2	5.40	123.68	119.90
46	LG	78	PHE	C-N-CA	5.39	135.18	121.70
1	C2	517	U	N1-C2-O2	5.39	126.57	122.80
1	C2	1082	C	C6-N1-C1'	-5.38	114.34	120.80
54	LO	27	LEU	CB-CG-CD2	-5.38	101.86	111.00
1	C2	482	U	C2-N1-C1'	5.37	124.15	117.70
1	C2	431	C	C2-N1-C1'	5.37	124.70	118.80
1	C2	322	G	P-O3'-C3'	5.36	126.14	119.70
4	C1	2846	U	N1-C2-O2	5.36	126.55	122.80
1	C2	1258	U	C2-N1-C1'	5.36	124.13	117.70
55	LP	173	ARG	CB-CG-CD	5.35	125.52	111.60
4	C1	1243	G	P-O5'-C5'	5.35	129.46	120.90
4	C1	3228	C	P-O3'-C3'	5.34	126.11	119.70
4	C1	315	C	C2-N1-C1'	5.34	124.68	118.80
4	C1	1858	A	O4'-C1'-N9	5.33	112.46	108.20
32	SZ	42	LEU	CA-CB-CG	5.33	127.56	115.30
4	C1	1349	G	N3-C4-N9	5.33	129.20	126.00
1	C2	172	C	C2-N1-C1'	5.32	124.66	118.80
4	C1	1232	C	C2-N3-C4	5.32	122.56	119.90
4	C1	1562	C	P-O3'-C3'	5.32	126.09	119.70
4	C1	3316	A	P-O3'-C3'	5.32	126.08	119.70
14	SH	9	LEU	CB-CG-CD2	5.32	120.05	111.00
4	C1	916	G	P-O3'-C3'	5.32	126.08	119.70
4	C1	2873	U	C2-N1-C1'	5.32	124.08	117.70
4	C1	2585	G	N3-C4-C5	-5.31	125.94	128.60
4	C1	1604	G	C8-N9-C1'	-5.30	120.11	127.00
1	C2	1742	U	C2-N1-C1'	5.30	124.06	117.70
1	C2	190	C	N1-C2-O2	5.30	122.08	118.90
4	C1	524	U	N3-C2-O2	-5.30	118.49	122.20
4	C1	282	G	P-O3'-C3'	5.29	126.05	119.70
1	C2	736	C	C2-N1-C1'	5.29	124.62	118.80
1	C2	278	U	P-O3'-C3'	5.29	126.05	119.70
4	C1	3104	U	N3-C2-O2	-5.29	118.50	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C1	922	U	C6-N1-C1'	-5.29	113.80	121.20
1	C2	767	U	C2-N1-C1'	5.28	124.04	117.70
4	C1	2137	U	C2-N1-C1'	5.28	124.03	117.70
55	LP	173	ARG	CA-CB-CG	5.28	125.00	113.40
84	CN	14	LEU	CA-CB-CG	5.26	127.39	115.30
47	LH	161	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	C2	640	U	P-O3'-C3'	5.26	126.01	119.70
15	SI	157	GLU	CA-CB-CG	5.25	124.96	113.40
4	C1	1820	U	P-O3'-C3'	5.25	126.00	119.70
1	C2	609	U	P-O3'-C3'	5.25	125.99	119.70
4	C1	270	U	N1-C2-O2	5.24	126.47	122.80
1	C2	1585	U	C2-N3-C4	5.24	130.15	127.00
1	C2	1799	U	C2-N1-C1'	5.24	123.99	117.70
4	C1	1258	U	O4'-C1'-N1	5.24	112.39	108.20
5	C4	26	C	N1-C2-O2	5.23	122.04	118.90
1	C2	500	C	N1-C2-O2	5.23	122.04	118.90
55	LP	52	LEU	CA-CB-CG	5.23	127.33	115.30
4	C1	1263	A	N7-C8-N9	5.23	116.42	113.80
1	C2	280	U	P-O3'-C3'	5.22	125.97	119.70
1	C2	1063	U	N1-C2-O2	5.22	126.46	122.80
4	C1	2189	U	N1-C2-O2	5.22	126.46	122.80
23	SQ	53	LEU	N-CA-CB	-5.22	99.97	110.40
4	C1	1577	G	N1-C6-O6	-5.21	116.77	119.90
43	LD	198	TYR	CA-CB-CG	5.21	123.29	113.40
4	C1	1262	G	OP2-P-O3'	5.20	116.65	105.20
6	C3	125	U	C2-N1-C1'	5.19	123.93	117.70
4	C1	1307	G	P-O3'-C3'	5.19	125.92	119.70
4	C1	1349	G	C8-N9-C1'	-5.18	120.27	127.00
1	C2	224	C	C6-N1-C2	-5.17	118.23	120.30
4	C1	2263	C	C5-C6-N1	5.17	123.59	121.00
4	C1	1243	G	C4-N9-C1'	5.17	133.22	126.50
4	C1	1608	C	C2-N1-C1'	5.17	124.48	118.80
1	C2	1243	G	N3-C4-N9	5.16	129.10	126.00
1	C2	1274	C	N1-C2-O2	5.16	121.99	118.90
65	LZ	103	GLN	CA-CB-CG	5.16	124.74	113.40
1	C2	1566	U	N3-C2-O2	-5.15	118.60	122.20
4	C1	3218	A	P-O3'-C3'	5.14	125.87	119.70
7	SA	17	LEU	CA-CB-CG	5.14	127.13	115.30
4	C1	3050	U	C2-N1-C1'	5.14	123.87	117.70
1	C2	530	C	N1-C2-O2	5.14	121.98	118.90
57	LR	157	GLU	OE1-CD-OE2	-5.13	117.14	123.30
1	C2	1560	U	O4'-C1'-N1	5.13	112.30	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	SF	161	ASP	CB-CG-OD1	5.13	122.92	118.30
4	C1	2842	U	N1-C2-O2	5.12	126.39	122.80
1	C2	654	C	N3-C2-O2	-5.12	118.31	121.90
1	C2	912	U	P-O3'-C3'	5.12	125.85	119.70
47	LH	179	ILE	CG1-CB-CG2	-5.12	100.15	111.40
57	LR	157	GLU	N-CA-CB	5.11	119.79	110.60
4	C1	969	C	N1-C2-O2	5.11	121.96	118.90
4	C1	1235	U	N1-C1'-C2'	5.10	120.62	114.00
4	C1	78	U	N1-C2-O2	5.09	126.36	122.80
4	C1	3269	U	P-O3'-C3'	5.09	125.81	119.70
1	C2	494	U	C2-N1-C1'	5.08	123.80	117.70
4	C1	1716	U	OP1-P-O3'	5.08	116.38	105.20
4	C1	2652	U	N1-C2-O2	5.08	126.36	122.80
4	C1	1872	C	N1-C2-O2	5.08	121.95	118.90
1	C2	1332	C	C2-N1-C1'	5.07	124.38	118.80
4	C1	3275	U	OP1-P-O3'	5.07	116.36	105.20
1	C2	539	G	P-O3'-C3'	5.06	125.78	119.70
1	C2	1214	U	N1-C2-O2	5.06	126.34	122.80
1	C2	1584	G	C8-N9-C1'	5.06	133.58	127.00
1	C2	1596	C	N1-C2-O2	5.06	121.94	118.90
4	C1	2726	C	N3-C2-O2	-5.06	118.36	121.90
4	C1	3104	U	N1-C2-O2	5.05	126.33	122.80
4	C1	3078	U	C2-N1-C1'	5.04	123.75	117.70
1	C2	141	U	P-O3'-C3'	5.04	125.75	119.70
4	C1	1240	A	N9-C4-C5	-5.04	103.78	105.80
4	C1	3217	C	C5-C6-N1	5.04	123.52	121.00
4	C1	3153	U	C2-N1-C1'	5.03	123.74	117.70
8	SB	61	LEU	CA-CB-CG	5.03	126.86	115.30
5	C4	1	G	N3-C4-C5	-5.02	126.09	128.60
1	C2	656	G	C2-N3-C4	5.01	114.41	111.90
1	C2	517	U	N3-C2-O2	-5.01	118.69	122.20
4	C1	1577	G	C5-C6-O6	5.01	131.60	128.60
1	C2	1214	U	C2-N1-C1'	5.00	123.71	117.70
1	C2	1742	U	P-O3'-C3'	5.00	125.71	119.70
15	SI	6	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
82	L1	16	LEU	Peptide
42	LC	144	LYS	Peptide

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Mol	Chain	Res	Type	Group
43	LD	270	LYS	Peptide
46	LG	79	GLN	Peptide
49	LJ	94	ARG	Peptide
50	LK	55	GLY	Peptide
50	LK	56	ILE	Peptide
50	LK	74	VAL	Peptide
50	LK	76	SER	Peptide
50	LK	83	THR	Peptide
51	LL	47	ALA	Peptide
51	LL	49	ARG	Peptide
65	LZ	101	PHE	Peptide
66	La	17	ALA	Peptide
66	La	66	ALA	Peptide
67	Lb	21	ILE	Peptide
74	Li	64	SER	Peptide
81	Lp	51	ALA	Peptide
83	P0	42	ARG	Peptide
83	P0	52	LEU	Peptide
83	P0	55	LYS	Peptide
12	SF	155	ALA	Peptide
14	SH	64	VAL	Peptide
16	SJ	105	LEU	Mainchain
19	SM	119	SER	Peptide
19	SM	130	THR	Peptide
21	SO	36	LYS	Peptide
23	SQ	113	ASP	Peptide
25	SS	60	GLU	Peptide
27	SU	51	VAL	Peptide
31	SY	51	GLU	Peptide
37	Se	44	PHE	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	
7	SA	204/252 (81%)	179 (88%)	24 (12%)	1 (0%)	25	61
8	SB	214/255 (84%)	200 (94%)	14 (6%)	0	100	100
9	SC	215/254 (85%)	205 (95%)	9 (4%)	1 (0%)	25	61
10	SD	221/240 (92%)	196 (89%)	24 (11%)	1 (0%)	25	61
11	SE	258/261 (99%)	234 (91%)	24 (9%)	0	100	100
12	SF	204/225 (91%)	181 (89%)	22 (11%)	1 (0%)	25	61
13	SG	216/236 (92%)	204 (94%)	12 (6%)	0	100	100
14	SH	183/190 (96%)	157 (86%)	24 (13%)	2 (1%)	12	44
15	SI	184/200 (92%)	176 (96%)	8 (4%)	0	100	100
16	SJ	183/197 (93%)	168 (92%)	15 (8%)	0	100	100
17	SK	90/105 (86%)	78 (87%)	7 (8%)	5 (6%)	1	8
18	SL	144/156 (92%)	133 (92%)	11 (8%)	0	100	100
19	SM	122/143 (85%)	86 (70%)	36 (30%)	0	100	100
20	SN	148/151 (98%)	137 (93%)	11 (7%)	0	100	100
21	SO	126/137 (92%)	107 (85%)	19 (15%)	0	100	100
22	SP	117/142 (82%)	99 (85%)	17 (14%)	1 (1%)	14	49
23	SQ	139/143 (97%)	119 (86%)	19 (14%)	1 (1%)	19	54
24	SR	111/136 (82%)	100 (90%)	11 (10%)	0	100	100
25	SS	143/146 (98%)	127 (89%)	16 (11%)	0	100	100
26	ST	141/144 (98%)	134 (95%)	7 (5%)	0	100	100
27	SU	99/121 (82%)	92 (93%)	7 (7%)	0	100	100
28	SV	85/87 (98%)	76 (89%)	9 (11%)	0	100	100
29	SW	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
30	SX	142/145 (98%)	131 (92%)	11 (8%)	0	100	100
31	SY	132/135 (98%)	117 (89%)	13 (10%)	2 (2%)	8	36
32	SZ	67/108 (62%)	63 (94%)	4 (6%)	0	100	100
33	Sa	95/119 (80%)	81 (85%)	14 (15%)	0	100	100
34	Sb	79/82 (96%)	69 (87%)	10 (13%)	0	100	100
35	Sc	61/67 (91%)	59 (97%)	2 (3%)	0	100	100
36	Sd	51/56 (91%)	49 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	Se	58/63 (92%)	52 (90%)	6 (10%)	0	100	100
38	Sf	31/152 (20%)	25 (81%)	5 (16%)	1 (3%)	3	19
39	Sg	311/319 (98%)	277 (89%)	34 (11%)	0	100	100
40	LA	250/254 (98%)	224 (90%)	26 (10%)	0	100	100
41	LB	384/387 (99%)	367 (96%)	17 (4%)	0	100	100
42	LC	359/362 (99%)	325 (90%)	33 (9%)	1 (0%)	37	70
43	LD	292/297 (98%)	276 (94%)	16 (6%)	0	100	100
44	LE	153/176 (87%)	139 (91%)	14 (9%)	0	100	100
45	LF	221/244 (91%)	217 (98%)	4 (2%)	0	100	100
46	LG	229/256 (90%)	206 (90%)	23 (10%)	0	100	100
47	LH	188/191 (98%)	179 (95%)	9 (5%)	0	100	100
48	LI	205/221 (93%)	194 (95%)	11 (5%)	0	100	100
49	LJ	167/174 (96%)	147 (88%)	18 (11%)	2 (1%)	11	41
50	LK	156/165 (94%)	137 (88%)	16 (10%)	3 (2%)	6	31
51	LL	192/199 (96%)	173 (90%)	15 (8%)	4 (2%)	5	28
52	LM	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
53	LN	201/204 (98%)	192 (96%)	9 (4%)	0	100	100
54	LO	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
55	LP	171/184 (93%)	167 (98%)	4 (2%)	0	100	100
56	LQ	183/186 (98%)	175 (96%)	8 (4%)	0	100	100
57	LR	172/189 (91%)	167 (97%)	5 (3%)	0	100	100
58	LS	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
59	LT	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
60	LU	96/121 (79%)	93 (97%)	3 (3%)	0	100	100
61	LV	132/137 (96%)	129 (98%)	3 (2%)	0	100	100
62	LW	61/155 (39%)	59 (97%)	2 (3%)	0	100	100
63	LX	118/142 (83%)	108 (92%)	10 (8%)	0	100	100
64	LY	122/127 (96%)	119 (98%)	3 (2%)	0	100	100
65	LZ	133/136 (98%)	121 (91%)	12 (9%)	0	100	100
66	La	146/149 (98%)	125 (86%)	19 (13%)	2 (1%)	9	37
67	Lb	56/59 (95%)	48 (86%)	8 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	Lc	98/105 (93%)	94 (96%)	4 (4%)	0	100	100
69	Ld	107/113 (95%)	101 (94%)	6 (6%)	0	100	100
70	Le	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
71	Lf	104/107 (97%)	97 (93%)	7 (7%)	0	100	100
72	Lg	110/121 (91%)	106 (96%)	4 (4%)	0	100	100
73	Lh	117/120 (98%)	109 (93%)	8 (7%)	0	100	100
74	Li	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
75	Lj	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
76	Lk	75/78 (96%)	71 (95%)	3 (4%)	1 (1%)	10	39
77	Ll	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
78	Lm	50/128 (39%)	50 (100%)	0	0	100	100
79	L2	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
79	Ln	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
80	Lo	103/106 (97%)	99 (96%)	4 (4%)	0	100	100
81	Lp	89/92 (97%)	82 (92%)	7 (8%)	0	100	100
82	L1	202/217 (93%)	149 (74%)	53 (26%)	0	100	100
83	P0	201/312 (64%)	184 (92%)	16 (8%)	1 (0%)	25	61
84	CN	110/560 (20%)	104 (94%)	6 (6%)	0	100	100
All	All	11507/13159 (87%)	10583 (92%)	894 (8%)	30 (0%)	38	70

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	SK	81	ASN
31	SY	32	ARG
49	LJ	95	ASN
51	LL	48	PRO
14	SH	30	SER
17	SK	88	PRO
22	SP	126	VAL
23	SQ	116	LEU
31	SY	52	LYS
50	LK	58	VAL
66	La	48	TYR
38	Sf	135	HIS
49	LJ	94	ARG

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Mol	Chain	Res	Type
51	LL	76	THR
51	LL	77	LEU
7	SA	30	GLN
14	SH	74	GLN
17	SK	54	TYR
50	LK	134	GLY
10	SD	91	VAL
17	SK	3	MET
51	LL	47	ALA
83	P0	38	MET
12	SF	100	ASN
17	SK	30	ALA
42	LC	339	LEU
76	Lk	17	ARG
9	SC	235	LEU
50	LK	140	GLY
66	La	18	GLY

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	
7	SA	165/210 (79%)	165 (100%)	0	100	100
8	SB	192/224 (86%)	191 (100%)	1 (0%)	86	94
9	SC	176/205 (86%)	176 (100%)	0	100	100
10	SD	182/195 (93%)	178 (98%)	4 (2%)	47	76
11	SE	221/222 (100%)	221 (100%)	0	100	100
12	SF	173/191 (91%)	172 (99%)	1 (1%)	84	93
13	SG	187/201 (93%)	186 (100%)	1 (0%)	86	94
14	SH	165/170 (97%)	157 (95%)	8 (5%)	21	55
15	SI	150/161 (93%)	148 (99%)	2 (1%)	65	85
16	SJ	158/166 (95%)	156 (99%)	2 (1%)	65	85
17	SK	73/98 (74%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	SL	129/137 (94%)	128 (99%)	1 (1%)	79	90
19	SM	88/119 (74%)	87 (99%)	1 (1%)	70	87
20	SN	127/128 (99%)	127 (100%)	0	100	100
21	SO	97/105 (92%)	97 (100%)	0	100	100
22	SP	98/118 (83%)	93 (95%)	5 (5%)	20	53
23	SQ	117/119 (98%)	109 (93%)	8 (7%)	13	42
24	SR	92/124 (74%)	91 (99%)	1 (1%)	70	87
25	SS	128/129 (99%)	126 (98%)	2 (2%)	58	82
26	ST	115/116 (99%)	115 (100%)	0	100	100
27	SU	94/114 (82%)	94 (100%)	0	100	100
28	SV	74/74 (100%)	74 (100%)	0	100	100
29	SW	110/111 (99%)	108 (98%)	2 (2%)	54	80
30	SX	119/120 (99%)	118 (99%)	1 (1%)	79	90
31	SY	112/113 (99%)	112 (100%)	0	100	100
32	SZ	61/89 (68%)	60 (98%)	1 (2%)	58	82
33	Sa	83/100 (83%)	83 (100%)	0	100	100
34	Sb	70/71 (99%)	70 (100%)	0	100	100
35	Sc	56/60 (93%)	56 (100%)	0	100	100
36	Sd	47/49 (96%)	47 (100%)	0	100	100
37	Se	51/54 (94%)	51 (100%)	0	100	100
38	Sf	27/135 (20%)	24 (89%)	3 (11%)	5	21
39	Sg	255/262 (97%)	251 (98%)	4 (2%)	58	82
40	LA	192/196 (98%)	192 (100%)	0	100	100
41	LB	318/323 (98%)	316 (99%)	2 (1%)	84	93
42	LC	288/289 (100%)	287 (100%)	1 (0%)	91	96
43	LD	243/245 (99%)	242 (100%)	1 (0%)	89	95
44	LE	135/153 (88%)	134 (99%)	1 (1%)	81	91
45	LF	187/205 (91%)	187 (100%)	0	100	100
46	LG	177/208 (85%)	176 (99%)	1 (1%)	84	93
47	LH	170/171 (99%)	170 (100%)	0	100	100
48	LI	177/187 (95%)	176 (99%)	1 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	LJ	147/150 (98%)	139 (95%)	8 (5%)	18	50
51	LL	154/159 (97%)	153 (99%)	1 (1%)	84	93
52	LM	108/109 (99%)	108 (100%)	0	100	100
53	LN	175/176 (99%)	175 (100%)	0	100	100
54	LO	160/162 (99%)	159 (99%)	1 (1%)	84	93
55	LP	139/146 (95%)	138 (99%)	1 (1%)	81	91
56	LQ	150/151 (99%)	149 (99%)	1 (1%)	81	91
57	LR	133/154 (86%)	133 (100%)	0	100	100
58	LS	156/156 (100%)	155 (99%)	1 (1%)	84	93
59	LT	136/137 (99%)	134 (98%)	2 (2%)	60	83
60	LU	85/107 (79%)	85 (100%)	0	100	100
61	LV	103/105 (98%)	103 (100%)	0	100	100
62	LW	55/129 (43%)	55 (100%)	0	100	100
63	LX	104/118 (88%)	103 (99%)	1 (1%)	73	88
64	LY	107/110 (97%)	107 (100%)	0	100	100
65	LZ	115/116 (99%)	114 (99%)	1 (1%)	75	89
66	La	118/119 (99%)	118 (100%)	0	100	100
67	Lb	46/47 (98%)	46 (100%)	0	100	100
68	Lc	84/88 (96%)	84 (100%)	0	100	100
69	Ld	94/97 (97%)	94 (100%)	0	100	100
70	Le	109/111 (98%)	109 (100%)	0	100	100
71	Lf	90/91 (99%)	90 (100%)	0	100	100
72	Lg	95/103 (92%)	91 (96%)	4 (4%)	25	59
73	Lh	103/105 (98%)	103 (100%)	0	100	100
74	Li	80/82 (98%)	79 (99%)	1 (1%)	65	85
75	Lj	67/71 (94%)	67 (100%)	0	100	100
76	Lk	67/69 (97%)	67 (100%)	0	100	100
77	Ll	45/46 (98%)	45 (100%)	0	100	100
78	Lm	47/116 (40%)	47 (100%)	0	100	100
79	L2	23/23 (100%)	23 (100%)	0	100	100
79	Ln	23/23 (100%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
80	Lo	90/91 (99%)	90 (100%)	0	100	100
81	Lp	71/72 (99%)	70 (99%)	1 (1%)	62	83
84	CN	109/533 (20%)	109 (100%)	0	100	100
All	All	9267/10539 (88%)	9189 (99%)	78 (1%)	77	90

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	SB	152	ARG
10	SD	143	ARG
10	SD	146	ARG
10	SD	148	LYS
10	SD	196	ARG
12	SF	203	LYS
13	SG	79	LYS
14	SH	7	LYS
14	SH	28	GLU
14	SH	35	LYS
14	SH	37	GLU
14	SH	39	ARG
14	SH	77	LEU
14	SH	79	ARG
14	SH	83	LYS
15	SI	12	SER
15	SI	141	ARG
16	SJ	23	ARG
16	SJ	154	LYS
18	SL	67	ARG
19	SM	85	LYS
22	SP	18	ARG
22	SP	20	VAL
22	SP	21	ASP
22	SP	35	LYS
22	SP	36	LEU
23	SQ	36	ILE
23	SQ	42	GLU
23	SQ	47	LYS
23	SQ	53	LEU
23	SQ	58	ASP
23	SQ	79	TYR
23	SQ	116	LEU

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Mol	Chain	Res	Type
23	SQ	118	ILE
24	SR	81	LYS
25	SS	56	LYS
25	SS	89	GLN
29	SW	55	ASP
29	SW	57	ARG
30	SX	114	LYS
32	SZ	90	LYS
38	Sf	132	LEU
38	Sf	134	ASN
38	Sf	143	LYS
39	Sg	51	ASP
39	Sg	312	VAL
39	Sg	314	GLN
39	Sg	316	MET
41	LB	331	ASN
41	LB	332	ARG
42	LC	197	ARG
43	LD	35	ARG
44	LE	100	LYS
46	LG	213	LYS
48	LI	156	ARG
49	LJ	9	MET
49	LJ	10	ARG
49	LJ	11	ASP
49	LJ	13	LYS
49	LJ	131	MET
49	LJ	153	LYS
49	LJ	154	THR
49	LJ	163	PHE
51	LL	194	GLU
54	LO	56	ASP
55	LP	171	ARG
56	LQ	182	LYS
58	LS	57	GLU
59	LT	83	ARG
59	LT	139	ARG
63	LX	85	GLN
65	LZ	93	LYS
72	Lg	44	CYS
72	Lg	47	CYS
72	Lg	79	SER

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Mol	Chain	Res	Type
72	Lg	87	GLU
74	Li	36	ARG
81	Lp	17	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
12	SF	116	HIS
13	SG	13	GLN
14	SH	29	ASN
16	SJ	112	GLN
17	SK	9	ASN
23	SQ	83	GLN
24	SR	83	GLN
31	SY	22	GLN
33	Sa	25	ASN
35	Sc	27	GLN
35	Sc	43	ASN
38	Sf	135	HIS
59	LT	134	GLN
63	LX	85	GLN
71	Lf	88	ASN
84	CN	41	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C2	1768/1800 (98%)	471 (26%)	39 (2%)
2	C7	2/3 (66%)	0	0
3	C5	74/75 (98%)	13 (17%)	0
4	C1	3201/3396 (94%)	632 (19%)	38 (1%)
5	C4	120/121 (99%)	11 (9%)	1 (0%)
6	C3	157/158 (99%)	28 (17%)	1 (0%)
All	All	5322/5553 (95%)	1155 (21%)	79 (1%)

All (1155) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C2	2	A
1	C2	4	C

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Mol	Chain	Res	Type
1	C2	17	C
1	C2	25	C
1	C2	26	A
1	C2	34	G
1	C2	42	G
1	C2	43	A
1	C2	45	U
1	C2	47	A
1	C2	56	U
1	C2	57	G
1	C2	61	A
1	C2	62	A
1	C2	63	G
1	C2	65	A
1	C2	67	A
1	C2	68	A
1	C2	69	G
1	C2	71	A
1	C2	73	U
1	C2	74	U
1	C2	75	U
1	C2	76	A
1	C2	78	A
1	C2	79	C
1	C2	81	G
1	C2	100	A
1	C2	104	A
1	C2	114	C
1	C2	115	G
1	C2	116	U
1	C2	126	A
1	C2	127	G
1	C2	129	U
1	C2	130	C
1	C2	131	C
1	C2	133	U
1	C2	134	U
1	C2	135	A
1	C2	138	A
1	C2	140	A
1	C2	141	U
1	C2	142	G

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Mol	Chain	Res	Type
1	C2	145	A
1	C2	155	U
1	C2	159	U
1	C2	168	A
1	C2	171	A
1	C2	176	C
1	C2	178	U
1	C2	179	A
1	C2	180	A
1	C2	188	A
1	C2	191	C
1	C2	192	U
1	C2	193	U
1	C2	194	U
1	C2	195	G
1	C2	198	A
1	C2	216	U
1	C2	217	A
1	C2	218	A
1	C2	223	U
1	C2	224	C
1	C2	225	A
1	C2	227	U
1	C2	228	G
1	C2	230	C
1	C2	232	U
1	C2	233	C
1	C2	234	G
1	C2	235	G
1	C2	236	A
1	C2	240	U
1	C2	241	U
1	C2	249	U
1	C2	250	C
1	C2	257	A
1	C2	260	U
1	C2	265	A
1	C2	272	U
1	C2	274	G
1	C2	276	C
1	C2	277	U
1	C2	278	U

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Mol	Chain	Res	Type
1	C2	279	G
1	C2	280	U
1	C2	281	G
1	C2	287	G
1	C2	299	A
1	C2	314	C
1	C2	316	A
1	C2	321	C
1	C2	322	G
1	C2	323	A
1	C2	330	G
1	C2	333	A
1	C2	337	G
1	C2	338	C
1	C2	352	A
1	C2	353	A
1	C2	359	A
1	C2	361	C
1	C2	370	A
1	C2	373	G
1	C2	388	G
1	C2	390	G
1	C2	400	A
1	C2	401	A
1	C2	402	C
1	C2	404	G
1	C2	416	A
1	C2	417	A
1	C2	419	G
1	C2	422	G
1	C2	423	G
1	C2	424	C
1	C2	425	A
1	C2	426	G
1	C2	434	G
1	C2	436	A
1	C2	439	U
1	C2	444	C
1	C2	446	A
1	C2	448	C
1	C2	452	A
1	C2	454	U

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Mol	Chain	Res	Type
1	C2	460	A
1	C2	468	A
1	C2	471	A
1	C2	477	A
1	C2	482	U
1	C2	483	A
1	C2	485	A
1	C2	487	G
1	C2	489	C
1	C2	491	C
1	C2	492	A
1	C2	493	U
1	C2	494	U
1	C2	496	G
1	C2	498	G
1	C2	499	U
1	C2	500	C
1	C2	502	U
1	C2	505	A
1	C2	506	A
1	C2	507	U
1	C2	510	G
1	C2	511	A
1	C2	517	U
1	C2	527	A
1	C2	534	A
1	C2	538	A
1	C2	539	G
1	C2	540	G
1	C2	541	A
1	C2	542	A
1	C2	544	A
1	C2	555	A
1	C2	556	A
1	C2	558	U
1	C2	565	C
1	C2	568	G
1	C2	572	C
1	C2	579	A
1	C2	580	A
1	C2	582	U
1	C2	594	A

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Mol	Chain	Res	Type
1	C2	595	G
1	C2	606	A
1	C2	610	G
1	C2	611	U
1	C2	617	U
1	C2	619	A
1	C2	620	A
1	C2	621	A
1	C2	622	A
1	C2	623	A
1	C2	624	G
1	C2	638	U
1	C2	639	U
1	C2	640	U
1	C2	641	G
1	C2	643	G
1	C2	648	G
1	C2	653	C
1	C2	654	C
1	C2	655	G
1	C2	678	A
1	C2	680	U
1	C2	681	U
1	C2	682	C
1	C2	683	C
1	C2	687	G
1	C2	693	U
1	C2	694	U
1	C2	696	C
1	C2	698	U
1	C2	700	C
1	C2	702	G
1	C2	703	G
1	C2	704	C
1	C2	705	U
1	C2	706	A
1	C2	707	A
1	C2	708	C
1	C2	709	C
1	C2	710	U
1	C2	711	U
1	C2	712	G

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Mol	Chain	Res	Type
1	C2	713	A
1	C2	714	G
1	C2	728	U
1	C2	729	G
1	C2	730	G
1	C2	731	C
1	C2	732	G
1	C2	733	A
1	C2	734	A
1	C2	736	C
1	C2	737	A
1	C2	738	G
1	C2	739	G
1	C2	741	C
1	C2	742	U
1	C2	743	U
1	C2	745	U
1	C2	756	A
1	C2	765	G
1	C2	766	U
1	C2	767	U
1	C2	774	A
1	C2	775	G
1	C2	778	G
1	C2	779	U
1	C2	780	A
1	C2	781	U
1	C2	782	U
1	C2	783	G
1	C2	787	G
1	C2	789	A
1	C2	812	A
1	C2	813	U
1	C2	814	A
1	C2	815	G
1	C2	819	G
1	C2	820	U
1	C2	821	U
1	C2	823	G
1	C2	833	U
1	C2	835	U
1	C2	840	U

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Mol	Chain	Res	Type
1	C2	841	U
1	C2	846	G
1	C2	851	U
1	C2	852	C
1	C2	855	A
1	C2	856	A
1	C2	857	U
1	C2	860	U
1	C2	863	A
1	C2	873	U
1	C2	899	G
1	C2	901	G
1	C2	902	G
1	C2	903	U
1	C2	912	U
1	C2	913	G
1	C2	929	A
1	C2	933	A
1	C2	934	C
1	C2	935	U
1	C2	942	G
1	C2	951	A
1	C2	960	U
1	C2	966	A
1	C2	970	A
1	C2	988	A
1	C2	992	A
1	C2	993	A
1	C2	998	A
1	C2	1003	A
1	C2	1004	U
1	C2	1005	A
1	C2	1020	A
1	C2	1021	C
1	C2	1023	A
1	C2	1024	U
1	C2	1026	A
1	C2	1028	C
1	C2	1039	A
1	C2	1052	U
1	C2	1053	G
1	C2	1058	U

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Mol	Chain	Res	Type
1	C2	1059	U
1	C2	1060	U
1	C2	1061	A
1	C2	1063	U
1	C2	1076	A
1	C2	1080	U
1	C2	1081	A
1	C2	1082	C
1	C2	1092	A
1	C2	1093	A
1	C2	1096	C
1	C2	1098	U
1	C2	1100	G
1	C2	1138	A
1	C2	1147	A
1	C2	1150	G
1	C2	1158	C
1	C2	1160	A
1	C2	1164	G
1	C2	1167	G
1	C2	1170	G
1	C2	1185	U
1	C2	1191	U
1	C2	1194	A
1	C2	1196	A
1	C2	1199	G
1	C2	1200	G
1	C2	1202	A
1	C2	1207	C
1	C2	1217	A
1	C2	1218	G
1	C2	1227	A
1	C2	1228	G
1	C2	1229	G
1	C2	1235	C
1	C2	1241	G
1	C2	1243	G
1	C2	1244	A
1	C2	1245	G
1	C2	1246	C
1	C2	1251	U
1	C2	1252	C

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Mol	Chain	Res	Type
1	C2	1256	A
1	C2	1257	U
1	C2	1274	C
1	C2	1275	A
1	C2	1276	U
1	C2	1285	U
1	C2	1286	U
1	C2	1291	G
1	C2	1301	U
1	C2	1314	U
1	C2	1315	U
1	C2	1316	G
1	C2	1318	G
1	C2	1321	A
1	C2	1322	A
1	C2	1325	A
1	C2	1337	A
1	C2	1344	A
1	C2	1345	A
1	C2	1346	A
1	C2	1348	A
1	C2	1349	G
1	C2	1354	G
1	C2	1361	U
1	C2	1363	U
1	C2	1364	G
1	C2	1367	G
1	C2	1370	U
1	C2	1371	A
1	C2	1372	U
1	C2	1373	C
1	C2	1382	A
1	C2	1383	G
1	C2	1389	C
1	C2	1390	U
1	C2	1398	U
1	C2	1399	C
1	C2	1400	A
1	C2	1402	G
1	C2	1414	U
1	C2	1415	U
1	C2	1425	A

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Mol	Chain	Res	Type
1	C2	1427	A
1	C2	1431	C
1	C2	1432	U
1	C2	1433	G
1	C2	1436	A
1	C2	1446	A
1	C2	1459	C
1	C2	1460	A
1	C2	1466	G
1	C2	1469	A
1	C2	1470	C
1	C2	1471	A
1	C2	1472	C
1	C2	1479	A
1	C2	1486	G
1	C2	1491	U
1	C2	1492	A
1	C2	1493	A
1	C2	1496	U
1	C2	1503	A
1	C2	1506	G
1	C2	1514	U
1	C2	1516	A
1	C2	1517	U
1	C2	1518	C
1	C2	1521	G
1	C2	1523	G
1	C2	1524	A
1	C2	1531	G
1	C2	1535	U
1	C2	1537	C
1	C2	1540	G
1	C2	1542	G
1	C2	1543	A
1	C2	1554	U
1	C2	1557	U
1	C2	1558	U
1	C2	1559	A
1	C2	1570	A
1	C2	1572	G
1	C2	1573	A
1	C2	1574	G

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Mol	Chain	Res	Type
1	C2	1576	A
1	C2	1577	A
1	C2	1583	A
1	C2	1584	G
1	C2	1585	U
1	C2	1590	G
1	C2	1601	G
1	C2	1610	G
1	C2	1611	A
1	C2	1614	A
1	C2	1616	G
1	C2	1622	G
1	C2	1631	A
1	C2	1634	C
1	C2	1635	A
1	C2	1636	C
1	C2	1637	C
1	C2	1657	U
1	C2	1658	G
1	C2	1678	A
1	C2	1688	U
1	C2	1693	A
1	C2	1700	C
1	C2	1701	A
1	C2	1703	C
1	C2	1708	U
1	C2	1709	C
1	C2	1715	G
1	C2	1717	G
1	C2	1743	U
1	C2	1753	A
1	C2	1756	A
1	C2	1757	G
1	C2	1760	G
1	C2	1762	A
1	C2	1766	A
1	C2	1767	G
1	C2	1769	U
1	C2	1771	U
1	C2	1780	G
1	C2	1782	A
1	C2	1783	C

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Mol	Chain	Res	Type
1	C2	1791	A
1	C2	1792	G
1	C2	1793	G
1	C2	1794	A
1	C2	1796	C
1	C2	1798	U
1	C2	1799	U
3	C5	13	C
3	C5	14	A
3	C5	16	H2U
3	C5	18	G
3	C5	20	A
3	C5	21	G
3	C5	45	7MG
3	C5	46	H2U
3	C5	47	5MC
3	C5	58	A
3	C5	62	G
3	C5	63	A
3	C5	75	A
4	C1	6	A
4	C1	13	A
4	C1	14	U
4	C1	26	A
4	C1	40	A
4	C1	43	A
4	C1	49	A
4	C1	59	G
4	C1	60	A
4	C1	65	A
4	C1	66	A
4	C1	67	A
4	C1	92	G
4	C1	109	A
4	C1	110	G
4	C1	111	C
4	C1	116	A
4	C1	120	G
4	C1	121	A
4	C1	122	A
4	C1	133	U
4	C1	134	U

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Mol	Chain	Res	Type
4	C1	135	C
4	C1	136	G
4	C1	150	A
4	C1	156	G
4	C1	157	A
4	C1	165	A
4	C1	166	C
4	C1	172	G
4	C1	173	G
4	C1	187	A
4	C1	190	U
4	C1	191	U
4	C1	200	C
4	C1	206	G
4	C1	210	U
4	C1	213	A
4	C1	218	G
4	C1	219	A
4	C1	234	G
4	C1	240	U
4	C1	241	G
4	C1	242	C
4	C1	243	G
4	C1	245	U
4	C1	249	U
4	C1	252	U
4	C1	269	G
4	C1	283	G
4	C1	286	U
4	C1	295	A
4	C1	305	U
4	C1	323	A
4	C1	329	U
4	C1	337	G
4	C1	339	C
4	C1	350	C
4	C1	374	A
4	C1	376	G
4	C1	390	G
4	C1	398	A
4	C1	399	A
4	C1	401	U

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Mol	Chain	Res	Type
4	C1	402	A
4	C1	403	C
4	C1	421	G
4	C1	422	A
4	C1	439	C
4	C1	440	A
4	C1	503	C
4	C1	517	G
4	C1	518	G
4	C1	521	A
4	C1	523	A
4	C1	535	G
4	C1	543	C
4	C1	544	C
4	C1	546	C
4	C1	547	G
4	C1	548	G
4	C1	551	A
4	C1	552	G
4	C1	555	U
4	C1	557	A
4	C1	558	U
4	C1	559	A
4	C1	578	A
4	C1	579	G
4	C1	589	A
4	C1	597	G
4	C1	600	G
4	C1	604	G
4	C1	609	G
4	C1	611	A
4	C1	620	U
4	C1	621	A
4	C1	622	A
4	C1	637	C
4	C1	638	C
4	C1	649	A
4	C1	660	A
4	C1	662	U
4	C1	667	C
4	C1	677	A
4	C1	681	U

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Mol	Chain	Res	Type
4	C1	690	A
4	C1	705	A
4	C1	712	G
4	C1	715	A
4	C1	716	A
4	C1	719	U
4	C1	738	A
4	C1	758	C
4	C1	763	G
4	C1	764	U
4	C1	765	C
4	C1	766	U
4	C1	767	U
4	C1	776	U
4	C1	777	U
4	C1	780	A
4	C1	781	G
4	C1	785	G
4	C1	786	A
4	C1	798	G
4	C1	801	A
4	C1	806	A
4	C1	808	A
4	C1	817	A
4	C1	830	A
4	C1	848	A
4	C1	849	C
4	C1	850	U
4	C1	861	C
4	C1	865	U
4	C1	874	U
4	C1	879	U
4	C1	896	A
4	C1	907	G
4	C1	908	G
4	C1	909	G
4	C1	914	A
4	C1	916	G
4	C1	917	A
4	C1	921	A
4	C1	923	C
4	C1	924	G

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Mol	Chain	Res	Type
4	C1	925	A
4	C1	933	A
4	C1	937	G
4	C1	944	C
4	C1	959	C
4	C1	960	U
4	C1	974	G
4	C1	979	U
4	C1	984	G
4	C1	991	G
4	C1	1000	C
4	C1	1001	G
4	C1	1002	A
4	C1	1010	G
4	C1	1013	G
4	C1	1015	U
4	C1	1017	C
4	C1	1018	G
4	C1	1020	G
4	C1	1024	G
4	C1	1028	U
4	C1	1029	G
4	C1	1036	A
4	C1	1037	C
4	C1	1041	U
4	C1	1047	A
4	C1	1049	C
4	C1	1063	G
4	C1	1064	A
4	C1	1065	A
4	C1	1072	G
4	C1	1081	U
4	C1	1083	G
4	C1	1087	G
4	C1	1093	A
4	C1	1094	U
4	C1	1095	U
4	C1	1096	U
4	C1	1097	G
4	C1	1098	A
4	C1	1103	A
4	C1	1104	G

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Mol	Chain	Res	Type
4	C1	1117	G
4	C1	1131	G
4	C1	1143	A
4	C1	1144	U
4	C1	1153	A
4	C1	1155	C
4	C1	1159	A
4	C1	1178	G
4	C1	1180	A
4	C1	1181	U
4	C1	1192	C
4	C1	1193	A
4	C1	1196	C
4	C1	1197	A
4	C1	1201	C
4	C1	1202	A
4	C1	1208	U
4	C1	1217	A
4	C1	1222	G
4	C1	1223	A
4	C1	1227	C
4	C1	1230	G
4	C1	1231	A
4	C1	1232	C
4	C1	1233	G
4	C1	1234	G
4	C1	1236	G
4	C1	1237	G
4	C1	1238	C
4	C1	1240	A
4	C1	1241	U
4	C1	1242	G
4	C1	1244	A
4	C1	1245	A
4	C1	1246	G
4	C1	1248	C
4	C1	1251	A
4	C1	1252	A
4	C1	1253	U
4	C1	1254	C
4	C1	1256	G
4	C1	1257	C

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Mol	Chain	Res	Type
4	C1	1258	U
4	C1	1259	A
4	C1	1260	A
4	C1	1261	G
4	C1	1262	G
4	C1	1263	A
4	C1	1264	G
4	C1	1267	U
4	C1	1269	U
4	C1	1270	A
4	C1	1271	A
4	C1	1272	C
4	C1	1273	A
4	C1	1274	A
4	C1	1275	C
4	C1	1278	A
4	C1	1279	C
4	C1	1280	C
4	C1	1282	G
4	C1	1283	C
4	C1	1285	G
4	C1	1286	A
4	C1	1287	A
4	C1	1305	U
4	C1	1307	G
4	C1	1308	A
4	C1	1309	U
4	C1	1313	G
4	C1	1325	U
4	C1	1330	A
4	C1	1332	A
4	C1	1348	U
4	C1	1349	G
4	C1	1351	U
4	C1	1352	A
4	C1	1355	A
4	C1	1356	U
4	C1	1357	G
4	C1	1386	A
4	C1	1392	G
4	C1	1399	A
4	C1	1400	G

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Mol	Chain	Res	Type
4	C1	1418	A
4	C1	1419	A
4	C1	1434	G
4	C1	1435	A
4	C1	1437	C
4	C1	1443	G
4	C1	1446	A
4	C1	1450	G
4	C1	1477	A
4	C1	1481	A
4	C1	1483	G
4	C1	1487	G
4	C1	1488	G
4	C1	1496	C
4	C1	1502	C
4	C1	1508	C
4	C1	1536	G
4	C1	1539	A
4	C1	1555	U
4	C1	1556	C
4	C1	1557	A
4	C1	1560	G
4	C1	1562	C
4	C1	1563	C
4	C1	1566	A
4	C1	1568	U
4	C1	1569	U
4	C1	1572	U
4	C1	1573	G
4	C1	1575	A
4	C1	1576	G
4	C1	1580	A
4	C1	1581	C
4	C1	1582	C
4	C1	1583	A
4	C1	1587	A
4	C1	1590	G
4	C1	1593	A
4	C1	1605	A
4	C1	1607	U
4	C1	1619	A
4	C1	1620	U

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Mol	Chain	Res	Type
4	C1	1629	U
4	C1	1639	C
4	C1	1642	A
4	C1	1643	A
4	C1	1645	U
4	C1	1657	C
4	C1	1683	A
4	C1	1716	U
4	C1	1717	U
4	C1	1724	U
4	C1	1725	C
4	C1	1736	G
4	C1	1741	A
4	C1	1750	A
4	C1	1751	G
4	C1	1760	A
4	C1	1761	C
4	C1	1765	U
4	C1	1766	G
4	C1	1770	G
4	C1	1775	G
4	C1	1778	G
4	C1	1780	G
4	C1	1794	G
4	C1	1797	A
4	C1	1808	G
4	C1	1814	A
4	C1	1816	A
4	C1	1819	U
4	C1	1820	U
4	C1	1821	U
4	C1	1835	A
4	C1	1839	A
4	C1	1840	U
4	C1	1841	A
4	C1	1842	A
4	C1	1846	C
4	C1	1849	C
4	C1	1866	C
4	C1	1867	A
4	C1	1879	A
4	C1	1880	U

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Mol	Chain	Res	Type
4	C1	1881	A
4	C1	1893	A
4	C1	1906	G
4	C1	1952	G
4	C1	1953	G
4	C1	1954	G
4	C1	2094	C
4	C1	2102	U
4	C1	2111	G
4	C1	2112	U
4	C1	2113	A
4	C1	2114	C
4	C1	2121	G
4	C1	2122	G
4	C1	2131	A
4	C1	2140	U
4	C1	2144	A
4	C1	2158	A
4	C1	2169	G
4	C1	2171	G
4	C1	2176	U
4	C1	2188	A
4	C1	2201	G
4	C1	2205	U
4	C1	2206	G
4	C1	2207	A
4	C1	2208	A
4	C1	2209	U
4	C1	2210	G
4	C1	2223	A
4	C1	2225	U
4	C1	2228	A
4	C1	2235	C
4	C1	2249	G
4	C1	2250	G
4	C1	2255	A
4	C1	2256	A
4	C1	2257	C
4	C1	2272	G
4	C1	2273	G
4	C1	2281	A
4	C1	2282	U

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Mol	Chain	Res	Type
4	C1	2288	G
4	C1	2307	G
4	C1	2310	U
4	C1	2313	A
4	C1	2314	U
4	C1	2315	G
4	C1	2334	U
4	C1	2335	G
4	C1	2336	U
4	C1	2372	A
4	C1	2373	A
4	C1	2374	C
4	C1	2375	G
4	C1	2385	G
4	C1	2388	U
4	C1	2393	G
4	C1	2397	A
4	C1	2398	A
4	C1	2402	A
4	C1	2403	G
4	C1	2404	A
4	C1	2411	U
4	C1	2419	A
4	C1	2435	G
4	C1	2437	G
4	C1	2439	A
4	C1	2443	A
4	C1	2445	A
4	C1	2450	G
4	C1	2453	U
4	C1	2454	G
4	C1	2455	U
4	C1	2456	A
4	C1	2457	G
4	C1	2458	A
4	C1	2459	A
4	C1	2460	U
4	C1	2461	A
4	C1	2463	G
4	C1	2467	G
4	C1	2468	A
4	C1	2472	U

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Mol	Chain	Res	Type
4	C1	2474	G
4	C1	2475	G
4	C1	2477	G
4	C1	2479	C
4	C1	2480	A
4	C1	2486	A
4	C1	2487	U
4	C1	2490	C
4	C1	2491	A
4	C1	2493	U
4	C1	2495	C
4	C1	2497	U
4	C1	2498	U
4	C1	2499	U
4	C1	2501	U
4	C1	2503	G
4	C1	2505	U
4	C1	2506	U
4	C1	2514	U
4	C1	2515	A
4	C1	2526	C
4	C1	2530	G
4	C1	2537	U
4	C1	2538	U
4	C1	2539	C
4	C1	2540	A
4	C1	2541	U
4	C1	2542	U
4	C1	2543	U
4	C1	2544	U
4	C1	2547	A
4	C1	2548	C
4	C1	2549	G
4	C1	2552	C
4	C1	2554	A
4	C1	2555	G
4	C1	2561	A
4	C1	2569	A
4	C1	2570	U
4	C1	2571	U
4	C1	2572	C
4	C1	2573	G

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Mol	Chain	Res	Type
4	C1	2585	G
4	C1	2586	G
4	C1	2593	A
4	C1	2594	C
4	C1	2606	G
4	C1	2607	G
4	C1	2614	G
4	C1	2629	U
4	C1	2651	G
4	C1	2652	U
4	C1	2656	A
4	C1	2674	A
4	C1	2677	G
4	C1	2678	A
4	C1	2689	A
4	C1	2691	A
4	C1	2694	A
4	C1	2696	A
4	C1	2704	A
4	C1	2714	G
4	C1	2719	U
4	C1	2728	G
4	C1	2737	C
4	C1	2752	U
4	C1	2753	G
4	C1	2755	C
4	C1	2772	C
4	C1	2777	G
4	C1	2778	G
4	C1	2788	C
4	C1	2791	G
4	C1	2796	G
4	C1	2800	G
4	C1	2801	A
4	C1	2803	A
4	C1	2810	C
4	C1	2814	G
4	C1	2816	G
4	C1	2817	A
4	C1	2818	U
4	C1	2821	C
4	C1	2842	U

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Mol	Chain	Res	Type
4	C1	2844	C
4	C1	2845	A
4	C1	2849	C
4	C1	2859	U
4	C1	2860	U
4	C1	2867	C
4	C1	2871	G
4	C1	2872	A
4	C1	2875	U
4	C1	2876	C
4	C1	2887	A
4	C1	2898	G
4	C1	2899	C
4	C1	2911	A
4	C1	2923	U
4	C1	2933	A
4	C1	2935	U
4	C1	2936	A
4	C1	2942	C
4	C1	2947	G
4	C1	2957	G
4	C1	2971	A
4	C1	2981	U
4	C1	2983	C
4	C1	2984	C
4	C1	2996	U
4	C1	2997	G
4	C1	3003	G
4	C1	3012	A
4	C1	3056	U
4	C1	3059	G
4	C1	3078	U
4	C1	3079	U
4	C1	3086	A
4	C1	3092	C
4	C1	3101	G
4	C1	3104	U
4	C1	3109	G
4	C1	3119	U
4	C1	3122	A
4	C1	3130	A
4	C1	3131	U

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Mol	Chain	Res	Type
4	C1	3142	A
4	C1	3143	C
4	C1	3151	U
4	C1	3154	C
4	C1	3155	U
4	C1	3156	U
4	C1	3157	U
4	C1	3165	A
4	C1	3170	A
4	C1	3173	G
4	C1	3174	A
4	C1	3175	U
4	C1	3176	G
4	C1	3179	U
4	C1	3181	C
4	C1	3186	A
4	C1	3187	A
4	C1	3196	U
4	C1	3207	U
4	C1	3209	A
4	C1	3217	C
4	C1	3218	A
4	C1	3219	G
4	C1	3228	C
4	C1	3229	G
4	C1	3243	A
4	C1	3245	A
4	C1	3247	G
4	C1	3259	U
4	C1	3263	G
4	C1	3269	U
4	C1	3270	U
4	C1	3273	A
4	C1	3276	G
4	C1	3281	U
4	C1	3287	U
4	C1	3288	G
4	C1	3289	G
4	C1	3294	A
4	C1	3295	A
4	C1	3303	G
4	C1	3304	U

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Mol	Chain	Res	Type
4	C1	3307	A
4	C1	3313	U
4	C1	3316	A
4	C1	3317	U
4	C1	3318	G
4	C1	3319	U
4	C1	3320	A
4	C1	3335	A
4	C1	3341	U
4	C1	3345	G
4	C1	3351	U
4	C1	3352	U
4	C1	3353	G
4	C1	3354	U
4	C1	3355	U
4	C1	3356	G
4	C1	3369	G
4	C1	3375	A
4	C1	3378	C
4	C1	3382	U
4	C1	3389	U
4	C1	3390	G
5	C4	7	G
5	C4	29	C
5	C4	53	U
5	C4	54	U
5	C4	55	A
5	C4	65	G
5	C4	73	C
5	C4	74	C
5	C4	102	A
5	C4	112	G
5	C4	121	U
6	C3	23	U
6	C3	34	U
6	C3	35	C
6	C3	38	U
6	C3	48	A
6	C3	51	G
6	C3	59	A
6	C3	62	C
6	C3	63	G

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Mol	Chain	Res	Type
6	C3	80	A
6	C3	81	U
6	C3	82	U
6	C3	83	C
6	C3	85	G
6	C3	86	U
6	C3	87	G
6	C3	90	U
6	C3	95	G
6	C3	104	A
6	C3	106	C
6	C3	111	A
6	C3	113	U
6	C3	125	U
6	C3	126	A
6	C3	138	A
6	C3	151	C
6	C3	152	G
6	C3	158	U

All (79) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C2	68	A
1	C2	77	U
1	C2	139	C
1	C2	141	U
1	C2	224	C
1	C2	278	U
1	C2	280	U
1	C2	313	U
1	C2	322	G
1	C2	352	A
1	C2	387	A
1	C2	400	A
1	C2	539	G
1	C2	541	A
1	C2	555	A
1	C2	557	G
1	C2	609	U
1	C2	639	U
1	C2	640	U

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Mol	Chain	Res	Type
1	C2	705	U
1	C2	711	U
1	C2	755	A
1	C2	819	G
1	C2	912	U
1	C2	928	U
1	C2	1023	A
1	C2	1226	A
1	C2	1256	A
1	C2	1273	G
1	C2	1274	C
1	C2	1344	A
1	C2	1382	A
1	C2	1430	U
1	C2	1471	A
1	C2	1573	A
1	C2	1633	A
1	C2	1636	C
1	C2	1742	U
1	C2	1791	A
4	C1	13	A
4	C1	239	G
4	C1	282	G
4	C1	439	C
4	C1	715	A
4	C1	763	G
4	C1	849	C
4	C1	916	G
4	C1	1064	A
4	C1	1097	G
4	C1	1232	C
4	C1	1240	A
4	C1	1241	U
4	C1	1253	U
4	C1	1259	A
4	C1	1263	A
4	C1	1307	G
4	C1	1355	A
4	C1	1554	U
4	C1	1562	C
4	C1	1716	U
4	C1	1815	U

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Mol	Chain	Res	Type
4	C1	1820	U
4	C1	2112	U
4	C1	2249	G
4	C1	2504	U
4	C1	2505	U
4	C1	2525	G
4	C1	2537	U
4	C1	2541	U
4	C1	3078	U
4	C1	3121	U
4	C1	3218	A
4	C1	3228	C
4	C1	3269	U
4	C1	3316	A
4	C1	3319	U
4	C1	3350	C
5	C4	52	G
6	C3	85	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	H2U	C5	46	3	18,21,22	3.08	4 (22%)	21,30,33	1.92	5 (23%)
3	5MC	C5	47	3	18,22,23	3.52	7 (38%)	26,32,35	1.02	2 (7%)
3	7MG	C5	45	3	22,26,27	3.74	10 (45%)	29,39,42	1.95	9 (31%)
3	1MA	C5	57	3	16,25,26	4.01	4 (25%)	18,37,40	1.72	3 (16%)
3	2MG	C5	10	3	18,26,27	2.25	8 (44%)	16,38,41	1.44	4 (25%)
3	T6A	C5	36	85,3	27,34,35	2.40	9 (33%)	29,49,52	2.11	5 (17%)
3	1MG	C5	9	3	18,26,27	2.63	6 (33%)	19,39,42	1.44	3 (15%)
3	M2G	C5	25	3	20,27,28	3.47	8 (40%)	22,40,43	1.56	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	H2U	C5	16	3	18,21,22	2.99	5 (27%)	21,30,33	2.05	5 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H2U	C5	46	3	-	6/7/38/39	0/2/2/2
3	5MC	C5	47	3	-	2/7/25/26	0/2/2/2
3	7MG	C5	45	3	-	0/7/37/38	0/3/3/3
3	1MA	C5	57	3	-	0/3/25/26	0/3/3/3
3	2MG	C5	10	3	-	0/5/27/28	0/3/3/3
3	T6A	C5	36	85,3	-	1/19/41/42	0/3/3/3
3	1MG	C5	9	3	-	0/3/25/26	0/3/3/3
3	M2G	C5	25	3	-	0/7/29/30	0/3/3/3
3	H2U	C5	16	3	-	0/7/38/39	0/2/2/2

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C5	57	1MA	C2-N3	14.63	1.46	1.29
3	C5	25	M2G	C2-N3	11.17	1.44	1.30
3	C5	46	H2U	C2-N1	9.48	1.49	1.35
3	C5	45	7MG	C8-N9	9.23	1.51	1.46
3	C5	16	H2U	C2-N1	9.11	1.48	1.35
3	C5	47	5MC	C6-C5	9.01	1.49	1.34
3	C5	45	7MG	C5-N7	7.93	1.44	1.35
3	C5	46	H2U	C2-N3	6.55	1.49	1.38
3	C5	47	5MC	C4-N3	6.43	1.45	1.34
3	C5	16	H2U	C2-N3	6.39	1.49	1.38
3	C5	9	1MG	C2-N3	6.34	1.46	1.34
3	C5	36	T6A	C6-N6	6.24	1.47	1.36
3	C5	9	1MG	C2-N2	6.20	1.45	1.34
3	C5	47	5MC	C2-N3	5.99	1.48	1.36
3	C5	25	M2G	C2-N2	5.86	1.46	1.35
3	C5	45	7MG	C2-N3	5.70	1.46	1.33
3	C5	45	7MG	C4-N3	5.47	1.47	1.34
3	C5	36	T6A	C10-N11	5.44	1.47	1.35
3	C5	36	T6A	C10-N6	5.29	1.48	1.37
3	C5	10	2MG	C2-N2	5.28	1.45	1.33
3	C5	45	7MG	C4-N9	5.15	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C5	25	M2G	C4-N3	5.10	1.49	1.37
3	C5	16	H2U	C4-N3	5.07	1.46	1.37
3	C5	46	H2U	C4-N3	5.05	1.46	1.37
3	C5	9	1MG	C4-N3	4.85	1.49	1.37
3	C5	45	7MG	C2-N2	4.65	1.45	1.34
3	C5	57	1MA	C2-N1	4.50	1.44	1.35
3	C5	47	5MC	C6-N1	4.47	1.45	1.38
3	C5	47	5MC	C4-N4	4.35	1.45	1.34
3	C5	25	M2G	C6-N1	4.12	1.44	1.37
3	C5	47	5MC	C2-N1	4.06	1.48	1.40
3	C5	57	1MA	C4-N3	3.92	1.49	1.37
3	C5	10	2MG	C4-N3	3.81	1.46	1.37
3	C5	45	7MG	C2-N1	3.71	1.46	1.37
3	C5	10	2MG	C6-N1	3.65	1.43	1.37
3	C5	45	7MG	C5-C6	3.54	1.52	1.43
3	C5	10	2MG	C2-N1	3.43	1.42	1.36
3	C5	36	T6A	C12-N11	3.38	1.53	1.45
3	C5	36	T6A	ODA-C13	3.35	1.32	1.22
3	C5	45	7MG	C6-N1	3.33	1.45	1.38
3	C5	25	M2G	O6-C6	-3.27	1.16	1.23
3	C5	25	M2G	C2-N1	3.17	1.44	1.36
3	C5	25	M2G	C5-C4	-2.96	1.35	1.43
3	C5	36	T6A	O10-C10	-2.81	1.17	1.23
3	C5	36	T6A	C12-C13	-2.78	1.47	1.52
3	C5	47	5MC	O2-C2	-2.70	1.18	1.23
3	C5	9	1MG	C5-C4	-2.67	1.36	1.43
3	C5	45	7MG	O6-C6	-2.53	1.18	1.23
3	C5	10	2MG	CM2-N2	2.53	1.50	1.45
3	C5	25	M2G	C5-C6	2.52	1.52	1.47
3	C5	36	T6A	C5-C4	-2.42	1.34	1.40
3	C5	10	2MG	C5-C4	-2.41	1.36	1.43
3	C5	57	1MA	C5-C4	-2.36	1.37	1.43
3	C5	10	2MG	O6-C6	-2.30	1.18	1.23
3	C5	16	H2U	O2-C2	-2.21	1.19	1.23
3	C5	46	H2U	O2-C2	-2.18	1.19	1.23
3	C5	10	2MG	C5-C6	2.14	1.51	1.47
3	C5	36	T6A	C2-N3	2.10	1.35	1.32
3	C5	16	H2U	O4-C4	-2.09	1.19	1.23
3	C5	9	1MG	C6-N1	2.04	1.43	1.39
3	C5	9	1MG	O6-C6	-2.03	1.18	1.22

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C5	16	H2U	C4-N3-C2	-7.09	119.91	125.79
3	C5	46	H2U	C4-N3-C2	-6.29	120.57	125.79
3	C5	36	T6A	N6-C10-N11	6.15	122.35	113.76
3	C5	36	T6A	N3-C2-N1	-5.44	120.17	128.68
3	C5	45	7MG	C5-C6-N1	4.92	119.66	110.99
3	C5	57	1MA	N1-C2-N3	-4.84	120.37	126.02
3	C5	45	7MG	C2-N3-C4	4.35	120.06	112.30
3	C5	25	M2G	N1-C2-N2	4.06	121.49	118.04
3	C5	36	T6A	C2-N1-C6	4.02	120.04	116.59
3	C5	57	1MA	C5-C6-N1	4.00	119.86	113.90
3	C5	36	T6A	N6-C6-N1	3.97	124.04	118.72
3	C5	9	1MG	C5-C6-N1	3.92	119.80	113.90
3	C5	46	H2U	N3-C2-N1	3.83	120.70	116.65
3	C5	45	7MG	C5-C4-N3	-3.72	121.04	128.13
3	C5	47	5MC	C5-C6-N1	-3.50	119.73	123.34
3	C5	10	2MG	C5-C6-N1	3.46	120.06	113.95
3	C5	25	M2G	C5-C6-N1	3.44	120.02	113.95
3	C5	16	H2U	N3-C2-N1	3.30	120.14	116.65
3	C5	45	7MG	C5-C4-N9	3.17	110.46	106.35
3	C5	36	T6A	O10-C10-N6	-3.05	118.46	123.62
3	C5	16	H2U	C5-C4-N3	2.99	120.01	116.65
3	C5	45	7MG	C4-C5-N7	2.90	109.56	105.53
3	C5	25	M2G	C8-N7-C5	2.84	108.40	102.99
3	C5	10	2MG	C8-N7-C5	2.83	108.37	102.99
3	C5	46	H2U	C5-C6-N1	2.82	120.89	111.61
3	C5	9	1MG	C8-N7-C5	2.79	108.31	102.99
3	C5	57	1MA	C8-N7-C5	2.64	108.01	102.99
3	C5	45	7MG	C2-N1-C6	-2.56	120.43	125.10
3	C5	16	H2U	O2-C2-N1	-2.54	119.92	123.11
3	C5	16	H2U	C5-C6-N1	2.51	119.90	111.61
3	C5	25	M2G	C2-N1-C6	-2.47	119.61	123.71
3	C5	45	7MG	O6-C6-C5	-2.43	121.59	127.54
3	C5	46	H2U	C5-C4-N3	2.33	119.27	116.65
3	C5	9	1MG	O6-C6-C5	-2.27	120.17	124.19
3	C5	25	M2G	O6-C6-C5	-2.23	120.02	124.37
3	C5	45	7MG	N9-C8-N7	2.22	106.56	103.38
3	C5	10	2MG	O6-C6-C5	-2.22	120.03	124.37
3	C5	10	2MG	CM2-N2-C2	-2.14	119.14	123.86
3	C5	47	5MC	CM5-C5-C6	-2.05	120.11	122.85
3	C5	46	H2U	O2-C2-N1	-2.04	120.54	123.11
3	C5	45	7MG	N9-C4-N3	2.03	128.50	125.47

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C5	46	H2U	O4'-C4'-C5'-O5'
3	C5	46	H2U	C3'-C4'-C5'-O5'
3	C5	46	H2U	O4'-C1'-N1-C6
3	C5	46	H2U	C2'-C1'-N1-C2
3	C5	46	H2U	C2'-C1'-N1-C6
3	C5	47	5MC	O4'-C4'-C5'-O5'
3	C5	47	5MC	C3'-C4'-C5'-O5'
3	C5	46	H2U	O4'-C1'-N1-C2
3	C5	36	T6A	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 332 ligands modelled in this entry, 325 are monoatomic - leaving 7 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	T1C	C2	1990	-	44,45,45	1.20	4 (9%)	53,72,72	0.92	2 (3%)
86	T1C	C1	3403	85	44,45,45	1.22	4 (9%)	53,72,72	1.09	4 (7%)
86	T1C	C1	3401	-	44,45,45	1.18	4 (9%)	53,72,72	1.44	8 (15%)
86	T1C	C1	3405	85	44,45,45	1.18	4 (9%)	53,72,72	1.35	5 (9%)
87	SPD	C1	3628	-	9,9,9	0.30	0	8,8,8	0.98	0
86	T1C	C1	3402	-	44,45,45	1.21	4 (9%)	53,72,72	1.17	4 (7%)
86	T1C	C1	3404	85	44,45,45	1.20	4 (9%)	53,72,72	0.99	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	T1C	C2	1990	-	-	8/22/80/80	0/4/4/4
86	T1C	C1	3403	85	-	13/22/80/80	0/4/4/4
86	T1C	C1	3401	-	-	11/22/80/80	0/4/4/4
86	T1C	C1	3405	85	-	11/22/80/80	0/4/4/4
87	SPD	C1	3628	-	-	5/7/7/7	-
86	T1C	C1	3402	-	-	13/22/80/80	0/4/4/4
86	T1C	C1	3404	85	-	7/22/80/80	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	C1	3402	T1C	C21-N21	5.52	1.48	1.33
86	C2	1990	T1C	C21-N21	5.52	1.48	1.33
86	C1	3401	T1C	C21-N21	5.47	1.48	1.33
86	C1	3403	T1C	C21-N21	5.47	1.48	1.33
86	C1	3404	T1C	C21-N21	5.44	1.47	1.33
86	C1	3405	T1C	C21-N21	5.38	1.47	1.33
86	C1	3402	T1C	C4-N4	2.37	1.52	1.47
86	C1	3404	T1C	C4-N4	2.35	1.52	1.47
86	C1	3405	T1C	O11-C11	2.25	1.28	1.23
86	C2	1990	T1C	O11-C11	2.23	1.28	1.23
86	C1	3402	T1C	O11-C11	2.23	1.28	1.23
86	C1	3401	T1C	O11-C11	2.22	1.27	1.23
86	C1	3404	T1C	O11-C11	2.21	1.27	1.23
86	C1	3403	T1C	O11-C11	2.19	1.27	1.23
86	C1	3401	T1C	C7-N7	2.16	1.48	1.42
86	C2	1990	T1C	C4-N4	2.13	1.52	1.47
86	C1	3402	T1C	C7-N7	2.11	1.48	1.42
86	C1	3403	T1C	C7-N7	2.10	1.48	1.42
86	C2	1990	T1C	C7-N7	2.06	1.48	1.42
86	C1	3405	T1C	C4-N4	2.06	1.52	1.47
86	C1	3405	T1C	C7-N7	2.03	1.47	1.42
86	C1	3404	T1C	C7-N7	2.02	1.47	1.42
86	C1	3403	T1C	C4-N4	2.01	1.51	1.47
86	C1	3401	T1C	C4-N4	2.01	1.51	1.47

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	C1	3401	T1C	C11-C1B-C12	4.63	122.47	118.80
86	C1	3405	T1C	C1-C1C-C12	4.47	115.12	109.88
86	C1	3402	T1C	C1C-C1-C2	4.39	122.72	115.75
86	C1	3401	T1C	C1C-C1-C2	4.23	122.47	115.75
86	C1	3405	T1C	C11-C1B-C12	4.09	122.03	118.80
86	C1	3405	T1C	O1C-C1C-C12	-3.97	103.79	110.14
86	C1	3401	T1C	C1C-C41-C4	3.86	116.91	111.64
86	C1	3403	T1C	C11-C1B-C12	3.74	121.76	118.80
86	C2	1990	T1C	C1-C1C-C12	3.34	113.80	109.88
86	C1	3402	T1C	C11-C1B-C12	2.99	121.17	118.80
86	C1	3405	T1C	C21-C2-C1	2.97	124.48	120.97
86	C1	3405	T1C	C1C-C41-C4	2.91	115.62	111.64
86	C1	3401	T1C	O1C-C1C-C12	-2.67	105.87	110.14
86	C1	3404	T1C	C11-C1B-C12	2.62	120.87	118.80
86	C1	3403	T1C	C51-C5-C41	-2.61	105.90	110.49
86	C1	3401	T1C	C1-C1C-C12	2.60	112.94	109.88
86	C1	3401	T1C	C51-C5-C41	-2.60	105.92	110.49
86	C2	1990	T1C	C11-C1B-C12	2.44	120.73	118.80
86	C1	3401	T1C	O1C-C1C-C41	-2.39	107.16	110.09
86	C1	3402	T1C	O1C-C1C-C12	-2.35	106.39	110.14
86	C1	3404	T1C	C8-C7-N7	-2.31	117.81	120.91
86	C1	3403	T1C	C1-C1C-C12	2.30	112.58	109.88
86	C1	3401	T1C	C72-N7-C71	-2.04	109.56	116.12
86	C1	3402	T1C	O12-C12-C1B	-2.00	121.16	123.90
86	C1	3403	T1C	C1C-C41-C4	2.00	114.37	111.64

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	C2	1990	T1C	C92-C91-N9-C9
86	C2	1990	T1C	C3-C2-C21-O21
86	C2	1990	T1C	C3-C2-C21-N21
86	C2	1990	T1C	C1-C2-C21-O21
86	C2	1990	T1C	C1-C2-C21-N21
86	C1	3401	T1C	C94-C93-N92-C92
86	C1	3401	T1C	C95-C93-N92-C92
86	C1	3401	T1C	C96-C93-N92-C92
86	C1	3401	T1C	C41-C4-N4-C43
86	C1	3401	T1C	C1-C2-C21-O21
86	C1	3401	T1C	C1-C2-C21-N21
86	C1	3402	T1C	C92-C91-N9-C9
86	C1	3402	T1C	C1-C2-C21-O21

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Mol	Chain	Res	Type	Atoms
86	C1	3402	T1C	C1-C2-C21-N21
86	C1	3403	T1C	C92-C91-N9-C9
86	C1	3403	T1C	C3-C4-N4-C43
86	C1	3403	T1C	C3-C2-C21-O21
86	C1	3404	T1C	C91-C92-N92-C93
86	C1	3404	T1C	C1-C2-C21-O21
86	C1	3404	T1C	C1-C2-C21-N21
86	C1	3405	T1C	C92-C91-N9-C9
86	C1	3405	T1C	C3-C2-C21-O21
86	C1	3405	T1C	C3-C2-C21-N21
86	C1	3405	T1C	C1-C2-C21-O21
86	C1	3405	T1C	C1-C2-C21-N21
86	C2	1990	T1C	O91-C91-N9-C9
86	C1	3405	T1C	O91-C91-N9-C9
87	C1	3628	SPD	C3-C4-C5-N6
86	C1	3402	T1C	O91-C91-N9-C9
86	C1	3403	T1C	O91-C91-N9-C9
87	C1	3628	SPD	C4-C5-N6-C7
87	C1	3628	SPD	N6-C7-C8-C9
86	C1	3405	T1C	O91-C91-C92-N92
86	C1	3405	T1C	N9-C91-C92-N92
86	C1	3401	T1C	C10-C9-N9-C91
86	C1	3403	T1C	O91-C91-C92-N92
86	C1	3401	T1C	C8-C9-N9-C91
86	C1	3404	T1C	O91-C91-N9-C9
86	C1	3403	T1C	N9-C91-C92-N92
86	C1	3402	T1C	O91-C91-C92-N92
86	C1	3402	T1C	N9-C91-C92-N92
86	C1	3401	T1C	C91-C92-N92-C93
86	C1	3402	T1C	C91-C92-N92-C93
86	C1	3405	T1C	C91-C92-N92-C93
86	C1	3403	T1C	C41-C4-N4-C43
86	C1	3403	T1C	C41-C4-N4-C42
86	C1	3403	T1C	C3-C4-N4-C42
86	C1	3401	T1C	C3-C2-C21-N21
86	C1	3403	T1C	C3-C2-C21-N21
86	C1	3404	T1C	C3-C2-C21-N21
86	C1	3401	T1C	C3-C2-C21-O21
86	C1	3402	T1C	C3-C2-C21-O21
86	C1	3404	T1C	C92-C91-N9-C9
86	C1	3403	T1C	C1-C2-C21-N21
87	C1	3628	SPD	C2-C3-C4-C5

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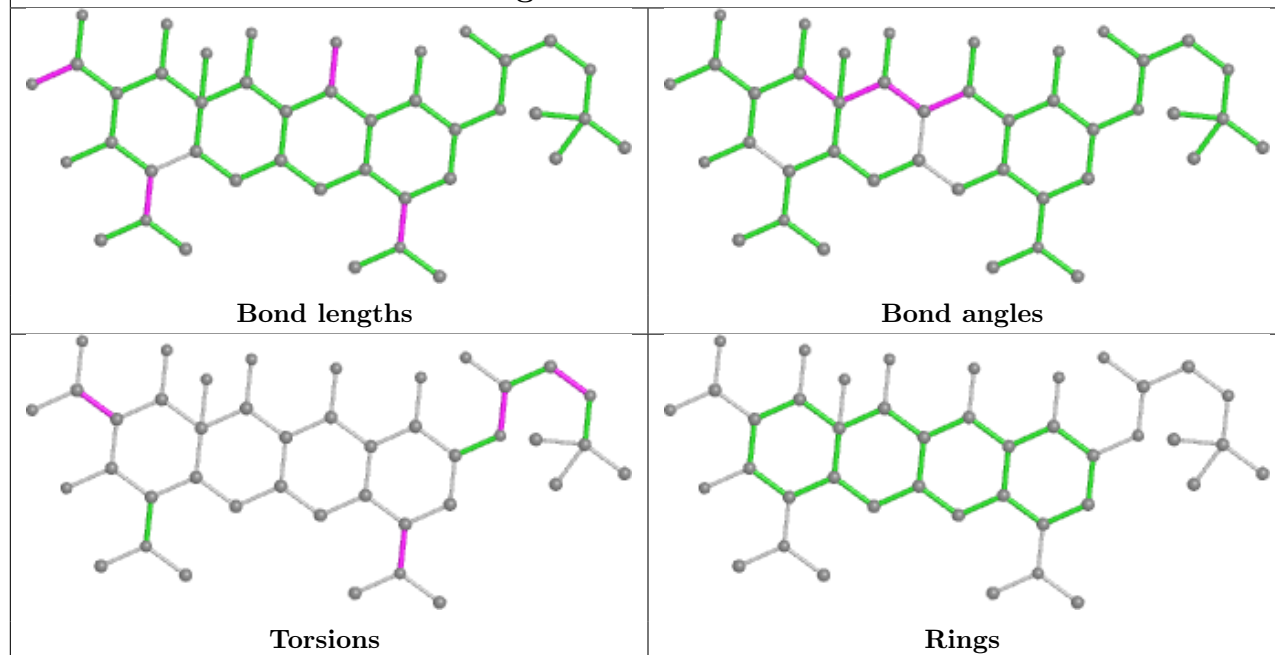
Mol	Chain	Res	Type	Atoms
86	C1	3403	T1C	C10-C9-N9-C91
86	C1	3402	T1C	C95-C93-N92-C92
86	C1	3405	T1C	C61-C7-N7-C71
86	C2	1990	T1C	C91-C92-N92-C93
87	C1	3628	SPD	C8-C7-N6-C5
86	C1	3402	T1C	C96-C93-N92-C92
86	C1	3402	T1C	C61-C7-N7-C71
86	C1	3402	T1C	C61-C7-N7-C72
86	C1	3405	T1C	C61-C7-N7-C72
86	C1	3402	T1C	C3-C2-C21-N21
86	C1	3404	T1C	C3-C2-C21-O21
86	C1	3403	T1C	C1-C2-C21-O21
86	C2	1990	T1C	C61-C7-N7-C72

There are no ring outliers.

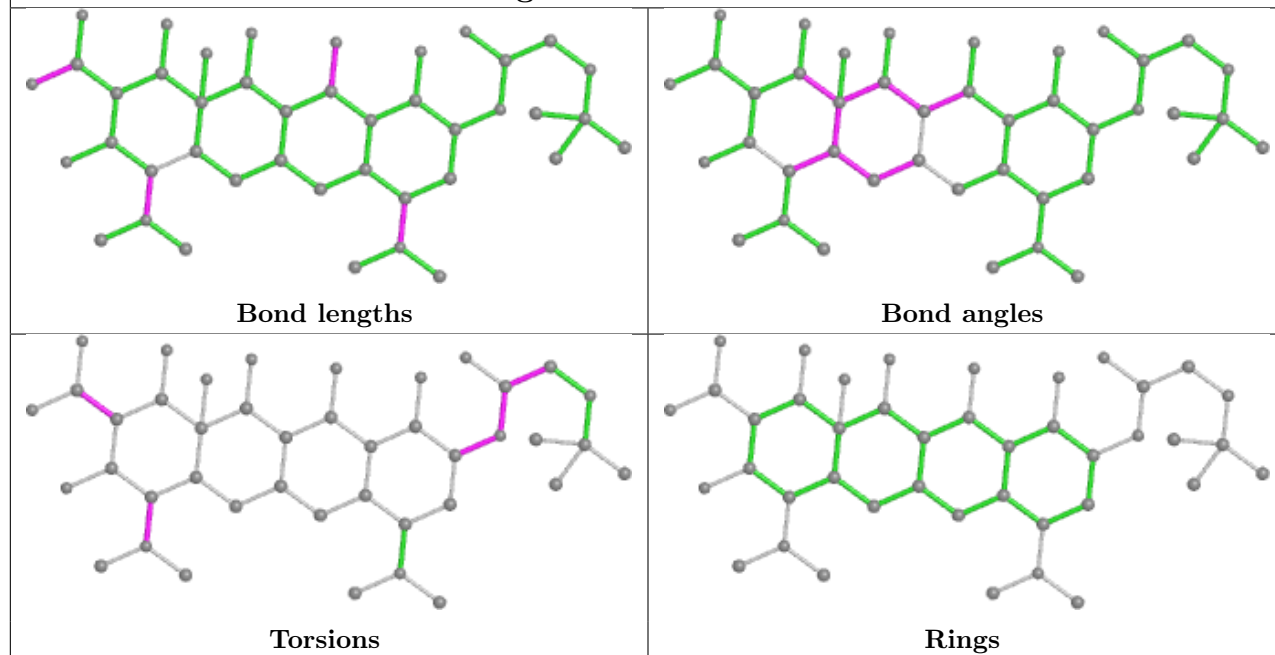
No monomer is involved in short contacts.

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.

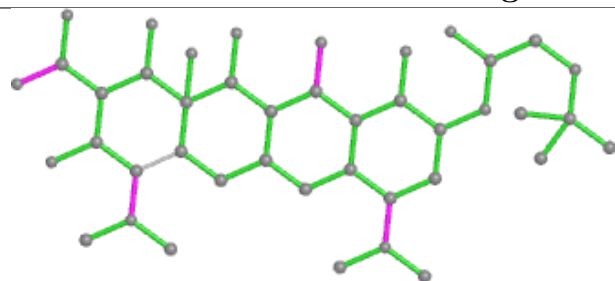
Ligand T1C C2 1990



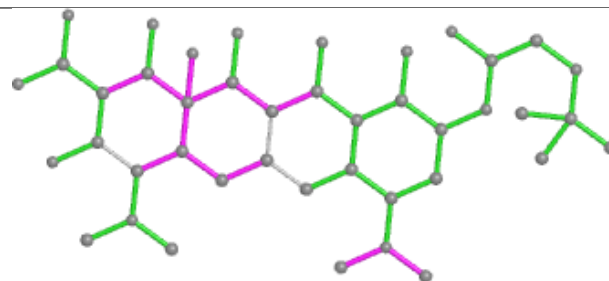
Ligand T1C C1 3403



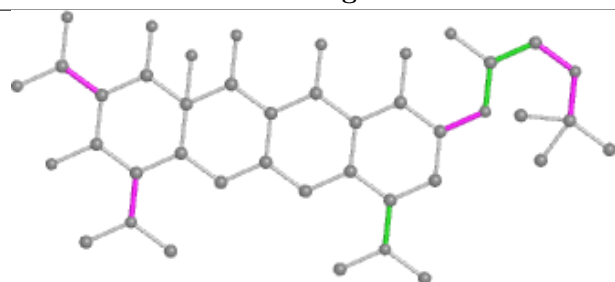
Ligand T1C C1 3401



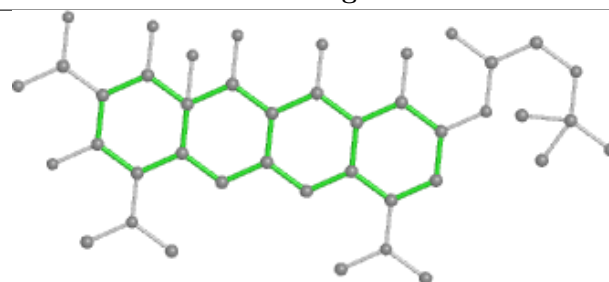
Bond lengths



Bond angles

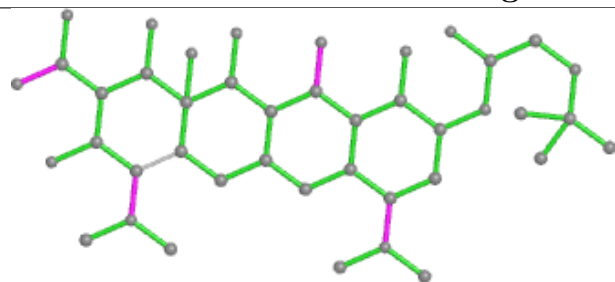


Torsions

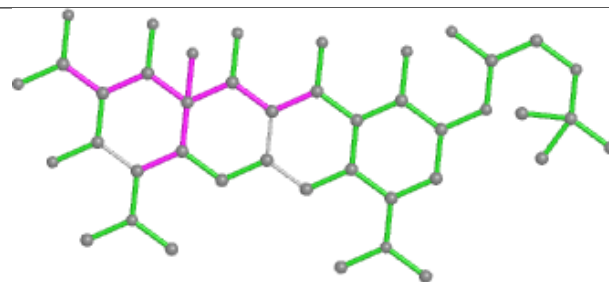


Rings

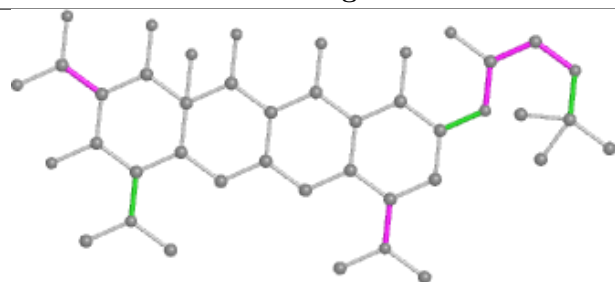
Ligand T1C C1 3405



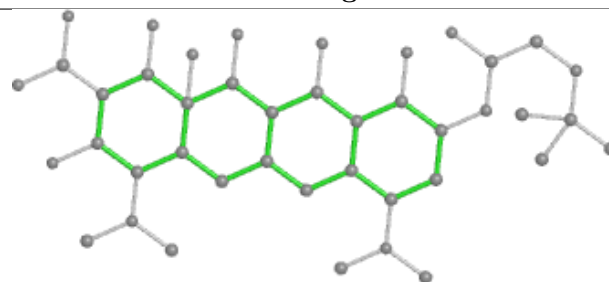
Bond lengths



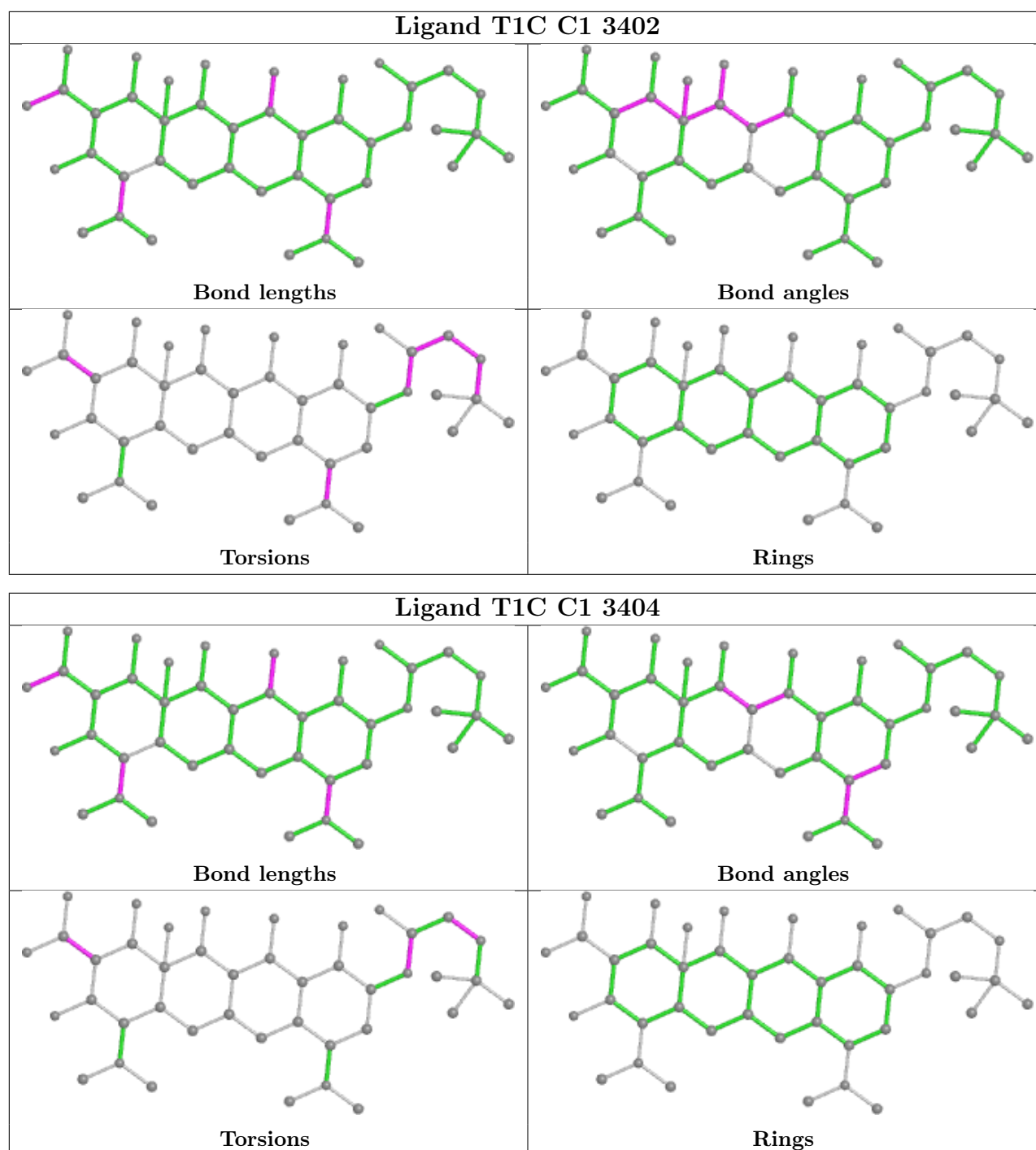
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

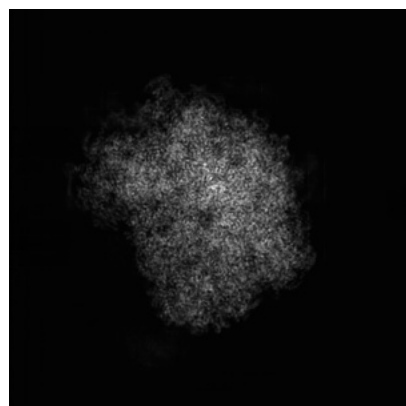
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36945. These allow visual inspection of the internal detail of the map and identification of artifacts.

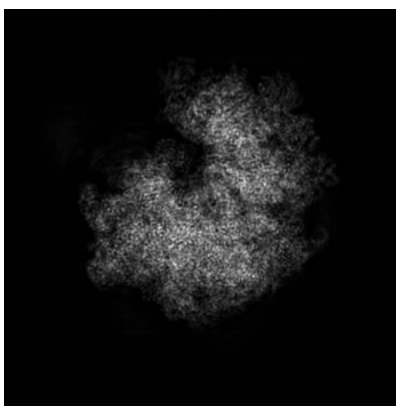
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

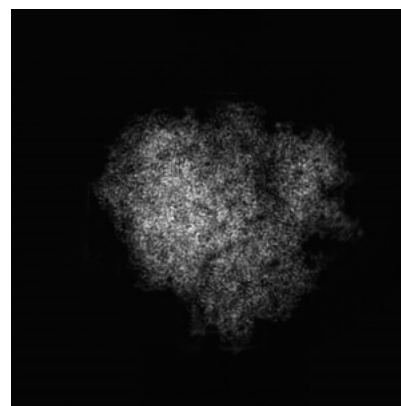
6.1.1 Primary map



X

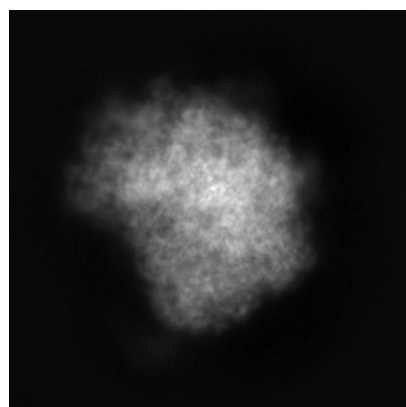


Y

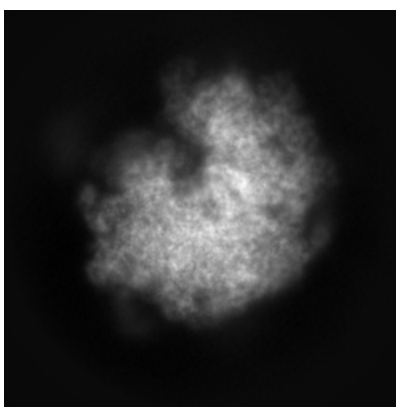


Z

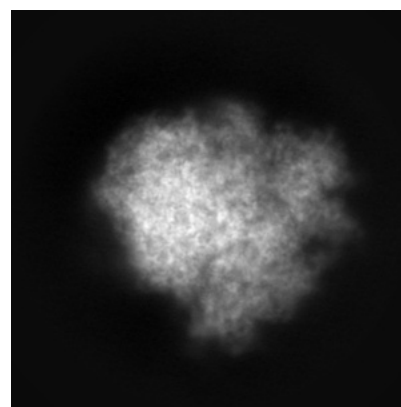
6.1.2 Raw map



X



Y



Z

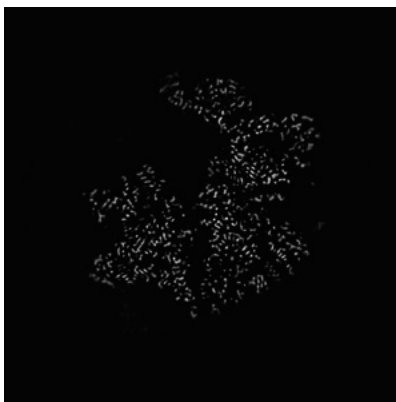
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240

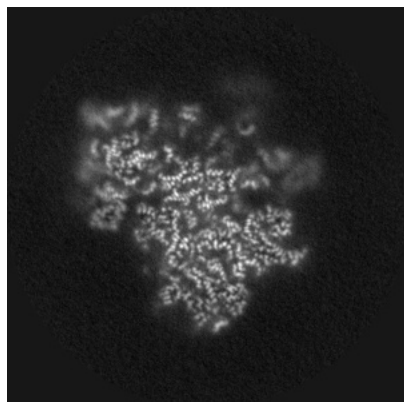


Y Index: 240

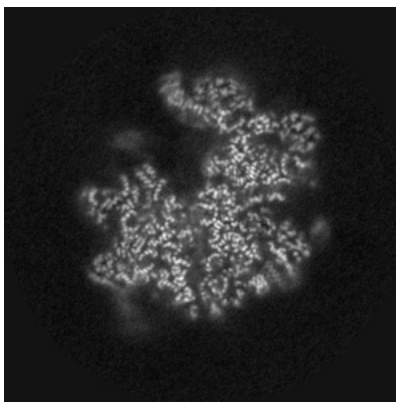


Z Index: 240

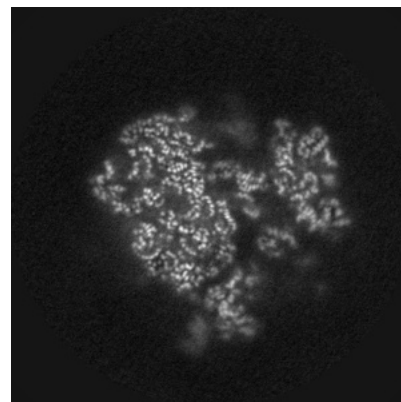
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

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

6.3 Largest variance slices [i](#)

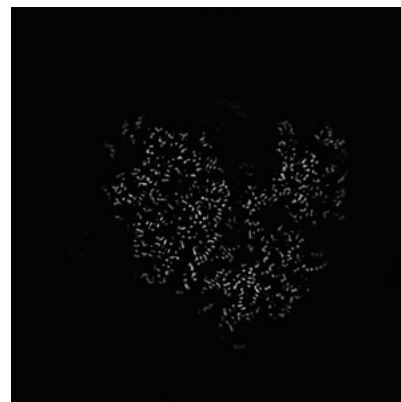
6.3.1 Primary map



X Index: 213

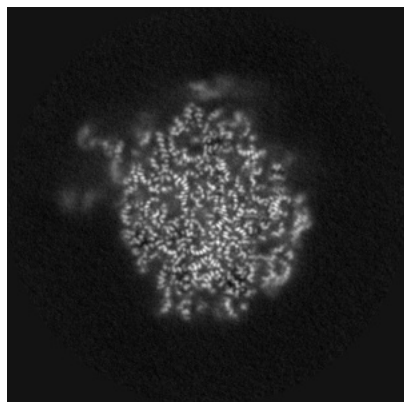


Y Index: 256

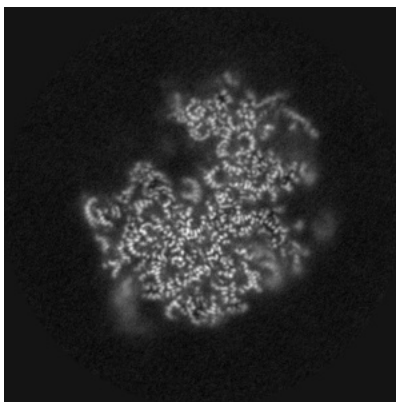


Z Index: 268

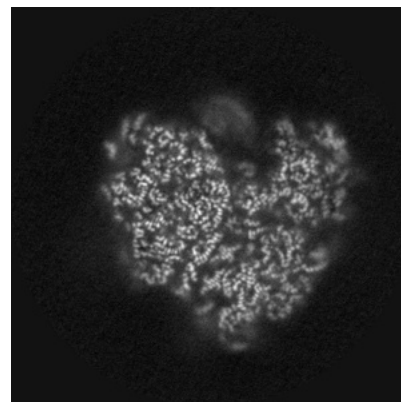
6.3.2 Raw map



X Index: 213



Y Index: 256

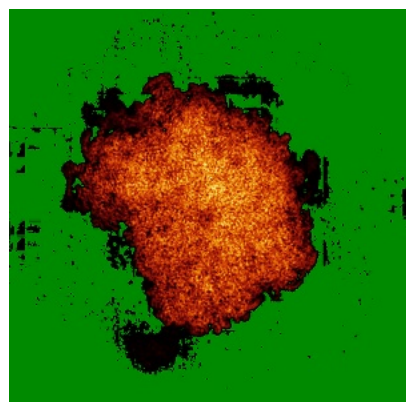


Z Index: 268

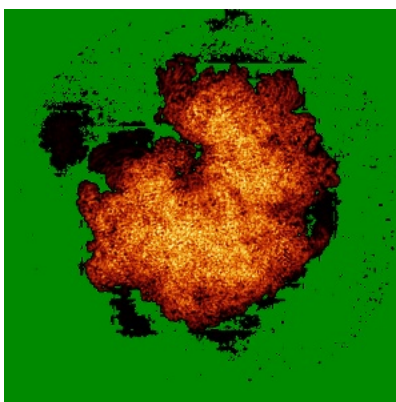
The images above show the largest variance slices of the map in three orthogonal directions.

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

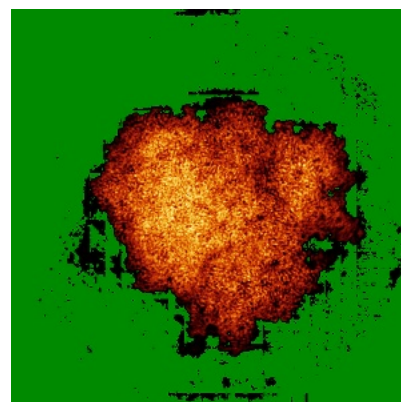
6.4.1 Primary map



X

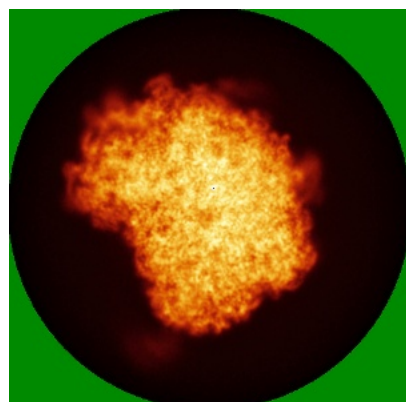


Y

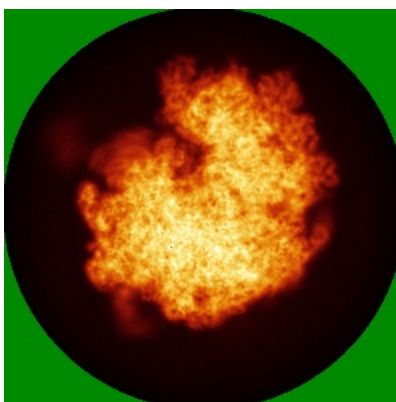


Z

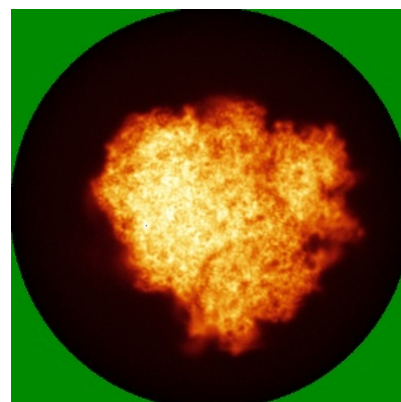
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



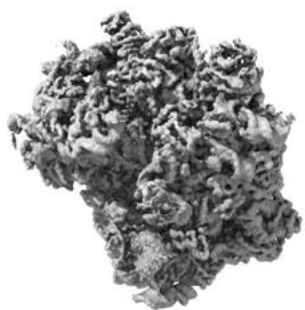
Y



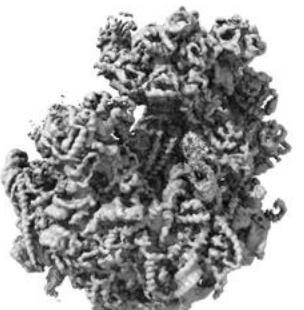
Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

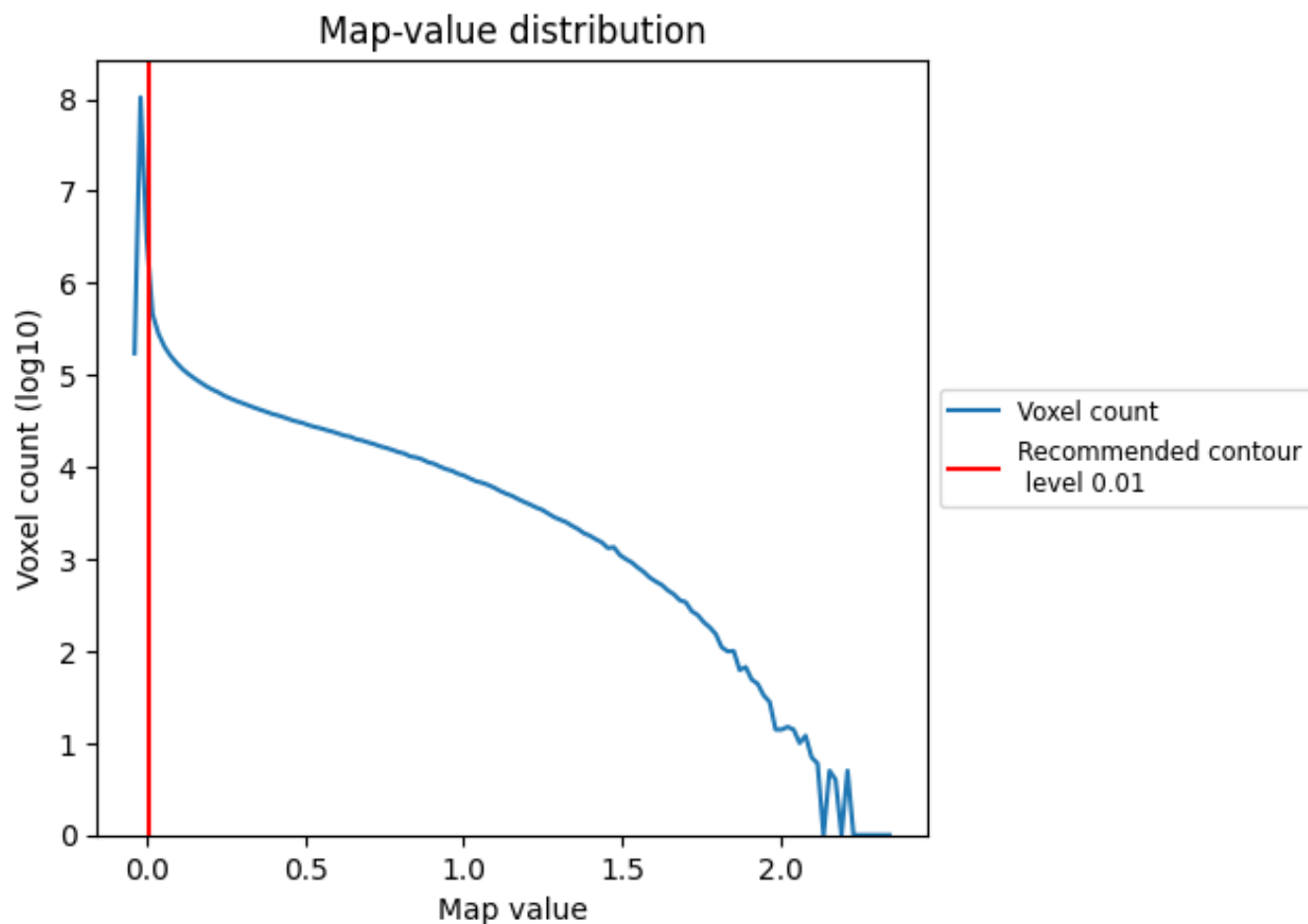
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

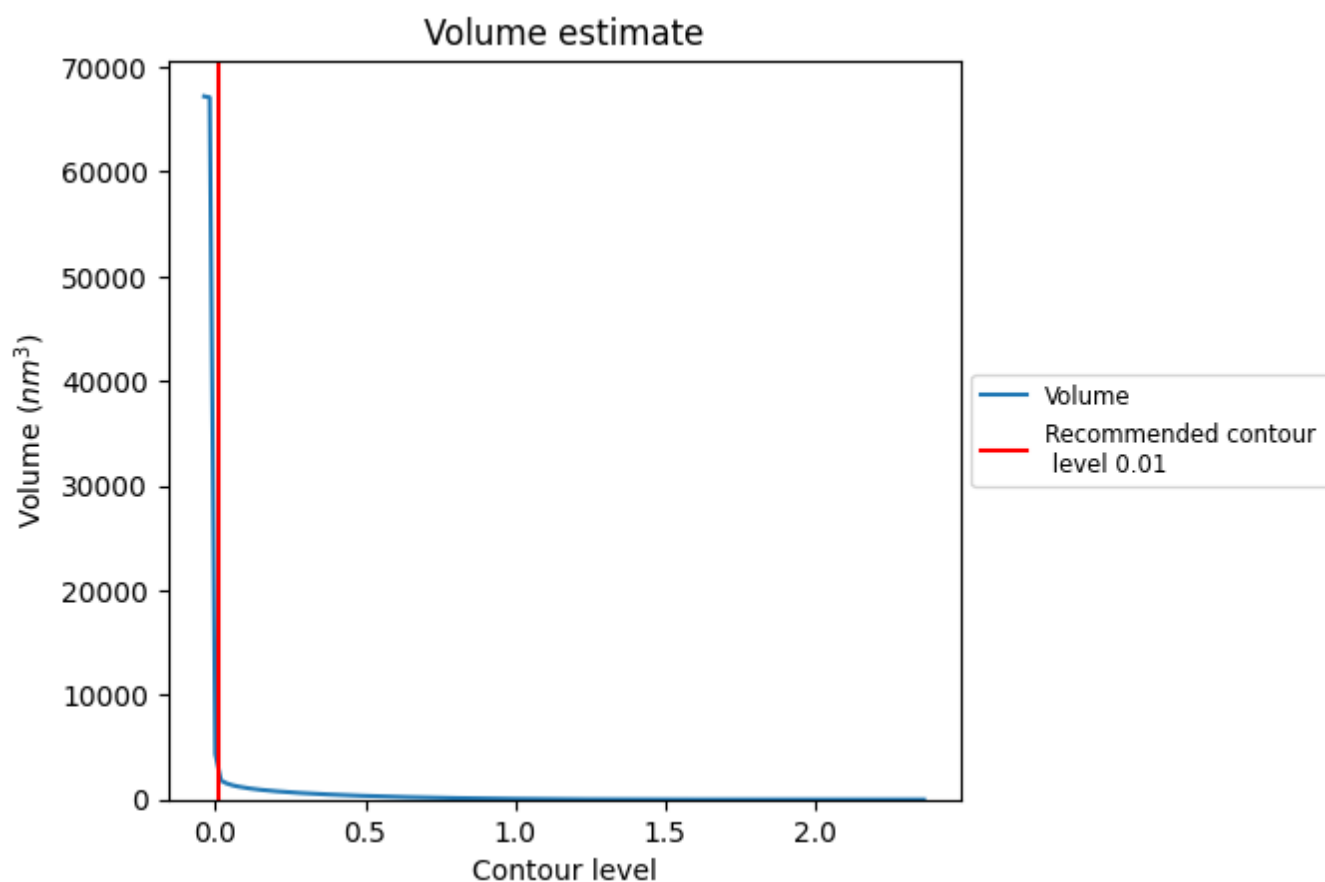
This section contains the results of statistical analysis of the map.

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.

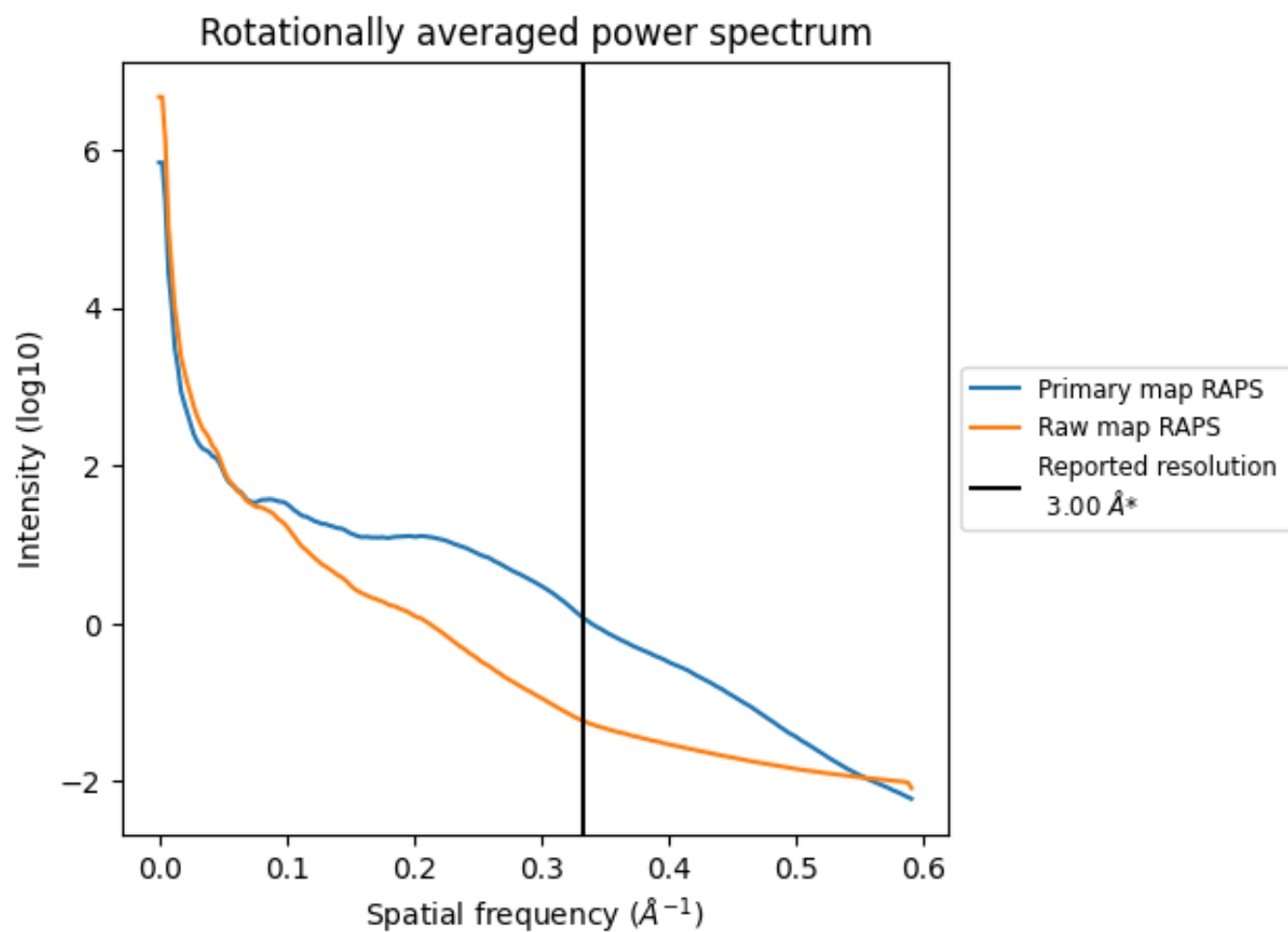
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3065 nm^3 ; this corresponds to an approximate mass of 2769 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 ⓘ

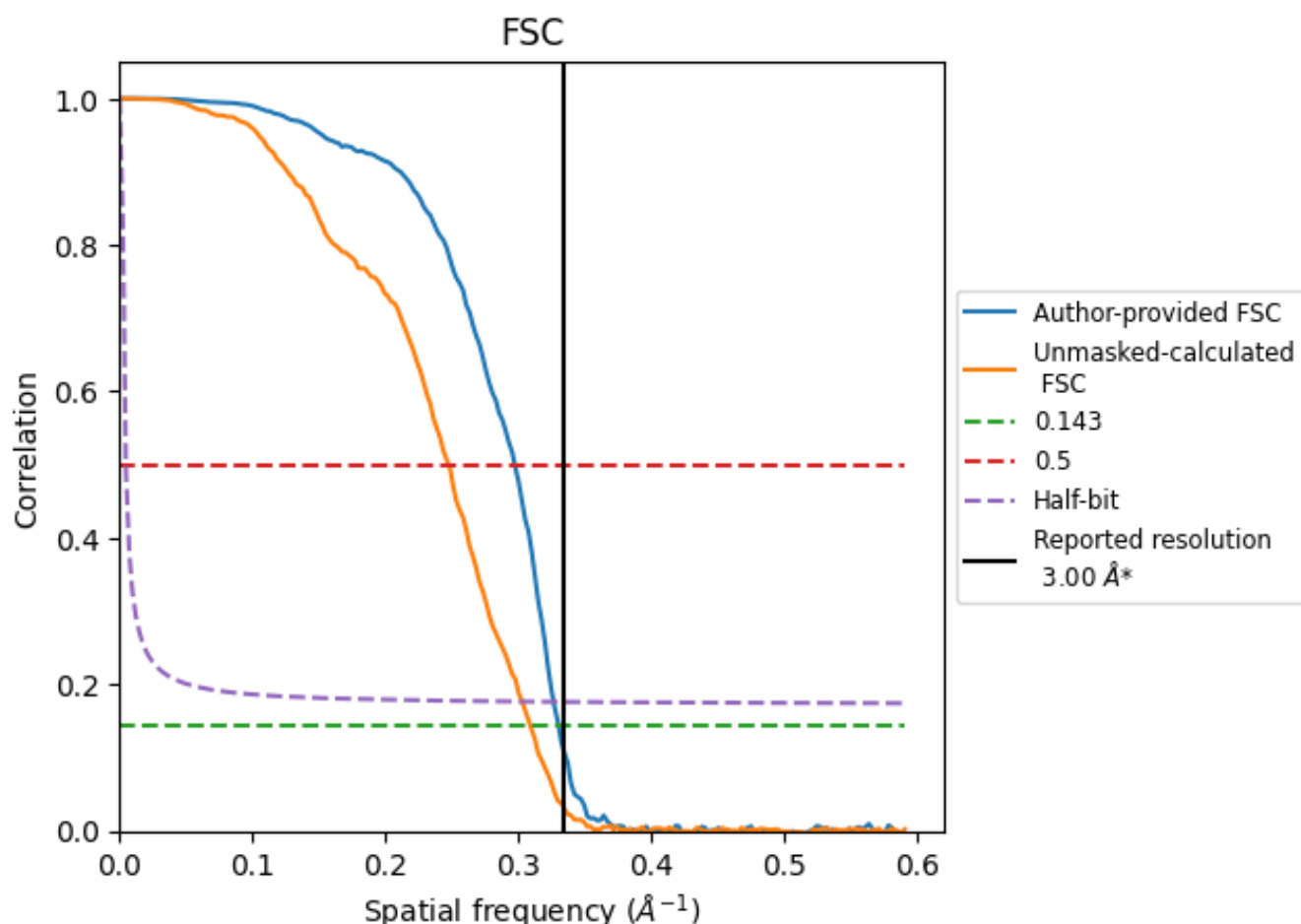


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

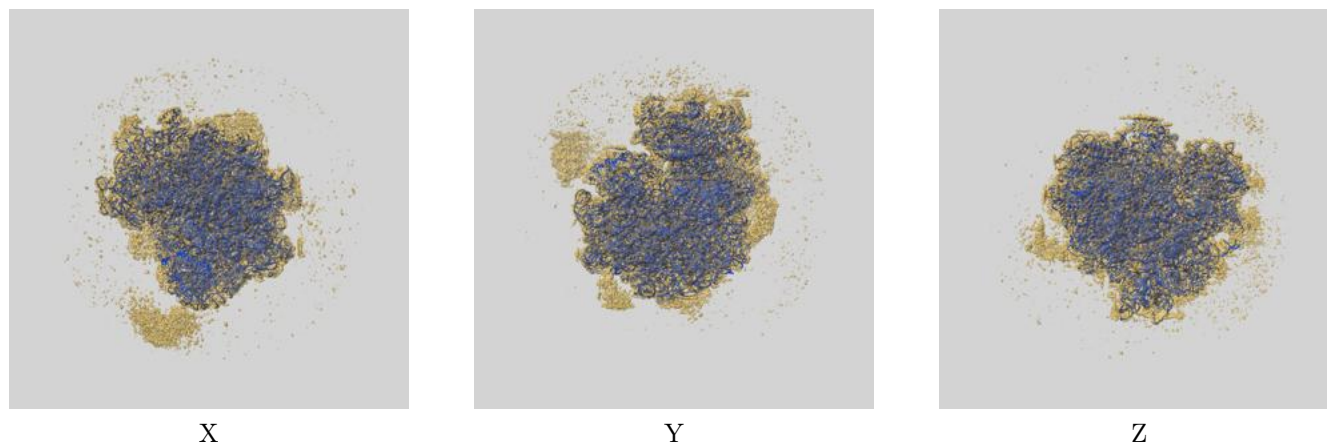
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.03	3.37	3.06
Unmasked-calculated*	3.24	4.04	3.30

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

9 Map-model fit [i](#)

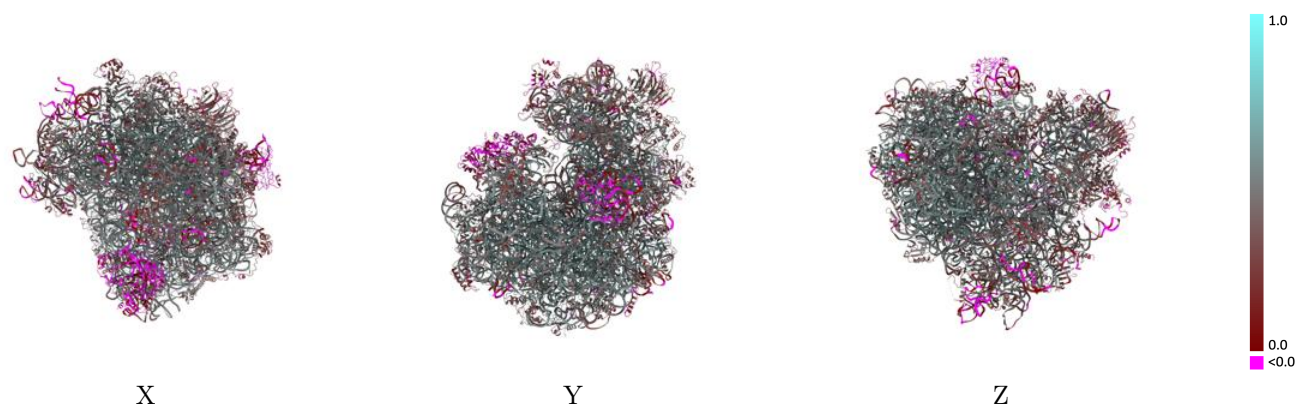
This section contains information regarding the fit between EMDB map EMD-36945 and PDB model 8K82. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



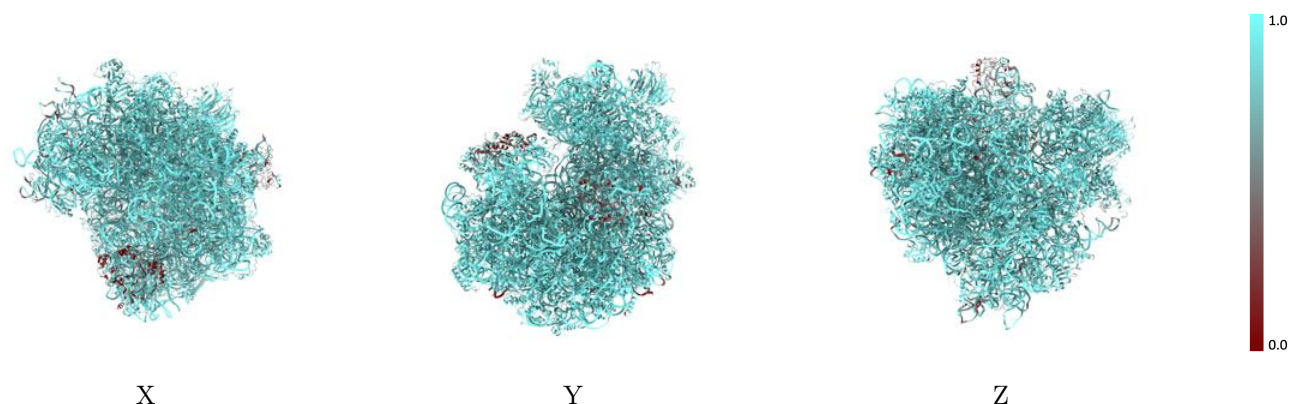
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



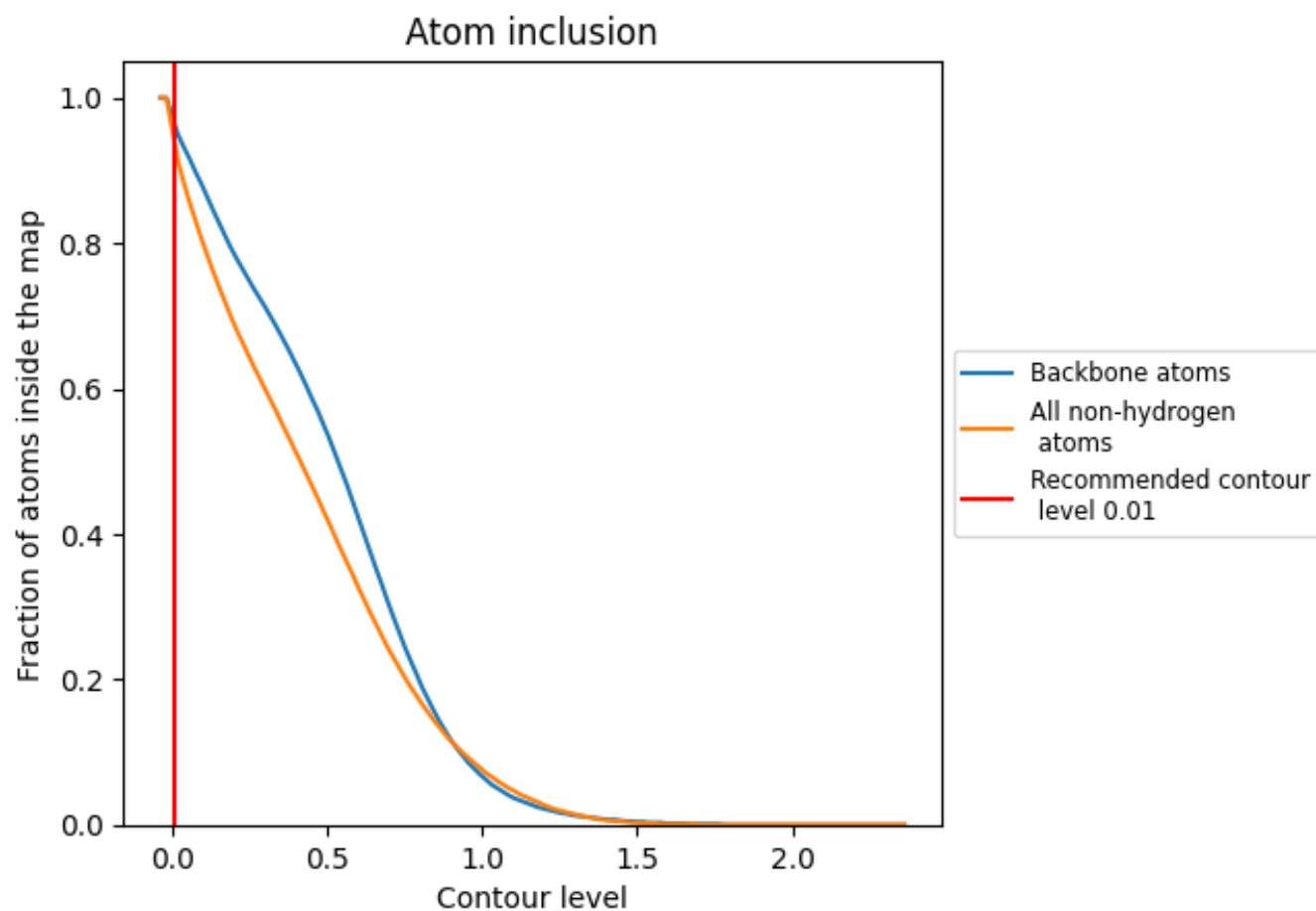
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9330	 0.4530
C1	 0.9650	 0.5090
C2	 0.9580	 0.4620
C3	 0.9820	 0.5350
C4	 0.9920	 0.5310
C5	 0.9480	 0.4580
C7	 1.0000	 0.5590
CN	 0.7270	 0.2950
L1	 0.3790	 -0.0680
L2	 0.6130	 0.2870
LA	 0.9440	 0.5020
LB	 0.9350	 0.4740
LC	 0.9380	 0.4510
LD	 0.8690	 0.3370
LE	 0.9050	 0.3950
LF	 0.9460	 0.4710
LG	 0.9160	 0.4020
LH	 0.9180	 0.4230
LI	 0.9020	 0.4290
LJ	 0.9120	 0.4070
LK	 0.3750	 -0.0300
LL	 0.9300	 0.4450
LM	 0.9250	 0.4390
LN	 0.9590	 0.5190
LO	 0.9550	 0.4860
LP	 0.9350	 0.4850
LQ	 0.9420	 0.4720
LR	 0.9380	 0.4810
LS	 0.9310	 0.4710
LT	 0.9290	 0.4650
LU	 0.9170	 0.4060
LV	 0.9080	 0.4630
LW	 0.9170	 0.4710
LX	 0.9250	 0.4630
LY	 0.9220	 0.4320





















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Chain	Atom inclusion	Q-score
LZ	 0.9130	 0.4250
La	 0.9540	 0.4870
Lb	 0.8830	 0.4080
Lc	 0.9020	 0.4380
Ld	 0.8840	 0.4360
Le	 0.9300	 0.4780
Lf	 0.9570	 0.5090
Lg	 0.9320	 0.4900
Lh	 0.9050	 0.4340
Li	 0.9020	 0.4010
Lj	 0.9730	 0.5400
Lk	 0.8990	 0.3960
Ll	 0.9470	 0.4730
Lm	 0.9310	 0.4650
Ln	 0.8910	 0.4330
Lo	 0.9230	 0.4630
Lp	 0.9060	 0.4620
P0	 0.5110	 0.0120
SA	 0.9340	 0.4020
SB	 0.9050	 0.3940
SC	 0.9280	 0.4420
SD	 0.8720	 0.3340
SE	 0.9070	 0.3970
SF	 0.8830	 0.3540
SG	 0.8670	 0.3200
SH	 0.8770	 0.3190
SI	 0.9180	 0.4380
SJ	 0.8970	 0.3920
SK	 0.8860	 0.3090
SL	 0.9110	 0.4550
SM	 0.7640	 0.0910
SN	 0.9200	 0.4400
SO	 0.9260	 0.4350
SP	 0.8630	 0.3220
SQ	 0.9040	 0.3890
SR	 0.9020	 0.3690
SS	 0.8710	 0.3250
ST	 0.8920	 0.3610
SU	 0.8600	 0.3220
SV	 0.9010	 0.3780
SW	 0.9480	 0.4860
SX	 0.8990	 0.4400

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Chain	Atom inclusion	Q-score
SY	 0.8620	 0.3510
SZ	 0.8760	 0.3060
Sa	 0.9260	 0.4570
Sb	 0.9370	 0.4190
Sc	 0.8550	 0.3490
Sd	 0.9340	 0.4670
Se	 0.8040	 0.3400
Sf	 0.7590	 0.0760
Sg	 0.8800	 0.2950